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COMMENT

Comment on 'Dynamical properties of a two-dimensional Coulomb fluid'

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Abstract. Agarwal and co-workers have reported on dynamical properties of a classical two-dimensional, one-component homogeneous plasma with a logarithmic potential for an arbitrary $\Gamma = \beta e^2$. Some of their results may now be compared with those obtained analytically for $\Gamma = 2$. In addition, their phenomenological response function can be analysed with respect to the third moment and compressibility sum rules. This analysis indicates the extent of the validity of their response function.

A few years ago, Agarwal and co-workers [1] published an interesting paper on the dynamical properties of a classical two-dimensional one-component homogeneous plasma with a logarithmic potential for an arbitrary coupling strength $\Gamma = \beta e^2$. Here β is the inverse temperature and e is the electron charge. This work represents an important advance in understanding of this system. To our knowledge, no one has since reported any further progress on it. Their work gives information on, among others, the longitudinal component of the third moment and the plasmon dispersion relation. We are primarily concerned with these two results. For simplicity, this system will be referred to as 2D Γ.

The frequency moments are static properties. Therefore, one can show that they depend on the static structure factor S_k, where $\boldsymbol{k}$ is the wavevector. For 2D Γ arbitrary, one does not know the analytic expression of S_k. Hence, Agarwal and co-workers [1] have given their results in a series expansion in k.

The main purpose of our Comment is to indicate that their results for $\Gamma = 2$ can be tested against analytical solutions now available at this particular value of the coupling strength. Jancovici [2] has obtained an analytic expression for S_k if $\Gamma = 2$. Hence, certain static quantities, e.g., the third moment, can be expressed analytically. More difficult is the plasmon dispersion relation. To obtain it, Agarwal and co-workers relied on a response function which they termed phenomenological. We find that this response function when $\Gamma = 2$ satisfies two important necessary conditions. Hence, it deserves more than a phenomenological label that the authors themselves have given. Perhaps more important, this response function has been used in other problems [3–6]. We, therefore, believe that the significance of our analysis goes beyond their paper.

We first deal with the third moment sum rule. The expression for the longitudinal component of the third frequency moment is well known. For 2D $\Gamma = 2$ it may be expressed in a simplified form shown below.

$$M_3(k) = \langle \omega^3(k) \rangle / \langle \omega(k) \rangle = 3a + 1 - I_k, \quad (1)$$

where

$$I_k = N^{-1} \sum_{q \neq 0, k} (\boldsymbol{k} \cdot \boldsymbol{q})^2 / k^2 q^2 [S(q) - S(q-k)] \quad (2)$$

and $a = k^2/4$. Here N is the number of electrons and $S(q)$ is the static structure factor. We have set the plasma frequency $\omega_p \equiv \sqrt{2\pi n e^2/m} = 1$, where n is the number density and m is the mass of the electron. We have further expressed the wavevector $\boldsymbol{k}$ in units of the inverse ion sphere radius $r_0^{-1} = (\pi n)^{1/2}$, so that it is now dimensionless. For 2D $\Gamma = 2$, we find that $a = k^2/4$ is a natural and simplifying unit rather than a dimensionless $\boldsymbol{k}$. Our equation (1) corresponds to that of equation (1) of Agarwal and co-workers [1].

A few years ago, it was shown [2] that for 2D $\Gamma = 2$

$$S_k = 1 - e^{-a}. \quad (3)$$

Using (3), one can show that [7, 8]

$$2I_k = 1 - a^{-1}(1 - e^{-a}). \quad (4)$$

Hence,

$$M_3(k) = 3a + \tfrac{1}{2}[1 + a^{-1}(1 - e^{-a})]. \quad (5)$$

It follows directly that

$$M_3(k) = 1 + \tfrac{11}{16}k^2 + \tfrac{1}{192}k^4 - \tfrac{1}{3072}k^6 + O(k^8). \quad (6)$$

The above expansion agrees with the one given in [1] for $\Gamma = 2$ (their equation (11)) except the coefficient of k^4. Theirs is given as $1/48\Gamma = \frac{1}{96}$. There is perhaps a typographical error in their coefficient of k^4.

We now deal with the response function. The plasmon dispersion relation is obtained from the frequency-dependent response function $\chi_k(\omega)$, where ω is the frequency. In general, this quantity is not exactly known. Agarwal and co-workers [1] introduced an interesting phenomenological one, which is a function of x, not just ω, where $x = \omega\tau$ and τ is a parameter defined as

$$\tau^{-2} = M_3(k) - \Omega^2 \quad (7)$$

where $\Omega^2 = aS_k^{-1}$ if $\Gamma = 2$. We shall distinguish their response function (equation (21)) by a superscript A. It is given as

$$\chi_k^A(\omega) = \chi_k^A(x) = 2\beta a \tau^2 Z(x) / [1 - (1 - 2aS_k^{-1}\tau^2) Z(x)] \quad (8)$$

where Z is the plasma dispersion function (see below) [9].

The response function is usually expressed in terms of an ideal response function $\chi_k^0(\omega)$ as follows:

$$\chi_k(\omega) = \chi_k^0(\omega) / \{1 - v_k[1 - G_k(\omega)]\chi_k^0(\omega)\} \quad (9)$$

where v_k is the Fourier transform of the Coulomb interaction and $G_k(\omega)$ is a dynamic local field [10]. For 2D $\Gamma = 2$, one has the following: $v_k = 2\pi e^2/k^2$, $\chi_k^0(\omega) = -n\beta W(u)$, $u = 2\omega/k$, where

$$W(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \frac{x e^{-x^2/2}}{x - u - \mathrm{i}\varepsilon}. \tag{10}$$

Hence, Z and W are related as $Z(y) = W(\sqrt{2}y)$. Putting together, we express (9) as

$$\chi_k(\omega) = \chi_k(u) = -n\beta W(u)/\{1 + a^{-1}[1 - G_k(u)]W(u)\}. \tag{11}$$

We see that (8) shows some resemblance to (11). But the comparison is not yet possible because (8) is given as a function of x. Thus it is necessary to find the meaning of their parameter τ in terms of standard quantities, e.g., $G_k = G_k(\omega = 0)$. For classical systems at $\Gamma = 2$, G_k is related to S_k as follows [9]:

$$S_k^{-1} = 1 + (1 - G_k)/a. \tag{12}$$

Hence, using (3) and (5) in (7) we get

$$\tau^{-2} = 2a + G_k - I_k = 2a[1 + \eta_2(k)] \tag{13}$$

where we have introduced

$$G_k - I_k = 2a\eta_2(k). \tag{14}$$

Since both G_k and I_k are exactly known for 2D $\Gamma = 2$, $\eta_2(k)$ is known exactly. Finally

$$x = \omega\tau = \omega/\sqrt{2a(1 + \eta_2)} = u/\sqrt{2(1 + \eta_2)}. \tag{15}$$

That is, the frequency in their response function is scaled. This is not necessarily unphysical or undesirable. However, it must be handled consistently to avoid the appearance of its effect on some higher order terms.

Using (13) in (8), we obtain

$$\beta^{-1}\chi_k^{\mathrm{A}}(x) = Z(x)/\{1 + a^{-1}[1 - G_k^{\mathrm{A}}(x)]Z(x)\} \tag{16}$$

where we have defined

$$G_k^{\mathrm{A}}(x) = G_k - a\eta_2[Z^{-1}(x) - 1] \tag{17}$$

which may be regarded as their dynamic local field. It too resembles the second-order dynamic local field given by us [8, 11], i.e.,

$$G_k^{(2)}(u) = G_k - a\eta_2(W^{-1}(u) + u^2 - 1). \tag{18}$$

The significance of (18) is that if it is used in (11), the resulting response function will satisfy the first and third moment sum rules [11] as well as the compressibility sum rule.

The plasmon dispersion relation can be obtained directly from (16) by setting $\mathrm{Re}[\chi_k^{\mathrm{A}}(x)]^{-1} = 0$. That is,

$$a(1 + \eta_2)Z^{-1}(x) + 1 - G_k - a\eta_2 = 0. \tag{19}$$

For $x \to \infty$, the dispersion function has the following asymptotic expansion:

$$Z^{-1}(x) = -2x^2 + 3 + 3x^{-2} + \mathrm{O}(x^{-4}). \tag{20}$$

Now from (3), (4) and (12), one has

$$G_k = \tfrac{1}{2}a - \tfrac{1}{12}a^2 + 0a^3 + \mathrm{O}(a^4) \tag{21}$$

and

$$\eta_2(k) = \tfrac{1}{8} + 0a - \tfrac{1}{96}a^2 + \tfrac{1}{360}a^3 + \mathrm{O}(a^4). \tag{22}$$

Together with (20)–(22), we get from (19)

$$\omega_{\mathrm{p}}^2(k)^{\mathrm{A}} = 1 + \tfrac{11}{16}k^2 + \tfrac{1}{16}(\tfrac{1}{12} + \tfrac{243}{32})k^4 + \mathrm{O}(k^6). \tag{23}$$

The coefficient of k^2 agrees with the one originally given in [1], but the coefficient of k^4

does not. Theirs (see their equation (24)) is given as $\frac{1}{48}\Gamma^{-1} - \frac{9}{4}(1/\Gamma + \frac{1}{16})^2$. For $\Gamma = 2$, it is $\frac{1}{16}(\frac{1}{6} - \frac{729}{64})$, a negative value. We believe this is an error. If (18) were used in (11), one would obtain [8]

$$\omega_p^2(k) = 1 + \tfrac{11}{16}k^2 + \tfrac{1}{16}(\tfrac{1}{12} + \tfrac{27}{4})k^4 + O(k^6). \tag{24}$$

The two expansions (23) and (24) differ in the coefficient of k^4, and also in the coefficients of higher order terms. It comes from the frequency scaling introduced by Agarwal and co-workers mentioned earlier. Its effect begins to appear from the fourth order term of k.

Frequency moments are ordinarily defined with respect to the response function as [10]

$$\langle \omega^{2\nu+1}(k)\rangle = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, \omega^{2\nu+1}\, \mathrm{Im}\, \chi_k(\omega) \qquad \nu = 0, 1, 2, \ldots . \tag{25}$$

The above moments can also be obtained from an equation of motion, hence independently of the response function. It is known, for example $\langle\omega(k)\rangle = nk^2/m$. The third moment for 2D $\Gamma = 2$ is given by (1). We shall use (16) to test whether it satisfies the first and third moment sum rules for 2D $\Gamma = 2$.

The scaled frequency in the response function (16) may be 'unscaled' as follows:

$$\langle \omega^{2\nu+1}(k)\rangle^{A} = \frac{-1}{\pi}(k^2 s^2/m\beta)^{\nu+1}\int_{-\infty}^{\infty} dy\, y^{2\nu-1}\, \mathrm{Im}\, \chi_k^{A}(y/\sqrt{2}) \tag{26}$$

where $s^2 = 1 + \eta_2(k)$. Adopting the conventional sign [9], we write the right-hand side of (16) as $(-1/n\beta)\,\chi_k^{A}(x)$ and obtain

$$\langle \omega^{2\nu+1}(k)\rangle^{A} = (n\beta/\pi)(k^2 s^2/m\beta)^{\nu+1}\int_{-\infty}^{\infty} dy\, y^{2\nu+1}\, \mathrm{Im}\, F(y) \tag{27}$$

where

$$F(y) = W(y)/\{1 + a^{-1}[1 - G_k^{A}(y)]W(y)\} \tag{28}$$

and

$$G_k^{A}(y) = G_k - a\eta_2[W^{-1}(y) - 1]. \tag{29}$$

By expanding the denominator of $F(y)$ for $y \to \infty$, we get

$$\mathrm{Im}\, F(y) = s^{-2}[\mathrm{Im}\, W(y) + c_2^{A} y^{-2}\, \mathrm{Im}\, W(y) + O(y^{-4})] \tag{30}$$

where

$$c_2^{A} = (1 - I_k - 3a\eta_2)/as^2 = c_2. \tag{31}$$

To obtain (31) we have used (14).

Now by substituting (30) in (27) we can evaluate the moments for any ν. We shall do so for $\nu = 0$ and 1 only:

$$\langle\omega(k)\rangle^{A} = (n\beta/\pi)(k^2 s^2/m\beta)s^{-2}\int_{-\infty}^{\infty} dy\, y\, \mathrm{Im}\, W(y)$$

$$= nk^2/m = \langle\omega(k)\rangle. \tag{32}$$

$$\langle\omega^3(k)\rangle^{A} = (n\beta/\pi)(k^2 s^2/m\beta)^2 s^{-2}\left(\int_{-\infty}^{\infty} dy\, y^3\, \mathrm{Im}\, W(y) + c_2^{A}\int_{-\infty}^{\infty} dy\, y\, \mathrm{Im}\, W(y)\right)$$

$$= n\beta(k^2 s/m\beta)^2(3 + c_2) = \langle\omega^3(k)\rangle. \tag{33}$$

In evaluating (32 and 33), the integrands with negative powers of y can be shown to vanish [8]. We see that the response function of Agarwal and co-workers [1] satisfies the first and third moment sum rules. In this manner one may further show that it does not, however, satisfy the fifth and higher moment sum rules.

Finally we turn to the compressibility sum rule. It is well known that the isothermal compressibility K_T is related to the screened static susceptibility χ_k^{sc} via the following relation [12]

$$-n^2K_T = \lim_{k\to 0} \chi_k^{\text{sc}}. \tag{34}$$

Now the screened static susceptibility is related to the static response function as [12]

$$\chi_k^{\text{sc}} = \chi_k/(1 + v_k\chi_k) = \chi_k^0/(1 + v_kG_k\chi_k^0) \tag{35}$$

where $\chi_k = \chi_k(\omega = 0)$ and $G_k = G_k(\omega = 0)$. Thus, to satisfy the compressibility sum rule it is sufficient to possess a correct small-k form of G_k.

For 2D $\Gamma = 2$ one can calculate the isothermal compressibility from its equation of state. We find that

$$\lim_{k\to 0} \chi_k^{\text{sc}} = -2n\beta. \tag{36}$$

If we insert the exact form of G_k in the static limit of the response function of Agarwal and co-workers we should obtain (36). That their frequency is scaled becomes immaterial since this sum rule is concerned with the static limit only. From (16), taking $\omega = 0$, i.e., $x = 0$, and adopting the conventional form, we get

$$(-1/n\beta)\chi_k^{\text{A}} = 1/[1 + a^{-1}(1 - G_k)] \tag{37}$$

where $G_k^{\text{A}}(0) = G_k$, since $Z(x = 0) = 1$. Hence

$$\chi_k^{\text{sc}} = n\beta/(-1 + G_k/a). \tag{38}$$

Now using (21), we recover (36) by taking the small-k limit of (38).

We have noted that the phenomenological response function due to Agarwal and co-workers is distinguished by its use of a scaled frequency. Nevertheless we see that it satisfies some of the necessary conditions for the response function, e.g., the first and third moment sum rules, in the manner of our second-order response function. The frequency scaling will cause a disagreement between this work and others more conventional in some of dynamical properties, e.g., dispersion relation.

A response function which can satisfy the third moment and compressibility sum rules represents a significant advance. In the recent literature there has been much confusion over developing what may be termed a consistent theory [13, 14]. For example, it has been realised that a generalised RPA theory cannot be made to satisfy the third moment sum rule [15, 16]. As we have elucidated here, but perhaps not previously recognised, the work of Agarwal and co-workers [1] is an improvement. It is in the right direction toward the construction of a consistent dynamical theory of the many-body problem.

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References

[1] Agarwal G K, Pathak K N and Ranganathan S 1984 *J. Phys. C: Solid State Phys.* **17** 2537
[2] Jancovici B 1981 *Phys. Rev. Lett.* **46** 386
[3] Abramo M C and Tosi M P 1974 *Nuovo Cimento* B **21** 5073
[4] Agarwal G K and Pathak K N 1982 *J. Phys. C: Solid State Phys.* **15** 5063
[5] Singh H B, Sharma A and Pathak K N 1979 *Phys. Rev.* A **19** 899
[6] Pathak K N 1984 *J. Phys. C: Solid State Phys.* **17** 2833
[7] De Leeuw S W, Perram J W and Smith E R 1983 *Physica* A **119** 441
[8] Hong J, Park J and Lee M H 1989 *Phys. Rev.* B **30** 1528
[9] Ichimaru S 1973 *Basic Principles of Plasma Physics* (Reading, MA: Benjamin) p 56
[10] Mahan G D 1981 *Many-Particle Physics* (New York: Plenum) p 440
[11] Hong J and Lee M H 1985 *Phys. Rev. Lett.* **55** 2375
[12] Pines D and Nozieres P 1966 *Theory of Quantum Liquids* (Reading, MA: Benjamin) pp 106, 205
[13] Iwamoto N 1984 *Phys. Rev.* A **30** 3289
[14] Iwamoto N, Krotscheck E and Pines D 1984 *Phys. Rev.* B **29** 3936
[15] Vaishya J S and Gupta A K 1973 *Phys. Rev.* B **7** 4300
[16] Pathak K N and Vashishta P 1973 *Phys. Rev.* B **7** 3649