Reconstruction of internal longitudinal conductivity of non-ideal plasmas by exact relations and sum rules

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Abstract. The classical method of moments is applied to the analysis of the external and internal dynamic conductivities of dense plasmas. The Nevanlinna formula with only one non-zero $f$–sum rule taken into account reproduces the Drude-Lorentz model expression for the internal conductivity. The inclusion of the second non-zero sum rule produces a new model which includes the non-monotonicity of the conductivity beyond the domain of applicability of the Drude-Lorentz model. An extensive mathematical analysis of recent simulation data and reflectivity measurements of shock-compressed dense xenon plasmas is carried out.

1. The Drude-Lorentz model from the point of view of the theory of moments

The classical model for the (internal) conductivity of dense plasmas and metals,

$$\sigma_{DL}(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

is characterized by two static parameters, the static conductivity $\sigma_0 = \sigma(\omega = 0) = n_e e^2 m^{-1} = (4\pi)^{-1}\omega_p^2 \tau$ and the relaxation time $\tau$. Here $n_e$ is the number density of electrons in the system, $-e$ and $m$ are the electronic charge and mass, and $\omega_p$ is the plasma frequency.

The static conductivity value can be obtained as [1]:

$$\sigma_0 = \lim_{\omega \to 0} \frac{\text{Re} \sigma_{\text{ext}}(\omega)}{\omega^2},$$

where $\sigma_{\text{ext}}(\omega)$ is the external dynamic conductivity of the Coulomb system related to the internal conductivity through the well-known relation$^4$ [2]:

$$\sigma(\omega) = \frac{\sigma_{\text{ext}}(\omega)}{1 - i\frac{4\pi}{\omega}\sigma_{\text{ext}}(\omega)}.$$
Mathematically, the DL function, \( \sigma_{DL}(z) \) is a simple Nevanlinna (response) function with a single simple pole in the lower half-plane. In addition, the real part of \( \sigma_{DL}(z) \) possesses a single finite frequency moment, which is known also as the \( f \)-sum rule:

\[
\mu_0 = \int_{-\infty}^{\infty} \text{Re} \sigma(\omega) \, d\omega = \frac{\omega_p^2}{4}. \quad (4)
\]

It is also known that the real part of the internal conductivity must have a finite second frequency moment

\[
\mu_2 = \int_{-\infty}^{\infty} \omega^2 \text{Re} \sigma(\omega) \, d\omega = \frac{\omega_p^2 \Omega^2}{4}. \quad (5)
\]

All odd-order frequency moments are equal to zero due to parity, and higher order moments diverge.

An explicit expression for the frequency \( \Omega \) is related to static correlations in a plasma, and is model-dependent [1, 3, 4, 5]. In particular, it was shown [3] that in a completely ionized hydrogen-like plasma, the moment (5) is proportional to the probability to encounter an electron at the point where an ion is:

\[
\mu_2 = \frac{\omega_p^4}{12N^2V} \sum_{i,j} N_i \langle \delta(r_i - r_j) \rangle_0. \quad (6)
\]

Here \( N \) is the number of charges of each species in the volume \( V \) occupied by plasma, \( \langle \cdots \rangle_0 \) stands for the equilibrium average. This value can be evaluated in the RPA [3] to give:

\[
\mu_2 = \frac{\omega_p^4}{12} \left\{ 1 + \frac{\beta e^2}{\lambda_T (1 + \lambda_T/\lambda_D)} \right\}, \quad (7)
\]

where \( \beta^{-1} = k_B T \) is the plasma temperature in energy units, \( \lambda_T = \hbar/2\sqrt{\beta/m} \) is the electronic thermal wavelength, and \( \lambda_D^2 = 4\pi e^2 / \beta \sum_{j=0}^{s-1} Z_j n_j \) is the plasma Debye radius. The plasma is presumed to consist of electrons (\( j = 0 \)) and \( s \) ionic species with charge numbers \( Z_i \), so that \( n_e = \sum_{i=1}^{s} Z_i n_i \).

Nevertheless, the classical theory of moments [6, 1] permits to describe the class of functions which possess the second moment (5), and thus to go beyond the DL model. Precisely, if the distribution density \( \text{Re} \sigma(\omega) \) we are looking for has \( 2r + 1 \) finite moments

\[
\mu_k = \int_{-\infty}^{\infty} \omega^k \text{Re} \sigma(\omega) \, d\omega, \quad k = 0, 1, 2, \ldots, 2r, \quad (8)
\]

then the Nevanlinna theorem establishes a one-to-one correspondence between the set of such densities or, due to the Kramers-Kronig relations, complex conductivities

\[
\sigma(z) = \frac{1}{\pi i} \int_{-\infty}^{\infty} \frac{\text{Re} \sigma(x)}{x - z} \, dx, \quad (9)
\]

and all Nevanlinna-class functions \( q(z) \) such that \( \lim_{z \to 0} q(z)/z = 0, \, \text{Im} z > 0 \), [6]

\[
\sigma(z) = \frac{i}{\pi} \frac{E_{r+1}(z) + q(z) E_r(z)}{D_{r+1}(z) + q(z) D_r(z)}. \quad (10)
\]

Here \( D_k(z) \) are orthogonal polynomials with respect to the measure \( \text{Re} \sigma \) [7]:

\[
\int_{-\infty}^{\infty} D_n(\omega) D_m(\omega) \text{Re} \sigma(\omega) \, d\omega = \delta_{nm} \| D_n \|^2, \quad n, m = 0, 1, \ldots, 2r, \quad (11)
\]
and $E_n(z)$ are their conjugate polynomials:
\[ E_n(z) = \int_{-\infty}^{\infty} \frac{D_n(z) - D_n(t)}{z-t} \text{Re} \sigma(t) \, dt. \]  
(12)

In our case, $r = 1$ and we have:
\[
\begin{align*}
D_0(z) &= \frac{1}{\sqrt{\mu_0}}, \quad D_1(z) = \frac{z}{\sqrt{\mu_2}}, \quad D_2(z) = \sqrt{\frac{\mu_0 \mu_2}{\Delta_2}} \left( z^2 - \Omega^2 \right), \\
E_0(z) &= 0, \quad E_1(z) = \sqrt{\frac{\mu_0^2}{\mu_2}}, \quad E_2(z) = \mu_0 \sqrt{\frac{\mu_0 \mu_2}{\Delta_2}} z,
\end{align*}
\]
(13)
where $\Delta_2 > 0$ is a parameter to disappear by an adequate renormalization of $q(z)$.

Notice first that if we put $r = 0$ in (10), then we obtain the generalized DL model expression:
\[
\sigma_1(z) = \frac{i \omega_p^2}{4 \pi} \frac{1}{z + q(z)}.
\]
(14)
Thus the classical DL conductivity is recovered if we substitute the function $q(z)$ in (14) by its static value $q(0) = i/\tau$.

Notice also that the existence of two (even) finite frequency moments of the conductivity real part implies the following asymptotic expansion for the complex conductivity:
\[
\sigma(z \to \infty) \simeq \frac{i \omega_p^2}{4 \pi z} + \frac{i \omega_p^2 \Omega^2}{4 \pi z^3}.
\]
(15)

### 2. Two-moment modelling

Generally speaking, we have no phenomenological considerations for the determination of the Nevanlinna parameter function $q(z)$ in Eq. (10).

To go beyond the classical DL model with a constant relaxation time\(^5\) without violating the sum rules, we introduce here the following simple model expression for the Nevanlinna parameter function:
\[
q(z) = -\zeta \omega_p \Omega^2 \tau \frac{z}{z + i \zeta \omega_p},
\]
\[\zeta > 0\] being a model parameter. Then, for the conductivity we get:
\[
\begin{align*}
\sigma_2(z) &= \frac{i \omega_p^2}{4 \pi} \frac{z^2 + i \zeta \omega_p (z + i \Omega^2 \tau)}{z^3 + i \zeta \omega_p (z^2 - \Omega^2) - i \Omega_1^2 z}, \\
\Omega_1^2 &= \Omega^2 (1 + \zeta \omega_p \tau).
\end{align*}
\]
(16)

Notice that this conductivity model expression possesses a correct static value and satisfies two sum rules (4,5).

\(^5\) For the latest review on the frequency-dependent inverse relaxation time, see [8].
Table 1. Fit of the parameter $\zeta$ in the expression (16) corresponding to experimental data of reflectivity obtained with a laser with $\lambda = 1.06 \, \mu m$, for a $Xe$ plasma.

| Experimental data | Two-moment model |
|-------------------|------------------|
| $p \,(GPa)$ | $T \,(K)$ | $\rho \,(g \cdot cm^{-3})$ | $R$ | $\log_{10}(\zeta)$ | $R$ |
| 1.6 | 30050 | 0.51 | 0.096 | $-0.408$ | 0.096 |
| 3.1 | 29570 | 0.97 | 0.12 | $-0.730$ | 0.12 |
| 5.1 | 30260 | 1.46 | 0.18 | $-0.848$ | 0.18 |
| 7.3 | 29810 | 1.98 | 0.26 | $-0.836$ | 0.26 |
| 10.6 | 29250 | 2.70 | 0.36 | $-0.749$ | 0.36 |
| 16.7 | 28810 | 3.84 | 0.47 | $-0.460$ | 0.43 |

Table 2. Fit of the parameter $\zeta$ in the expression (16) corresponding to experimental data of reflectivity obtained with a laser with $\lambda = 0.694 \, \mu m$, for a $Xe$ plasma.

| Experimental data | Two-moment model |
|-------------------|------------------|
| $p \,(GPa)$ | $T \,(K)$ | $\rho \,(g \cdot cm^{-3})$ | $R$ | $\log_{10}(\zeta)$ | $R$ |
| 4.1 | 33000 | 1.1 | 0.11 | $-0.570$ | 0.11 |
| 9.1 | 32000 | 2.2 | 0.18 | $-0.445$ | 0.18 |
| 20.0 | 29000 | 4.1 | 0.43 | 0. | 0.35 |

3. Numerical analysis and conclusions

3.1. Reflectivity measurements

In Refs. [9, 8] and [10, 11], we find the results of experimental measurements of reflectivity for dense shock-compressed xenon plasmas at pressures $1.6 \div 20 \, GPa$ and temperatures around $30 kK$ using laser beams with wavelengths $1.06 \, \mu m$ and $0.694 \, \mu m$, respectively.

To check our model, we can apply the expression for the reflectivity derived from the Fresnel formula in the long-wavelength case,

$$ R = \left| \frac{\sqrt{\varepsilon(\omega)} - 1}{\sqrt{\varepsilon(\omega)} + 1} \right|^2, $$

where the dielectric function can be written as

$$ \varepsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma_2(\omega), $$

i.e., just considering the longitudinal conductivity.

In Tables 1 and 2 the experimental results on the reflectivity according to [9, 8] and [10, 13], respectively, are compared to our fit with the varying model parameter $\zeta$ of (16) to reproduce the reflectivity data quantitatively. In particular, for the last points in both sets of measurements, for $16.7 \, GPa$ and $20.0 \, GPa$, we can see that it is impossible to get the value of $0.47$ and $0.43$, respectively, since the maximum of the function occurs at $0.43 \, \log_{10}(\zeta) = -0.460$ for the first case, and at $0.35$, though at these points the curve which shows the reflectivity as a function of $\zeta$ is quite flat in both cases. Anyway, both values are inside the experimental error interval.
3.2. Comparison with simulation data

The characteristic feature of the new simulation data of [12] is the non-monotonicity of the dynamic internal conductivity beyond the domain of applicability of the DL model.

Here we report a comparison of our results obtained from equation (16) to the data of [12] and [13]. We show that the presence of the free parameter \( \zeta \) permits us to obtain at least a qualitative agreement with these data.

**Figure 1.** Dynamic conductivity for an Al plasma, using computed moments from numerical data of [12]: \( \rho = 0.025 \, \text{g/cm}^3 \), \( T = 30000 \, \text{K} \), and \( \zeta = 0.0198 \).

**Figure 2.** Dynamic conductivity for an Al plasma, using computed moments from numerical data of [12]: \( \rho = 0.5 \, \text{g/cm}^3 \), \( T = 20000 \, \text{K} \), and \( \zeta = 10 \).

In Figures 1 and 2 we can observe the shape of the model expression (16) as a function of frequency corresponding to thermodynamic conditions of figures 4 and 3b, respectively, of [12]. The values of the moments were obtained by numerical integration of the results reported in this reference, the quantitative behavior of the graphs depends strongly on these values.

In particular for Figure 1, the peak which appears at high frequencies and for high values of \( \zeta \), moves to lower frequencies as the value of the parameter diminishes; the qualitative behavior of the dynamic conductivity does not depend too much on the parameter \( \zeta \). Notice that the position of this peak tends to a finite value of frequency as \( \zeta \rightarrow 0 \) which effectively coincides with that of figure 4 of [12] (see Figure 1). Nevertheless, as the value of \( \zeta \) decreases, the effective width of the function for low values of frequencies also decreases, and the DL behavior vanishes.

On the other hand, for conditions corresponding to Figure 2 we see a different behavior: for any value of the model parameter \( \zeta \) the conductivity shows a non-monotonic dependence on the frequency.

If we put \( \zeta \rightarrow \infty \), the corresponding limiting form of the real part of Eq. (16) has a maximum at a finite non-zero value of frequency if, and only if, \( \Omega \tau < \sqrt{2} \); that is the situation in Figure 2.

In addition to this direct comparison of our model to the simulation data of [12], we used the Kramers-Kronig relations to calculate the corresponding external dynamic conductivity and the value of the static conductivity according to Eq. (2). The latter, coincided with the simulation data near \( \omega = 0 \), with a precision of higher than 2%, see Table 3.

In Ref. [13] we find numerical results for the internal and external conductivities in the long-wavelength limiting case, obtained from MD simulations of a xenon plasma for the same thermodynamic conditions as in the first measurement of [10, 11]. As we can see in Figures 3, the internal (effectively called in [13] transversal) conductivity for this simulation presents a Drude-like behavior. Nevertheless, if we take the value adjusted for the reflectivity calculation
Numerical data of [13]

Figure 3. Dynamic conductivity for a Xe plasma, using computed moments from numerical data of [13]. Thermodynamic conditions corresponds to the first point of Table 2: \( \sigma_0/\omega_p = 0.3390, \zeta = 0.27 \).

Table 3. Static conductivity obtained from the simulation data of [12] directly, \( \sigma_0 \), and evaluated according to Eq. (2).

| Conditions | \( \sigma_0/\omega_p \) | \( \sigma_0/\omega_p \) (Eq. (2)) |
|------------|----------------|------------------|
| Fig. 1     | 0.1323         | 0.1319           |
| Fig. 2     | 0.0706         | 0.0720           |

in Table 2, \( \zeta = 10^{-0.570} \approx 0.27 \), we observe that our two-moment model predicts a peak near \( \omega/\omega_p = 2.3 \).

4. Conclusions
We have outlined some basic features of an alternative approach to the investigation of Strongly Coupled Coulomb Systems based on exact relations and sum rules. The mathematical nature of this approach permits its application to Coulomb systems in which all characteristic lengths, like the Debye radius, the De Broglie wavelength, the Wigner-Seitz radius are of the same order of magnitude of about 1Å. Under such conditions the coupling parameter is at least of the order of 1, and the electron subsystem is degenerate, so that the traditional kinetic constructions based on the employment of the Landau or Balescu equations are no longer applicable; the experimental studies of such systems are difficult to carry out, and the interpretation of their results is often uncertain.

We have shown that the present approach is capable of capturing of basic features in the behavior of dynamic properties of these systems with extreme thermodynamic parameters. In the case of the internal conductivity which we considered as an example, we manage to achieve even a semi-quantitative agreement with experimental data within the error margin of the latter.

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