UDC 533.9

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The loss function of dense plasmas and sum rules

Abstract. Mathematical, particularly, asymptotic properties of the RPA and RPA with dynamic local field corrections of the coupled plasma dielectric function are analyzed within the method of moments which satisfies some exact relations. Particularly *f*-sum rule,higher-order sum rules and other conservation laws. Thehigher-order sum rules take into account the correlations in the system under scrutiny, so if the system dynamic characteristics, e.g., the dielectric function, do not satisfy these rules which are effectively additional conservation laws, it is difficult to expect the corresponding model to be adequate in the strong-coupling domain.Some other drawbacks and advantages of the above models are pointed out.

Keywords: coupled plasmas, dielectric function, loss function, sum rules, method of moments.

Introduction

The extension of numerous models for the description of the coupled or non-ideal plasma dynamic properties onto the density-temperature domain characteristic for the inertial fusion bound experiments [1] is a hot problem nowadays. Particularly, the diagnostics methods applied in these experimental studies require a reliable method of reconstruction of the dynamic structure factor, and the method of moments [2-8] has demonstrated its advantages here with respect to other approaches recently [9].

We believe the sum rules can help us to answer these questions and determine the level of accuracy of dynamic theories of non-perturbative systems [10]. Certainly, the f-sum rule related to the density conservation is a pillar of any such model, but there are other pillars. These are other conservation laws and higher-order sum rules. The latter take into account the correlations in the system under scrutiny, and if the system dynamic characteristics, e.g., the dielectric function, do not satisfy these rules which are effectively additional conservation laws, it is difficult to expect the corresponding model to be adequate in the strong-coupling domain. The advantage of the approach based on the theory of moments is that the constructed (inverse) dielectric function satisfies all sum rules taken into account automatically. The disadvantage is related to the necessity to model a phenomenologically unknown and not measurable parameter function with certain mathematical properties, the Nevanlinna parameter function (NPF). The latter can be either reconstructed from available dynamic data, like it was done in [9] by the local constraints method, see [8] and references therein, or modelled on the basis of additional exact properties and/or limiting properties, like it was suggested in [11]. The point or the hope is that the main physical properties of the dynamic characteristic reconstructed on the basis of sum rules depend on the NPF model weakly.

As we will show, in one-component plasmas the RPA with an adequate dynamic local-field correction does comply with the higher-order sum rule.

The loss function

Modelling of the dielectric function, $\varepsilon(k,\omega)$ (DF), or the inverse dielectric function, $\varepsilon^{-1}(k,\omega)$ (IDF), of strongly coupled Coulomb systems is actively discussed in the literature, in particular, because the corresponding loss function

$$\mathcal{L}(k,\omega) = -Im\varepsilon^{-1}(k,\omega)/\omega \geq 0, \quad (2.1)$$

which is an even function of the real frequency, ω, determines the polarizational stopping power of such systems [13]. The non-negativity of the loss function stems from the similar property of $\left(-Im\varepsilon^{-1}(k,\omega)\right)$ for positive frequencies which in turn follows from the fluctuation-dissipation theorem since the (charge-charge) dynamic structure factor (DSF), $S_{cc}(k,\omega)$, is non-negative by definition:

$$\mathcal{L}(k,\omega) = \pi\beta\phi(k)b(\beta\hbar\omega)S_{cc}(k,\omega). \quad (2.2)$$

Here $\beta^{-1} = k_B T$ is the system temperature in energy units, k_B and $\hbar$ are the Boltzmann and Planck constants, $\phi(k) = 4\pi e^2/k^2$; the function $b(x) = (1-\exp(-x))/x$ is obviously strictly positive. We presume the system we consider to be in thermal equilibrium, uniform, and unmagnetized.

The analyticity of the prolongation of the IDF onto the upper half-plane of the complex frequency $w = \omega + i\delta$, $\delta > 0$, is due to the causality principle and the Kramers-Kronig relations are always valid for this function:

$$\varepsilon^{-1}(k,w) = 1 + \int_{-\infty}^{\infty} \frac{Im\varepsilon^{-1}(k,\omega)}{\omega - w}\frac{d\omega}{\pi}, Imw > 0. \quad (2.3)$$

Additionally,

$$\varepsilon^{-1}(k,0) = \lim_{\delta\downarrow 0}\varepsilon^{-1}(k,i\delta) = 1 + P\int_{-\infty}^{\infty} Im\varepsilon^{-1}(k,\omega)\frac{d\omega}{\pi\omega} \quad (2.4)$$

where P implies the principal value of the integral.

Consider the sum rules for the IDF which are effectively the (non-negative) power moments of the loss function [4-8]:

$$C_l(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^l \mathcal{L}(k,\omega)\,d\omega, \quad l = 0,1,2,\ldots. \quad (2.5)$$

The odd order moments vanish due to the symmetry of the loss function.

The expression for the zero moment follows immediately from (2.4) since the loss function can be considered continuous at $\omega = 0$:

$$C_0(k) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{Im\varepsilon^{-1}(k,\omega)}{\omega}d\omega = 1 - \varepsilon^{-1}(k,0) > 0. \quad (2.6)$$

The inequalities of the form

$$\varepsilon^{-1}(k,0) \leq 1 \Leftrightarrow \varepsilon(k,0) \geq 1, \quad \varepsilon(k,0) < 0 \quad (2.7)$$

also follow directly from (2.4), see [14,15] and references therein; the values of $\varepsilon(k,0)$ between 0 and 1 turn out to be forbidden and the causality conditions corresponding to the action of the external charge on the system do not preclude negative values for a static dielectric function (DF) of the system. If the static DF, $\varepsilon(k,0)$, becomes negative then the analyticity of the DF in the half-plane $Im\omega > 0$ might brake down.

We are interested here in taking into account not only the sum rules, but other exact relations as well. We wish to consider multi-species systems and the method of moments does not involve essentially the local-field corrections and expresses the dynamic properties in terms of the system static characteristics like the static structure factors and the moments themselves. Therefore we are not explicitly bounded, e.g., by the Niklasson condition or the compressibility sum rule [16,17] though the latter is important for the correct solution of the Ornsten-Zernicke equation, e.g. in the hypernetted approximation we use to compute the system partial static structure factors. The exact relation which directly influences our expression for the TCP IDF is, along the Kramers-Kronig relations, the Perel'-Eliashberg exact asymptotic form [18] (particularly, in a hydrogen-like two-component completely ionized plasma with the neutrality condition $n_e = Zn_i$):

$$Im\varepsilon\left(k,\omega \gg (\beta\hbar)^{-1}\right) \simeq A\left(\omega_p/\omega\right)^{9/2}, \quad A = 3^{-5/4}\sqrt{2}Zr_s^{3/4}. \quad (2.8)$$

The Brueckner parameter $r_s = a/a_B$ is determined by the electronic Wigner-Seitz radius $a = (3/4\pi n_e)^{1/3}$, $a_B = \hbar^2/m_e e^2$ is the Bohr radius, $\omega_p = \sqrt{4\pi n_e e^2/m_e}$ being the (electronic) plasma frequency. At high frequencies the asymptotic forms of the DF and IDF differ only in the sign so that the loss function behaves at high frequencies as $\omega^{-11/2}$. This implies that in a real system the sixth and higher even order power moments must diverge. The result (2.8) was rediscovered in [19](a), see also [19](b).

Observe also that due to the f-sum rule,

$$C_2 = \omega_p^2 .$$

We will apply the method of moments to the set

$$\left\{C_0\left(k\right), 0, C_2, 0, C_4\left(k\right)\right\}, \qquad (2.9)$$

and use the characteristic frequencies

$$\omega_1\left(k\right) = \sqrt{C_2 / C_0\left(k\right)} = \omega_p / \sqrt{1-\varepsilon^{-1}\left(k,0\right)}, \quad \omega_2\left(k\right) = \sqrt{C_4\left(k\right)} / \omega_p. \qquad (2.10)$$

Notice that due to the non-negativity of the loss function and the Cauchy-Schwarz inequality, the above set of moments (2.9) is positive-definite and thus the corresponding Hamburger moment problem of reconstruction of the loss function is solvable [2,3]. Since, due to (3), we can rewrite the IDF as

$$\varepsilon^{-1}\left(k,w\right) = \varepsilon^{-1}\left(k,0\right) - \frac{w}{\pi}\int_{-\infty}^{\infty} \frac{\mathcal{L}\left(k,\omega\right)d\omega}{\omega - w}, \qquad (2.11)$$

the Nevanlinna theorem and formula determine the non-canonical solutions of the Hamburger moment problem for the IDF as well.

It is important also that the explicit exact forms of these convergent moments can be derived independently of a particular DF or IDF model of an equilibrium plasma.The latter limitation can be avoided [20](a) applying the matrix version of the method of moments [20](b) in the species space [20](c).

The asymptotic expansion of the IDF along any ray in the upper half-plane *Imw>0* can be easily constructed from (2.11):

$$\varepsilon^{-1}\left(k,w\to\infty\right) \simeq \varepsilon^{-1}\left(k,0\right) + \frac{1}{\pi}\int_{-\infty}^{\infty}\left(1+\frac{\omega}{w}+\left(\frac{\omega}{w}\right)^2+\cdots\right)\mathcal{L}\left(k,\omega\right)d\omega = 1+\frac{\omega_p^2}{w^2}+\frac{\omega_p^2\omega_2^2\left(k\right)}{w^4}+\cdots. \qquad (2.12)$$

Similarly, if the dielectric function itself is a response function, i.e., if $\varepsilon\left(k,0\right)>1$,

$$\varepsilon\left(k,w\to\infty\right) \simeq 1-\frac{\omega_p^2}{w^2}-\frac{\omega_p^2\left[\omega_2^2\left(k\right)-\omega_p^2\right]}{w^4}+\cdots, \qquad (2.13)$$

so that for

$$\mathcal{P}\left(k,\omega\right) = Im\varepsilon\left(k,\omega\right)/\omega, \qquad (2.14)$$

which is also presumed to be non-negative and even for any real frequency ω,

$$M_l\left(k\right) = \frac{1}{\pi}\int_{-\infty}^{\infty}\omega^l\mathcal{P}\left(k,\omega\right)d\omega, \quad l=0,2,4, \quad M_0\left(k\right)=\varepsilon\left(k,0\right)-1, \quad M_2=\omega_p^2, \quad M_4\left(k\right)=C_4\left(k\right)-C_2^2. \qquad (2.15)$$

Indeed, if

$$\varepsilon\left(k,w\right) = 1+\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{Im\varepsilon\left(k,\omega\right)}{\omega-w}d\omega, \quad Imw>0, \quad M_0\left(k\right)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{Im\varepsilon\left(k,\omega\right)}{\omega}d\omega = \varepsilon\left(k,0\right)-1; \qquad (2.16)$$

but the positivity of the 4th moment $M_4(k)$ does not follow from the Cauchy-Schwarz inequality in L^2.

Hence, the coefficients of the asymptotic expansion of a certain function along any ray in the upper half-plane coincide with the *convergent* power moments of the corresponding distribution density (the loss function in our case) only if we deal with a Nevanlinna function [2], i.e., with a response function. In general, there are no reasons for the loss function higher moments (for even l > 4) to diverge in one-component plasmas

(OCPs), particularly, in electron fluids, but we show that they do for some of the models we consider here. Due to the definition of an asymptotic expansion, such divergence does not mean that lower order sum rules are not satisfied; such an option was not considered in [21].

The zero moment in the RPA

The relation of the loss function zero moment to the static value of the plasma IDF is applicable to systems with arbitrary number of components. Within the RPA the static dielectric function is defined as

$$\varepsilon_{\text{RPA}}(k,0)=1+\frac{4}{\pi a_B k^3}\int_0^\infty p f_{\text{FD}}(p)\ln\left|\frac{k/2+p}{k/2-p}\right|dp. \quad (3.1)$$

Here

$$f_{\text{FD}}(\mathbf{p})=f_{FD}(p)=\left[\exp\left(\beta E(p)-\eta\right)+1\right]^{-1}$$

is the Fermi-Dirac distribution density with $E(\mathbf{p})=E(p)=\hbar^2p^2/(2m)$. The dimensionless chemical potential $\eta=\beta\mu$ is defined by the normalization equation $F_{1/2}(\eta)=2D^{3/2}/3$ with

$$F_\nu=\int_0^\infty\frac{x^\nu dx}{\exp(x-\eta)+1},$$
$$D=\beta E_F=\beta m v_F^2/2=\beta\hbar^2k_F^2/2m \quad (3.2)$$
$$=\beta\hbar^2\left(3\pi^2 n\right)^{2/3}/2m,$$

where $F_\nu(\eta)$, E_F, v_F, and k_F are the ν-th order Fermi integral, Fermi energy, velocity, and wavenumber, respectively.

For the reference, we provide here an exact explicit expression for the 4^{th} moment. In a coupled electron fluid (see [4,8] and references therein):

$$C_4^{\text{ocp}}(k)=\omega_p^4\left[1+W_0(k)\right], \quad (3.3)$$

and the correction of the fourth moment contains only two contributions:

$$W_0(k)=V(k)+U(k). \quad (3.4)$$

The first contribution is produced by the kinetic term of the system Hamiltonian. In the classical case, $V(k)$ coincides with the well-known Vlasov contribution to the dispersion relation, $V(k)=3k^2/k_D^2$. In a degenerate system

$$V(k)=\frac{\left\langle v_e^2\right\rangle k^2}{\omega_p^2}+\left(\frac{\hbar}{2m}\right)^2\frac{k^4}{\omega_p^2}, \quad (3.5)$$

where the average of the square of the (electron) velocity is expressed as $\left\langle v_e^2\right\rangle=\left(3F_{3/2}(\eta)\right)/\left(m\beta D^{3/2}\right)$. The second contribution to the fourth moment stems from the interaction contribution to the system Hamiltonian:

$$U(k)=\frac{1}{2\pi^2 n}\int_0^\infty p^2\left(S(p)-1\right)f(p,k)dp, \quad (3.6)$$

where we have introduced the angular factor,

$$f(p,k)=\frac{5}{12}-\frac{p^2}{4k^2}+\frac{\left(k^2-p^2\right)^2}{8pk^3}\ln\left|\frac{p+k}{p-k}\right|. \quad (3.7)$$

To describe experimental and simulation data within the moment approach, one should specify the characteristic frequencies (2.10) and the Nevanlinna parameter function [4-8]. But to apply the Mermin approximation, one first has to study other construction elements of (3.1).

The extended RPA

The extended Mermin approximation was suggested in [22](b) and [23]. The extension consists in the introduction into the RPA dielectric function $\varepsilon_{\text{RPA}}(k,w)$ of the dynamic local field correction (DLFC):

$$\varepsilon_{\text{xRPA}}(k,w)=1+\frac{\phi(k)\Pi(k,w)}{1-\phi(k)G(k,\omega)\Pi(k,w)},$$
$$\varepsilon_{\text{xRPA}}(k,0)=1+\frac{\phi(k)\Pi(k,0)}{1-\phi(k)G(k)\Pi(k,0)}, \quad (4.1)$$

General properties and, in particular, the asymptotic expansion of the DLFC were studied in detail by Kugler [25]. At least, within the interpolation model for the DLFC approximation [24] employed in [23], the odd-order power moments of the DLFC diverge while the even-order moments vanish:

$$G(k,w) = G(k,\infty) + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{ImG(k,\omega)}{\omega - w} d\omega \underset{w\to\infty}{\simeq} G(k,\infty). \quad (4.2)$$

The latter characteristic, in electron fluids without theself-energy and effective mass corrections [21].

Results and conclusions

We have presented in figures 1 and 2the RPA model and RPA model with DLFC of the unmagnetized one-component completely ionized plasma longitudinal dielectric function and compared them to the one generated by the method of moments which takes into account all known sum rules and other exact relations automatically, by construction.

The authors acknowledge the financial support of the Science Committee of the Ministry of Education and Sciences of the Republic of Kazakhstan under Grants No. 1128/GF, 1129/GF and 1099/GF, and express gratitude for the financial support provided by the Ministry by a grant “The Best Teacher”.

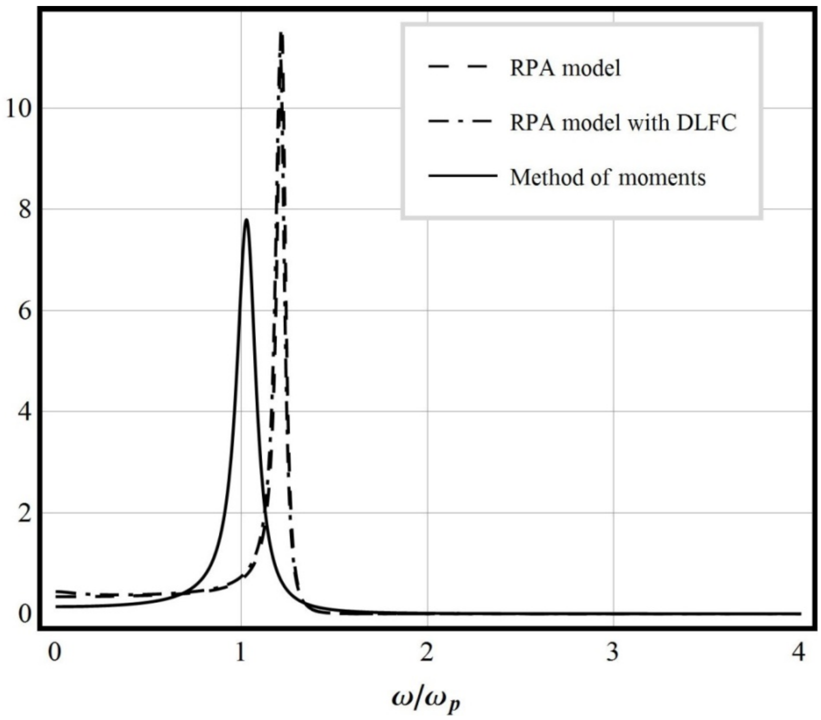

Figure 1 – The loss function calculated for different models of an electron fluid at Γ = 1, rs = 2.5256 and k =0.6 k_F.

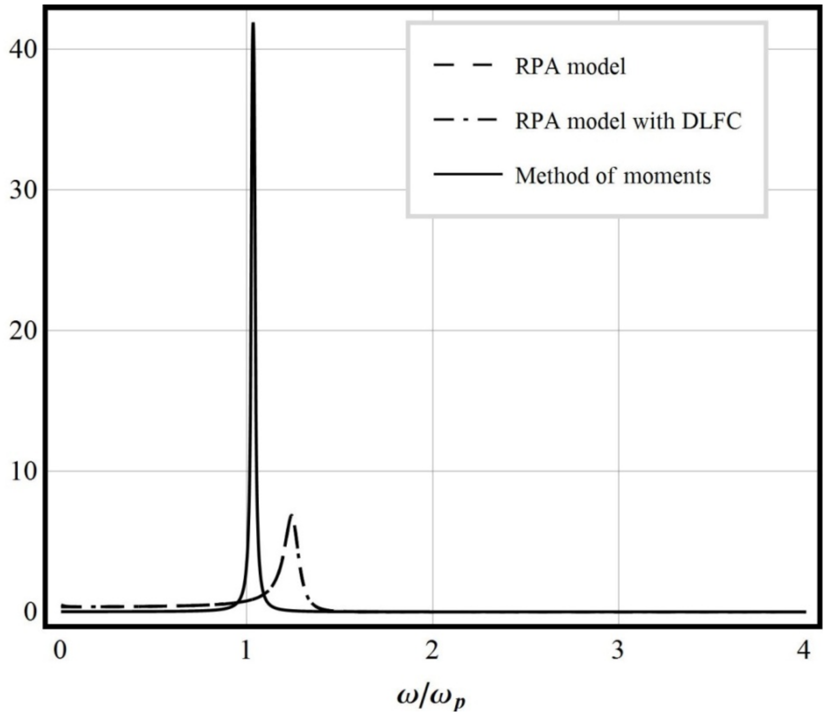

Figure 2 – As in Fig. 1 but for Γ = 0.1 and k = 0.11 k_F.

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