Dynamic properties of one-component strongly coupled plasmas

The moment approach with local constraints

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- We wish to outline a mathematical approach which could be employed in this context and, including, in other fields of research.
- We deal with the OCP dynamic properties as determined within the moment approach (based on the sum-rules and other exact relations) complemented by the local constrains in comparison with the MD simulation data of A. Wierling, T. Pschiwul, and G. Zwicknagel, Phys. Plasmas, **9**, 4871 (2002).

Problem

Let a positively defined integrable function (distribution density), $f(t)$, be given only by a set of its numerical values.
Find an analytic representation of $f(t)$ such that

1. *it were an imaginary part of the Nevanlinna class (response) function*

$$F(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(t)}{t - z} dt, \ \mathrm{Im}\, z > 0 \tag{1}$$

analytic in $\mathrm{Im}\, z > 0$, *continuous on the real axis* $\mathrm{Im}\, z = 0$ *and such that* $\lim_{z \to \infty} F(z)/z = 0, \ \mathrm{Im}\, z \geq 0$:
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2. $f(t)$ *would satisfy the local constraints at some real points* $(t_1, ..., t_p)$:

$$F(t_s + i0) = w_s, \ s = 1, .., p. \tag{2}$$

Fact

Assume that we are able to compute some power moments of the function in question,

$$c_k = \frac{1}{\pi} \int_{-\infty}^{\infty} t^k f(t)\, dt \ , \qquad k = 0, 1, ..., 2n, \tag{3}$$

then, asymptotically, along any ray in $\mathrm{Im}\, z \geq 0$,

$$F(z \to \infty) = -\frac{1}{\pi z} \int_{-\infty}^{\infty} \frac{f(t)}{1 - t/z} dt \simeq$$

$$\simeq -\frac{c_0}{z} - \frac{c_1}{z^2} - \frac{c_2}{z^3} - \cdots - \frac{c_{2n}}{z^{2n+1}} + \mathrm{o}\left(\frac{c_{2n}}{z^{2n+1}}\right). \tag{4}$$

Fact

Thus the above problem can be specified as a Hamburger truncated problem of moments solvable if and only if the set of moments $(c_0, ..., c_{2n})$ *is positive definite, i.e.,*

$$c_0 \geq 0, \qquad \det \begin{bmatrix} c_0 & c_1 \\ c_1 & c_2 \end{bmatrix} \geq 0,$$

$$\det \begin{bmatrix} c_0 & c_1 & c_2 \\ c_1 & c_2 & c_3 \\ c_2 & c_3 & c_4 \end{bmatrix} \geq 0, \cdots \tag{5}$$

$$\det \begin{bmatrix} c_0 & \cdots & c_n \\ \vdots & \ddots & \vdots \\ c_n & \cdots & c_{2n} \end{bmatrix} \geq 0.$$

Fact

If these conditions hold and if all of the above inequalities are strict, the Hamburger problem has two infinite sets of solutions: canonical and non-canonical

- A canonical solution is a linear combination of "masses" defined by the moment conditions (3), located at arbitrary points $(x_0, \ldots, x_{2n})$:

$$f_c(t) = \sum_{j=0}^{2n} m_j \delta(t - x_j) \ , \qquad F_c(z) = \sum_{j=0}^{2n} \frac{m_j}{\pi(x_j - z)} \ . \tag{6}$$

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- The non-canonical solutions are continuous and are described by the Nevanlinna theorem: there is a univocal correspondence between them and the functions $q_n(z)$ which belong to the same class:

$$q_n(z) = \int_{-\infty}^{\infty} \frac{dg(t)}{t - z}, \qquad \lim_{z\to\infty} q_n(z)/z = 0, \ \int_{-\infty}^{\infty} \frac{dg(t)}{1+t^2} < \infty, \ \mathrm{Im}\, z > 0.$$

Theorem

This correspondence is provided by the Nevanlinna formula,

$$\int_{-\infty}^{\infty} \frac{f(t)dt}{z-t} = \frac{E_{n+1}(z) + q_n(z) E_n(z)}{D_{n+1}(z) + q_n(z) D_n(z)} ,$$

Definitions

The polynomials

$$
\begin{aligned}
D_0 &= \frac{1}{\sqrt{c_0}} , \quad \Delta_{-1} = 1 , \quad \Delta_0 = c_0 , \\
D_k(t) &= \frac{1}{\sqrt{\Delta_{k-1}\Delta_{k+1}}} \det \begin{bmatrix} c_0 & \cdots & c_{k-1} & 1 \\ c_1 & \cdots & c_k & t \\ \vdots & \vdots & \vdots & \vdots \\ c_k & \cdots & c_{2k-1} & t^k \end{bmatrix} , \qquad (7) \\
\Delta_k &= \det \begin{bmatrix} c_0 & \cdots & c_k \\ \vdots & \vdots & \vdots \\ c_k & \cdots & c_{2k} \end{bmatrix} , \; k = 1, 2, ..., n
\end{aligned}
$$

form an orthogonal system with respect to each $f(t)$ satisfying (3);
$E_0 \equiv 0$, $E_k(t) = \int_{-\infty}^{\infty} \frac{D_k(t) - D_k(s)}{t-s} f(s) ds$, $k = 1, ..., n$,
is the corresponding set of conjugate polynomials.

- Notice that the zeros of each orthogonal polynomial $D_k(z)$ are real and by virtue of the Schwarz-Christoffel identity

$$D_n(z)E_{n+1}(z) - D_{n+1}(z)E_n(z) = \tag{8}$$

$$\Xi_n = \Delta_n \left(\Delta_{n-1}\Delta_{n+1}\right)^{-1/2} > 0 \ , \quad n = 0, 1, 2, \dots$$

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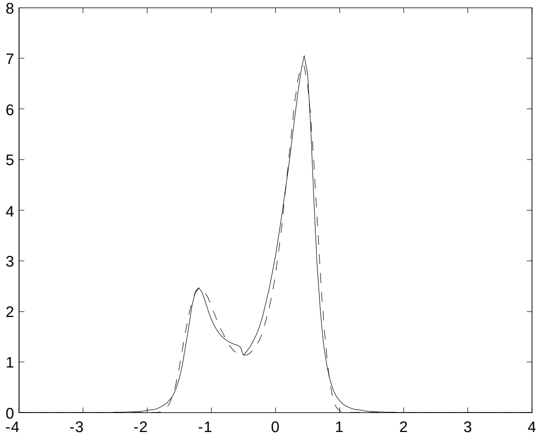
- We suggest to construct a non-canonical solution of the Hamburger problem and then find a parameter function $q_n(z)$ to satisfy the constraints

$$\lim_{\eta \downarrow 0} \int_{-\infty}^{\infty} \frac{f(t)dt}{t - t_s - i\eta} = \pi w_s, \; s = 1, .., p. \qquad (9)$$

  The latter can be done using a modification of the Schur algorithm of the theory of interpolations.

Example

The (irrational) reconstruction (solid line) of an asymmetric distribution density (dashed line) by three local constraints and five power moments:



Consider a physically interesting case of $n = 2$ and $p = 1$ and consider, for a given value of the wavenumber, $f(\omega) = S(k, \omega)$, the OCP dynamic strаucture factor (DSF). In our work we used the simulation data provided to us by G. Zwicknagel. We calculated the moments $c_0(k)$, $c_2(k)$, and $c_4(k)$ numerically.
Hence, by virtue of the Nevanlinna theorem,

$$\int_{-\infty}^{\infty} \frac{S(k, \omega)\, d\omega}{\omega - z} = -\frac{E_3(z) + Q(z) E_2(z)}{D_3(z) + Q(z) D_2(z)}, \quad \operatorname{Im} z > 0, \qquad (10)$$

$$\begin{aligned} &D_0(z) = 1, \quad D_1(z) = z, \quad D_2(z) = z^2 - \omega_1^2, \\ &D_3(z) = z^3 - z\omega_2^2, \quad E_0(z) \equiv 0, \quad E_1(z) = 1, \qquad (11) \\ &E_2(z) = z, \quad E_3(z) = z^2 - \Omega^2 \end{aligned}$$

$$\omega_1^2 = \frac{c_2}{c_0}, \quad \omega_2^2(k) = \frac{c_4}{c_2} = \omega_p^2 + \Omega^2, \; \Omega^2 \sim \Gamma. \qquad (12)$$

- Choose some real frequency $z = \omega_0 \in \mathbb{R}$ and calculate the interpolation parameters

$$s(\omega_0) = P.V. \int_{-\infty}^{\infty} \frac{S(k,\omega)\, d\omega}{\pi(\omega - \omega_0)} + iS(k,\omega_0) \in \mathbb{C}$$

and

$$a(\omega_0) = \omega_0 s(\omega_0) + 1.$$

It is important that, due to the fluctuation-dissipation theorem (FDT) and the Kramers-Kronig relations,

$$s_0 = s(\omega_0 = 0) = i/\tau\omega_p^2, \tag{13}$$

where the transport relaxation time τ is determined by the system static conductivity:

$$\sigma_0 = \omega_p^2 \tau / 4\pi\ . \tag{14}$$

- Invert the Nevanlinna formula to find

$$
\begin{aligned}
b(\omega_0) &= \frac{Q(\omega_0)}{\omega_p} = \\
&= -\frac{1}{\omega_p}\frac{s(\omega_0)\,D_3(\omega_0) + E_3(\omega_0)}{s(\omega_0)\,D_2(\omega_0) + E_2(\omega_0)} = \\
&= -\frac{\omega_0}{\omega_p} + \frac{a(\omega_0)\,\Omega^2/\omega_p}{\omega_0 a(\omega_0) - \omega_p^2 s(\omega_0)} \in \mathbb{C}
\end{aligned}
\tag{15}
$$

with

$$
b_0 = \frac{Q(0)}{\omega_p} = -\frac{\Omega^2}{s_0\omega_p^3} = i\frac{\tau\Omega^2}{\omega_p} := ih.
$$

- Observe that if we possess reliable numerical data on the DSF, we can make use of the relation (13) to find the static conductivity.

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- Our Shur-like algorithm reduces the search for the function $Q(z)$ to the construction of a contractive function $r(z)$ ($|r(z)| \leq 1$, the Caley transformation)

$$r(z) = \frac{Q(z) - i\omega_p}{Q(z) + i\omega_p} \tag{16}$$

such that

$$v = r(z = \omega_0) = \frac{b(\omega_0) - i}{b(\omega_0) + i}, |v| < 1. \tag{17}$$

- We choose

$$r(z) = \frac{u(z) + 1}{\overline{v}u(z) + v^{-1}}, \qquad (18)$$

with

$$u(z) = \exp\left\{\frac{\alpha}{\pi i}\int\limits_{\omega_0-1}^{\omega_0+1}\frac{1+tz}{t-z}\ln|t-\omega_0|\frac{dt}{t^2+1}\right\}, \ \alpha \in (0,1), \qquad (19)$$

which vanishes at $z = \omega_0$.

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which vanishes at $z=\omega_0$.

- Thus,

$$Q(z) = i\omega_p\frac{1+r(z)}{1-r(z)} = i\omega_p\frac{(\overline{v}+1)\,u(z)+v^{-1}+1}{(\overline{v}-1)\,u(z)+v^{-1}-1} \tag{20}$$

and when $\omega_0=0$, $u(0)=0$, while

$$Q_0 = Q(0) = i\tau\Omega^2\ . \tag{21}$$

The corresponding model expression for the DSF,

$$S(k,\omega) = \frac{n}{\pi} \frac{S(k)\,\omega_1^2\left(\omega_2^2 - \omega_1^2\right) \operatorname{Im} Q(k,\omega)}{\left|\omega\left(\omega^2 - \omega_2^2\right) + Q(k,\omega)\left(\omega^2 - \omega_1^2\right)\right|^2} \quad , \tag{22}$$

where

$$S(k) = \frac{1}{n} \int_{-\infty}^{\infty} S(k,\omega)\, d\omega = \frac{\pi c_0(k)}{n}$$

is the SSF, automatically, independently, of our choice of the parameter function $Q(k,\omega)$, satisfies the sum rules $c_0(k)$, $c_2(k)$, and $c_4(k)$ and interpolates between the static conductivity $\sigma_0 = \omega_p^2 \tau / 4\pi$ and the asymptotic expansion

$$S(k, z \to \infty) \simeq -\frac{c_0(k)}{z} - \frac{c_2(k)}{z^3} - \frac{c_4(k)}{z^5} + \cdots, \quad \operatorname{Im} z > 0. \tag{23}$$

- We can obtain a rational model for the Nevanlinna parameter function if we put, e.g.,

$$u(z) = z/(z + i\gamma)$$

with some positive parameter γ to be determined from the contractivity condition. Then

$$Q(z) = ih^2\omega_p \frac{z + i\delta}{z + ih\delta},$$

where

$$\delta = \frac{1}{2}(\gamma + h\gamma).$$

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$$\delta = \frac{1}{2}(\gamma + h\gamma).$$

- Alternatively, a non-rational model for the function $Q(z)$ follows from (20), (17), and (15).

We applied the Schur-like algorithm to reconstruct the DSF using 3 non-zero moments and 3 local constraints. The values of the numerical parameter $\alpha \in (0,1)$ of the auxiliary function

$$u_s(z) = \exp\left\{ \frac{\alpha}{\pi i} \int_{t_s-1}^{t_s+1} \frac{1+tz}{t-z} \ln|t-t_s| \frac{dt}{t^2+1} \right\}, \quad s=1,2,3 \qquad (24)$$

were obtained by the maximization of the Shannon entropy

$$\mathfrak{S}(\alpha) = -\int_{-\infty}^{+\infty} \psi(\alpha,t) \ln(\psi(\alpha,t))\, dt,$$

where the density $\psi(\alpha,t)$ is the one reconstructed within the algorithm. The density $\psi(\alpha,t)$ has no real poles and is positive over the whole real axis, hence it was quite easy to solve the equation $d\mathfrak{S}(\alpha)/d\alpha = 0$.

The numerical results were compared to the simulation data on the dynamic structure factor and are summarized in the following figures 2-6. In all figures the squares correspond to the simulation data.

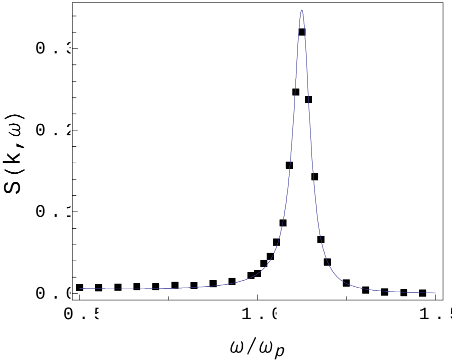

Figure 2. The OCP dynamic structure factor at $\Gamma = 0.5$ and $ka = 0.34725$.

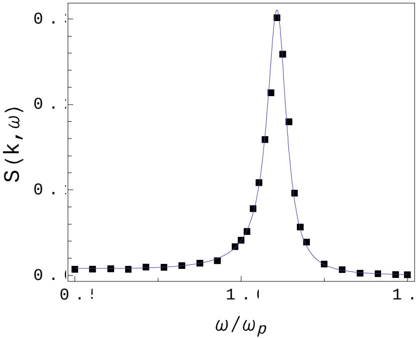

Figure 3. As in Fig. 2, but for
$\Gamma = 1$ and $ka = 0.49109$.

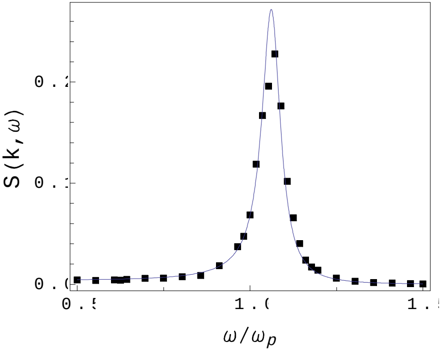

Figure 4. As in Fig. 2, but for $\Gamma = 2$ and $ka = 0.60145$.

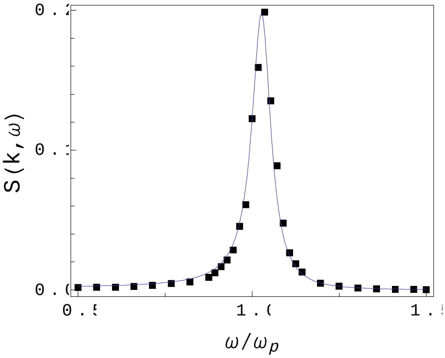

Figure 5. As in Fig. 2, but for $\Gamma = 4$ and $ka = 0.6945$.

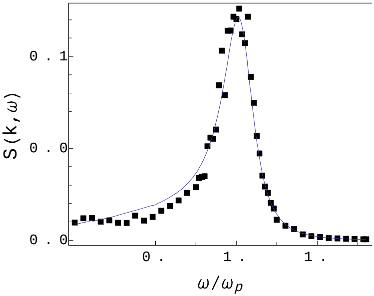

Figure 6. As in Fig. 2, but for $\Gamma = 8$ and $ka = 1.389$.

To study the characteristics of the plasmon mode we used the data on the Nevanlinna parameter function $Q(k,\omega)$ to solve the dispersion equation

$$z\left(z^2-\omega_2^2(k)\right)+Q(k,z)\left(z^2-\omega_1^2(k)\right)=0. \tag{25}$$

If the parameter function $Q(k,\omega)$ vanishes, the dispersion reduces to the frequency

$$\omega_2(k)=\sqrt{\omega_p^2+\Omega^2(k)}, \tag{26}$$

where the contribution $\Omega(k)$ accounts for the coupling in the system. Otherwise, we obtain complex solutions presented in Figs. 7.

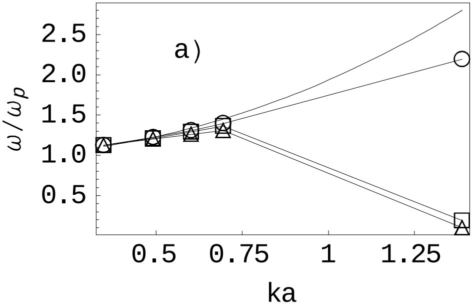

Figure 7a. The plasmon dispersion relation for $\Gamma = 0.5$. The triangles represent the positions of the maxima of the DSF, the squares stand for the real part of the solution of (25), the circles correspond to $\omega_2(k)/\omega_p$ (26), and the solid line was calculated by the interpolation formulas of P. Hansen.

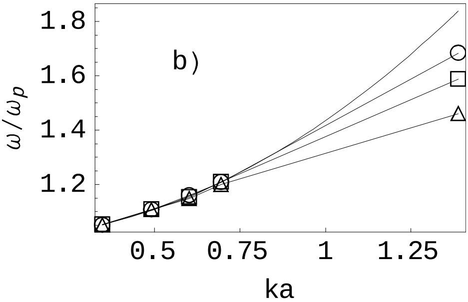

Figure 7b. As in Fig. 7a, but for $\Gamma = 1.0$.

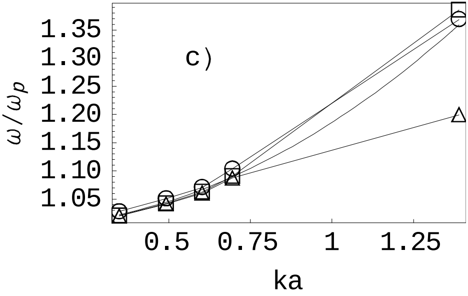

Figure. 7c. As in Fig. 7a, but for $\Gamma = 2.0$.

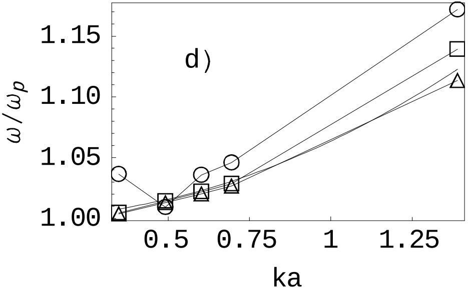

Figure. 7d. As in Fig. 7a, but for $\Gamma = 4.0$.

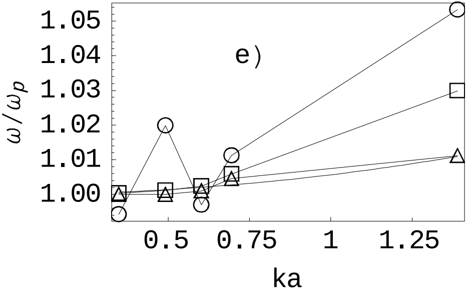

Figure. 7e. As in Fig. 7a, but for
$\Gamma = 8.0$.

The decay decrement of the Langmuir mode:

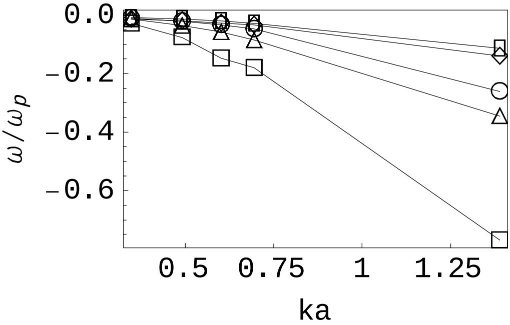

Figure 8. The mode decrement, i.e., the imaginary part of the solution of the dispersion equation (25) for $\Gamma = 0.5$ (squares), $\Gamma = 1.0$ (triangles), $\Gamma = 2.0$ (circles), $\Gamma = 4.0$ (diamonds), and $\Gamma = 8.0$ (rectangles).

Finally, we employed the results we recovered with respect to the plasma dielectric function (using the FDT), to calculate the reflectivity from this plasma layer:

$$R\left(\omega\right)=\left|\frac{\sqrt{\varepsilon(k,\omega)}-1}{\sqrt{\varepsilon(k,\omega)}+1}\right|^{2}. \qquad (27)$$

We neglected the influence of the transition layer from air to plasma, though additional studies are due in this sense. The results are presented in Fig. 9.

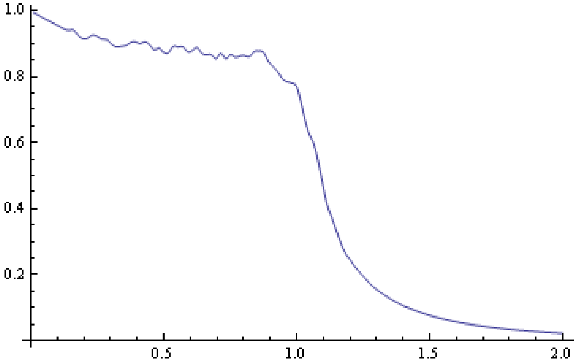

Figure. 9a. The plasma reflectivity as a function of frequency normalized to the plasma frequency ω_p for $\Gamma = 2$ and $ka = 0.60145$.

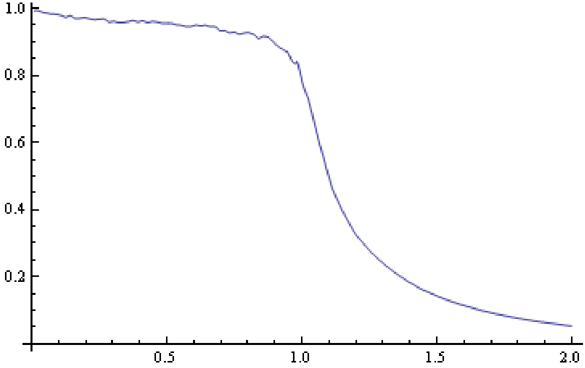

Figure. 9b. As in Fig. 9a, but for $\Gamma = 4$ and $ka = 0.6945$.

As it was expected, under these conditions, the reflectivity takes very high values and decreases rapidly as the oncoming radiation frequency becomes larger than the plasma frequency of the system.

We can conclude that an algorithm is presented which permits to obtain, at least in the cases we consider, a quantitative agreement between the simulation data on the plasma dynamic characteristics and their non-rational counterparts reconstructed by a few integral characteristics, the power moments and the local constraints. Further applicability and convergence properties of the approach are to be considered elsewhere.

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Thank you for your attention!

Спасибо за внимание!