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Yu.V.Arkhipov¹, A.B.Ashikbayeva^{1*}, A. Askaruly¹, A.E. Davletov¹, and I.M. Tkachenko²

¹IETP, Department of Optics and Plasma Physics, al-Farabi Kazakh National University,
Tole Bi 96, Almaty 050012, Kazakhstan;

²Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia,
Camino de Vera s/n, 46022 Valencia, Spain;

*assel02@mail.ru

Dynamic conductivity of Kelbg-pseudopotential-modelled plasmas

Abstract. The obtained results continue our work on the optical properties of Kelbg-pseudopotential-modelled plasmas [1]. Since the difficulty of the uncertainty in the determination of the Nevanlinna parameter function is overcome by developing a regular method for deriving the Nevanlinna parameter function which essentially stems from the asymptotic behavior of the simulated dynamic collision frequency in the classical method of moments, it is possible, on the basis of the dynamic collision frequency (DCF) of hydrogen-like plasmas to derive the dynamic conductivities. Here internal and external dynamic conductivities, i.e. their imaginary and real parts are presented. Some information on the method of moments (MM) is provided.

Keywords: strongly coupled plasma, method of moments, sum rule, dynamic conductivity, Nevanlinna parameter function.

Introduction

The ultimate goal of the last papers [1-6] was to check whether the available experimental and simulation data satisfy convergent sum rules and other exact relations which could be helpful in verifying the employed techniques. Simultaneously, it was a demonstration of the fruitfulness of the MM approach in describing dynamic properties of plasmas since the attained agreement with those data was indeed quite good. Nevertheless, the uncertainty in the determination of the Nevanlinna parameter function remains a weakness of the MM approach. In [1] this difficulty was overcome by developing a regular method for deriving the Nevanlinna parameter function which essentially stems from the asymptotic behavior of the simulated dynamic collision frequency. Then using the obtained results it is possible to calculate the imaginary and real parts of internal and external dynamic conductivities. The plasma parameters considered here are as in[1].

It is remarked that the theory of moments permits to reconstruct analytic functions, which appear in physics as response functions with their specific mathematical properties, i.e., the Nevanlinna class functions which are analytic in the upper half-plane with a positive imaginary (or real) part, from their integral characteristics.

Background

It was shown in [7] that the plasma dielectric function $\varepsilon(z)$ analytic properties strongly depend on the sign of the static DF $\varepsilon(0) = \lim_{\omega \to 0} \varepsilon(0, \omega)$. In the long-wavelength limit when the space dispersion can be neglected both direct (DF) and inverse (IDF) dielectric functions are continuous restrictions of the corresponding Nevanlinna or response functions $\varepsilon(k,z)$ and $\varepsilon^{-1}(k,z)$, Imz > 0, to the real axis $Imz = Im(\omega + i0^+) = 0$, respectively. This implies that both response functions satisfy the Kramers-Kronig relations (for Imz > 0):

$$\varepsilon(z) = 1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im}\varepsilon(\omega)d\omega}{\omega - z},$$

$$\varepsilon^{-1}(z) = 1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im}\varepsilon^{-1}(\omega)d\omega}{\omega - z}.$$
(1)

Particularly,

$$\varepsilon^{-1}(0) = 1 + \frac{1}{\pi} \lim_{\delta \downarrow 0} \int_{-\infty}^{\infty} \frac{\operatorname{Im} \varepsilon^{-1}(\omega) d\omega}{\omega - i\delta}, \quad (2)$$

but due to the parity of the inverse dielectric function (IDF), the integral $\int_{-\infty}^{\infty} (\mathrm{I} m \varepsilon^{-1}(\omega)/\pi \omega) d\omega$

converges and equals -1. On the other hand, if the system static conductivity exists,

$$\sigma_0 = \lim_{\omega \to 0} \lim_{k \to 0} \sigma^{int}(k, \omega),$$

the DF

$$\varepsilon(\omega) = \lim_{k \to 0} \varepsilon(k, \omega) = 1 + \frac{4\pi i}{\omega} \sigma^{int}(0, \omega)$$

diverges when $\omega \to 0$. Hence, we should and can consider the power moments of the loss function $L(\omega) = -\mathrm{Im}\varepsilon^{-1}(\omega)/\omega$:

$$c_l = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^l L(\omega) d\omega, \quad l = 0,2,4;$$
 (3)

whereas the function $P(\omega) = \text{Im}\varepsilon(\omega)/\omega$ possesses only "positive" convergent moments

$$m_l = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^l P(\omega) d\omega, \quad l = 2,4.$$
 (4)

The moments c_2 and m_2 coincide and, by virtue of the f-sum rule [8], are both equal to the square of the plasma frequency: $c_2 = m_2 = \omega_p^2 = 4\pi n_e e^2/m$. Comparing the asymptotic expansions of the functions $\varepsilon^{-1}(z)$ and $\varepsilon(z)$

$$\begin{split} \varepsilon^{-1}(z) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{L(\omega) d\omega}{1 - \frac{\omega}{z}} \underset{z \to \infty}{\cong} \frac{1}{\pi} \int_{-\infty}^{\infty} L(\omega) \left(1 + \frac{\omega}{z} + \frac{\omega^2}{z^2} + \frac{\omega^3}{z^3} + \frac{\omega^4}{z^4} + \cdots \right) d\omega = \\ &= 1 + \frac{\omega_p^2}{z^2} + \frac{c_4}{z^4} + \cdots; \quad \varepsilon(z) \underset{z \to \infty}{\cong} 1 - \frac{\omega_p^2}{z^2} - \frac{c_4 - \omega_p^4}{z^4} - \cdots. \end{split}$$

the relation between the fourth moments is easily found to be: $m_4 = c_4 - \omega_p^4$. The moment c_4 has been calculated in our previous publications, see, for example, [4], and, precisely, for model plasmas described by a pseudopotential

$$\varphi_{ab}(k) = \frac{4\pi e^2}{k^2} \zeta_{ab}(k), \quad a, b = e, i,$$

can be written as [7]:

$$c_4 = \omega_p^4 (1 + H), \quad H = -\frac{1}{6\pi^2 Z \sqrt{n_e n_i}} \int_0^\infty q^2 S_{ei}(q) \zeta_{ei}(q) dq > 0.$$
 (5)

Notice that in a purely Coulomb system $\zeta_{ei}(q) = -Z$ and this correction reduces to $H_{Coulomb} = h_{ei}(0)/3$, $h_{ei}(0) = g_{ei}(0) - 1$, $g_{ei}(r)$ being the electron-ion radial distribution function

[9-10]. The parameter $H_{Coulomb}$ was first evaluated in the modified random phase approximation in [11] and recently generalized in [12]:

$$H_{mRPA} = \frac{4}{3} Z r_s \sqrt{\Gamma} \left[3Z \Gamma^2 + 4r_s + 4\Gamma \sqrt{3(1+Z)r_s} \right]^{-1/2}.$$
 (6)

Dynamic collision frequency

The classical Drude-Lorentz model was generalized in [13], see also corresponding references therein. Precisely, the following long-wavelength model expression for the IDF was suggested:

$$\varepsilon_{gDL}^{-1}(z) = 1 + \frac{\omega_p^2}{z^2 - \omega_n^2 + iz\nu(z)}, \quad Imz \ge 0, \quad (7)$$

where v(z) is the dynamic collision frequency (DCF) defined in a way that the static conductivity

$$\sigma_0 = \lim_{\omega \to 0} \frac{\omega}{4\pi i} \left(\frac{1}{\varepsilon_{aDL}^{-1}(\omega)} - 1 \right) = \frac{\omega_p^2}{4\pi \nu(0)}. \tag{8}$$

Let us now, for a while, return to the dynamic properties of completely ionized plasmas without neglecting the effects of space dispersion. Then the IDF $\varepsilon^{-1}(k,\omega)$ is always a genuine response function which must satisfy the Kramers-Kronig relation

$$\varepsilon^{-1}(k,z) = 1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\operatorname{Im} \varepsilon^{-1}(k,\omega)}{\omega - z} d\omega$$
, $\operatorname{Im} z > 0$, (9)

with the limiting value at z = 0 understood as

$$\varepsilon^{-1}(k,\omega) = 1 + \frac{1}{\pi} P. V. \int_{-\infty}^{\infty} \frac{\operatorname{Im} \varepsilon^{-1}(k,\omega')}{\omega' - \omega} d\omega' + i \operatorname{Im} \varepsilon^{-1}(k,\omega). \tag{10}$$

Particularly, since the IDF imaginary part is an odd function of frequency, it should vanish at $\omega = 0$,

$$\varepsilon^{-1}(k,0) = 1 + \frac{1}{\pi} P.V. \int_{-\infty}^{\infty} \frac{\mathrm{Im}\varepsilon^{-1}(k,\omega)}{\omega} d\omega.$$
 (11)

We assume that the static dielectric function $\varepsilon(k,0)$ value exists and is finite. Then, we can rewrite the previous expression as [7]

$$\varepsilon^{-1}(k,0) = 1 + \frac{1}{\pi} P. V. \int_0^\infty \operatorname{Im} \varepsilon^{-1}(k,\omega) \frac{d\omega^2}{\omega^2}$$
 (12)

and take into account the inequalities

$$Im\varepsilon(k,\omega) \ge 0$$
, $Im\varepsilon^{-1}(k,\omega) \le 0$, (13)

which follow for $\omega \ge 0$ from the fluctuation-dissipation theorem [8].

The following inequalities,

$$\varepsilon^{-1}(k,0) \le 1 \Leftrightarrow \varepsilon(k,0) \ge 1, \quad \varepsilon(k,0) < 0, \quad (14)$$

are direct consequences of (12) valid for k > 0.

The situation changes if the case k = 0 is considered. Indeed, instead of (12) the following conditions for both the static IDF and DF must hold:

$$\varepsilon(0) = 1 + \frac{1}{\pi} P. V. \int_0^\infty \operatorname{Im} \varepsilon(0, \omega) \frac{d\omega^2}{\omega^2},$$

$$\varepsilon^{-1}(0) = 1 + \frac{1}{\pi} P. V. \int_0^\infty \operatorname{Im} \varepsilon^{-1}(0, \omega) \frac{d\omega^2}{\omega^2},$$
 (15)

so that, by virtue of (13), we have, in addition to (14), that

$$\varepsilon^{-1}(0) \le 1 \Leftrightarrow \varepsilon(0) \ge 1,$$
 (16)

and, thus, $\varepsilon(0)$ should never take negative values. Consequently, when k>0, the causality conditions corresponding to the action of the external charge on the system do not preclude the static dielectric function to be negative, only the values between 0 and 1 turn out to be forbidden. If the limit $k\to 0$ is initially taken, then, the causality principle prohibits the static DF to take values smaller than 1. Indeed, it was already shown [9] that $\varepsilon(0)=\infty$ or $\varepsilon^{-1}(0)=0$ which are due to the existence of the static conductivity.

The integrand in the principal value integral (11)

has a removable singularity, which means that it converges as a usual Riemann integral. The latter is actually the zero power moment of the loss function $\mathcal{L}(k,\omega) = -\mathrm{I} m \varepsilon^{-1}(k,\omega)/\omega$, which is an even function of the frequency well defined at $\omega = 0$:

$$C_0(k) = -\int_{-\infty}^{\infty} \frac{\operatorname{Im} \varepsilon^{-1}(k,\omega)}{\pi \omega} d\omega = 1 - \varepsilon^{-1}(k,0), (17)$$

and the first of the inequalities (14) implies the positivity of $C_0(k)$ with $C_0(k=0)=1$.

Even if the interparticle interaction potential is different from the bare Coulomb one and can be described by an effective potential, the second power moment of the loss function remains unchanged due to the *f*-sum rule [7-8] and is equal to the square of the system plasma frequency:

$$C_2 = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^2 \mathcal{L}(k, \omega) d\omega \equiv \omega_p^2 \approx \frac{4\pi e^2 n_e}{m}.$$
 (18)

Hence, the moment sequence $\{(1 - \varepsilon^{-1}(k,0)), 0, \omega_p^2\}$ is positive and the moment problem [14] of reconstruction of both the loss function and the IDF $\varepsilon^{-1}(k,z)$ is solvable [15]. The non-canonical continuous solution of the Hamburger moment problem in this case is easily found from the Nevanlinna formula [15]:

$$\varepsilon^{-1}(k,z) = 1 + \frac{\omega_1^2}{z^2 - \omega_1^2(k) + zQ_1(z;k)}, \quad Imz \ge 0.$$
 (19)

Here $\omega_1^2(k) = C_2/C_1(k)$ and $Q_1(z;k)$ is the Nevanlinna parameter function which belongs to a Nevanlinna class function such that along any ray in the upper half-plane, $\lim_{z\to\infty}Q_1(z;k)/z=0$. In the long-wavelength limiting case $\omega_1(0)=\omega_p$ model expression (7) is recovered if we choose $Q_1(z;0)=q_1(z)=i\nu(z)$. Moreover, for any k expressions (7) and (19) share the asymptotic expansion

$$\varepsilon^{-1}(k, z \to \infty) \cong 1 + \frac{\omega_p^2}{z^2} + O\left(\frac{1}{z^3}\right),$$
 (20)

which implies that both expressions satisfy the f-sum rule (18).

There are still some distinctions to be pointed out: (i) All three sum rules $\{(1 - \varepsilon^{-1}(k, 0)), 0, \omega_p^2\}$ are automatically satisfied by expression (19) for any proper choice of $q_1(k, z)$, while expression (7)

might satisfy the sum rules $\{1,0,\omega_p^2\}$ only for an as yet unknown DCF; for a constant $\nu(\omega) = \nu(0)$: = $\nu > 0$, these sum rules are satisfied. (ii) Expression (19) is easily generalized for the moment sequence

$$\{(1-\varepsilon^{-1}(k,0)), 0, \omega_n^2, 0, \omega_2^2(k)\omega_n^2\},$$
 (21)

i.e., the fourth sum rule which accounts for the correlations in the system, $C_4(k) = \int_{-\infty}^{\infty} \omega^2 \mathcal{L}(k,\omega) d\omega/\pi = \omega_2^2(k) \omega_p^2$ is satisfied. It is, however, unclear how the DCF $\nu(\omega) = \text{Re}\nu(\omega) + i\text{Im}\nu(\omega)$ could be chosen so that at least for k = 0, we had

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega^4 (\text{Re}\nu(\omega)) d\omega}{\left|\omega^2 - \omega_n^2 + i\omega\nu(\omega)\right|^2} = \omega_2^2(0) \omega_p^2. \tag{22}$$

(iii) Notice that for a constant collision frequency, the l.h.s. of (22) diverges, and its convergence might be guaranteed only if

$$\nu(\omega \to \infty) \cong a\omega^{-\alpha_r} + ib\omega^{-\alpha_i}$$
 (23)

with $\alpha_r > 1$ and $\alpha_i > -1$.

The fourth power moment

$$C_4(k) = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^4 \mathcal{L}(k, \omega) d\omega := \omega_2^2(k) \omega_p^2$$

has been known for a long time [6,10,16], $C_4(0) = c_4 = \omega_n^4(1+H)$.

The non-canonical solution of the Hamburger moment problem [15] for the positive sequence $\{1,0,\omega_p^2,0,\omega_p^4(1+H)\}$ can be written as

$$\varepsilon^{-1}(z) = 1 + \frac{\omega_p^2(z + Q_2(z))}{z(z^2 - \omega_p^2(1 + H)) + Q_2(z)(z^2 - \omega_p^2)}.$$
 (24)

The question to be answered now is whether the model expression for the IDF (7) satisfies not only the sum rules $\{1,0,\omega_p^2\}$, but also the fourth one $\omega_p^4(1+H)$. Numerical integration of the simulation data of [17] shows that the moment conditions (21) are satisfied with a high degree of accuracy. On the other hand, it is indeed interesting whether the Nevanlinna parameter function $Q_2(z)$ can be chosen such that expression (7) virtually turns into expression (24). It is straightforward to demonstrate that for the generalized Drude-Lorentz model IDF to $\omega_p^3(z)$ to satisfy the above five sum rules, the following relation between the DCF $\nu(z)$ and the Nevanlinna

function $Q_2(z)$ should hold:

$$\nu(z) = \frac{i\omega_p^2 H}{z + Q_2(z)}. (25)$$

The DCF $\nu(\omega)$ was studied, in a quite detailed way, for moderately coupled hydrogen plasmas. To describe these results in the context of relation (25), two model expressions are proposed below for the function $Q_2(z)$.

Nevanlinna parameter functions

Being a Nevanlinna class function which grows slower than |z| at $z \to \infty$, the parameter function $Q_2(z)$ is determined by the Riesz-Herglotz formula [15,18] as

$$Q_2(z) = \int_{-\infty}^{\infty} \frac{g(x)dx}{x-z},$$
 (26)

where the distribution density $g(x) \ge 0$ must be such that

$$\int_{-\infty}^{\infty} \frac{g(x)dx}{1+x^2} < \infty.$$

The main drawback of the MM is that the Nevanlinna parameter functions lack any phenomenological sense, i.e, they are not directly measurable quantities. Relation (26) is not a definition of the function $Q_2(z)$ as a measurable characteristic since the DCF is not measurable either. Thus, to reproduce the data on the DCF obtained in [13] and [17], one might try to determine an adequate distribution density g(x) from the asymptotic form of the DCF. Precisely, the values of the exponents α_r and α_i are found in [17] and it turns out that for the Kelbg potential $\alpha_r \approx 3.5$ while $\alpha_i \approx 1$, as for the Coulomb potential. For example, the asymptotic behavior is thoroughly reproduced by assuming

$$g_1(x) = \frac{b}{\pi} |x|^r,$$
 (27)

where b, and r are real parameters to be found. It is presumed that r is negative, but the integral in (26) converges only if $r \in (-1,0)$. Then

$$\frac{Q_{21}(z)}{\omega_p} = \frac{ib\left(\frac{z}{\omega_p}\right)^r}{\exp\left(\frac{\pi ir}{2}\right)\cos\left(\frac{\pi r}{2}\right)}.$$
 (28)

The weak point of such a model expression is

that the corresponding DCF vanishes at $\omega = 0$. Alternatively, we can assume

$$Q_{22}(z) = \frac{-1}{ih + Q_{21}(z)},\tag{29}$$

where the positive parameter h is to be determined from the relation (25) at $z \downarrow 0$:

$$\nu(0) = \omega_p^2 H/h. \tag{30}$$

In both cases the real part of the DCF decreases as $(\omega/\omega_p)^{r-2}$ whereas the DCF imaginary part goes to zero slower, namely as $(\omega/\omega_p)^{-1}$. Model expression (29) guarantees a finite positive value for the measurable parameter $\nu(0)$, but deviates from the asymptotic behavior for the Kelbg pseudopotential.

Dynamic conductivity and numerical results

The fluctuation dissipation theorem and the lingitudinal polarization function gives the relation between the internal conductivity and the dynamic colission frequency in the long wavelength limit [17]

$$\sigma^{int}(z) = \frac{\omega_p^2}{-iz + \nu(z)}.$$
 (31)

The internal and external conductivities are closely related by the expression [4]

$$\sigma^{int}(z) = \frac{\sigma^{ext}(z)}{1 - \frac{4\pi i}{z} \sigma^{ext}(z)}.$$
 (32)

The computed dynamic conductivities (31), (32) have real and imaginary parts. The comparisons between them and the simulation results [13] are presented on figures 1-4.

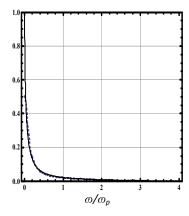


Figure 1- Real part of the internal dynamic conductivity obtained by (31) – full line compared to the simulation data [17] – dashed line

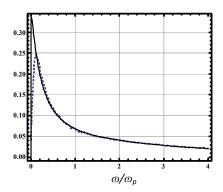


Figure 2 – Imaginary part of the internal dynamic conductivity obtained by (31) – full line compared to the simulation data [17] – dashed line

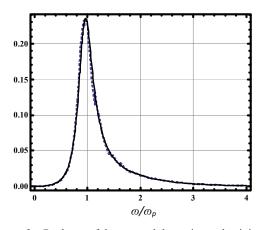


Figure 3 – Real part of the external dynamic conductivity obtained by (32) – full line compared to the simulation data [17] – dashed line

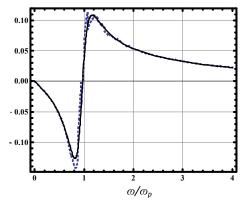


Figure 4 – Imaginary part of the external dynamic conductivity obtained by (32) – full line compared to the simulation data

[17] – dashed line

Conclusions

Using a model for the Nevanlinna parameter function [1] the plsma dynamic conductivities were

calculated within the moment approach and compared to the simulation data whichwas based on the application of the Kelbg pseudopotential to impose quantal characteristics on the MD method [17]. It is seen that the results on internal dynamic conductivitie agree with the simulation data quite well for both conductivities.

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