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New developments in the application of the method of moments in Plasma Physics

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This review article is based on a number of our research papers complemented by some mathematical developments which are usually not included to texts in Physics, and which can permit a reader to enter into the details of the self-consistent method of moments, recently suggested, and understand how it could be improved even further. The idea of the method of moments which appeared some 35 years ago is to employ several sum rules and other exact relations to determine the dynamic properties of strongly coupled classical or partially degenerate plasmas. Now this approach is complemented by new empirical and mathematical observations which permit to determine dynamic characteristics of strongly coupled completely ionized classical one-component plasmas without any data input from simulations or direct experiments and express the dynamic properties of the above systems entirely in terms of their static characteristics like the static structure factors. The obtained results are quite satisfactory and promising.

Key words: one-component plasmas, method of moments, dynamic structure factor.
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1 Introduction

The challenge of the contemporary statistical plasma physics is the description, analytical and numerical, of the transition from collisionless to collision-dominated regimes in different Coulomb systems, of the crossover from classical to Fermi liquid behavior in dense plasmas [1, 2]. We refer to warm and hot dense matter or strongly coupled plasmas characterized by a wide range of variation of temperature ($10^4 - 10^7$ K) and mass density ($10^{-2} - 10^4$ g/cm^3) spanning a few orders of magnitude. Under such conditions thermal, Coulomb coupling, and quantum effects compete between them and impede the construction of a bridge theory capable of including of all these effects into the description of static, kinetic, and dynamic properties of the above systems of high relevance for inertial fusion devices [3] and advanced laboratory studies, e.g., in ultracold plasmas [4], etc.

The standard (electron) coupling and degeneracy parameters defined, respectively, as

$$\Gamma = \beta e^2 / a , \quad D = \beta E_F , \tag{1}$$

vary in strongly coupled plasmas as follows:

$$\Gamma \in (4.9 \times 10^{-3}, 490),$$

$$D \in (1.4 \times 10^{-3}, 1.4 \times 10^{4}).$$

We employ above the Brueckner parameter

$$r_s = a / a_B \in (6.5 \times 10^{-2}, 6.5),$$

$a = (4\pi n/3)^{-1/3}$, a_B, and E_F are the electron Wigner-Seitz, Bohr radii and the Fermi energy, n being the number density of electrons; besides, the temperature $T = (k_B\beta)^{-1}$,

$$D = \frac{\Gamma}{2r_s}\left(\frac{9\pi}{4}\right)^{2/3} = 1.84158428\frac{\Gamma}{r_s}.$$

Throughout the text we will use the dimensionless wavenumber $q = ka$.

Despite the lack of small parameters, static structural and even kinetic characteristics of strongly coupled plasmas are relatively easy to determine numerically, see, e.g., [2, 5]. Nevertheless, currently, there are no first-principle physical approaches capable of producing reliable results on dynamic properties of such systems within the above gaps between ideal-gas and solid-state conditions. Good agreement in a relatively wide realm of variation of Γ and/or D is finally achieved using up to four adjustable parameters [6]. Numerical data on the dynamic local-corrections remains unexplained theoretically [7].

The well-known model of the Quasi-Localized Charge Approximation [8] satisfies only the interaction-related sum rule and fails to describe the energy dissipation processes.

We suggest an alternative mathematical approach capable of taking all sum rules (which might be considered complementary conservation laws) into account automatically and to include into the scheme the collective mode decay. Specifics of physical systems are included into the sum rules calculated independently and rigorously using standard methods of quantum statistics, say within the Kubo linear-reaction theory. This approach seminal papers were published more than 30 years ago [9]; further development was proposed in the papers [10-13], and the book [14]. They were based on the classical monographs [15] and [16].

A new, self-consistent version of this method was suggested recently [17] applied to the direct determination of dynamic properties of one-component classical strongly coupled plasmas in terms of their static ones, without any adjustment to the dynamic data. The validity of the approach was confirmed by comparison with available simulation results. In addition, the robustness of the method was confirmed by applying several schemes of calculation of the plasma static structure factor, which provided results in good agreement with each other, within the precision of the simulations themselves.

The method of moments is based on the Nevanlinna theorem which establishes a unilateral correspondence between the dynamic characteristic in question and a non-phenomenological (Nevanlinna parameter) function of a certain mathematical class, see below. The above results were achieved in [17] and numerous relevant publications within a significant simplification: the Nevanlinna parameter function (NPF) was approximated by its static value. This simplification, in one-component plasmas, is equivalent [10] to the substitution of the dynamic local-field correction by its static value. It also impedes the extension of the approach to low coupling systems traditionally described within the random-phase approximation (RPA).

The aim of the present paper is two-fold: (i) provide a detailed introduction into the mathematical aspects of the method of moments and (ii) suggest and check some model expressions for the NPF both in classical and quantum–mechanical settings. The liquid systems we consider are presumed to be in thermal equilibrium and unmagnetized. Generalizations to more complex systems can be carried out within the matrix method of moments [14].

The paper is organized in the following way. In the next Section we provide mathematical details of the moment approach. Then, some dynamical models of the NPF are proposed and analyzed. Finally, we arrive to some conclusions important for further development of the method.

2 The mathematical introduction.

2.1 Nevanlinna (response) functions and their mathematical properties [4].

Definition 1 (*The Nevanlinna class of functions $\mathfrak{R}$): A function $F(z) \in \mathfrak{R}$ if*

1. $F(z)$ is analytic in $\operatorname{Im} z > 0$;
2. $\operatorname{Im} F(z) \geq 0$ in $\operatorname{Im} z > 0$.

Definition 2 *Let $t \in \mathbb{R}$ be a random variable with a distribution function $\sigma(t)$. If*

$$\sigma(t) = \int_{-\infty}^{t} f(s)ds \qquad (2)$$

the function $f(t)$ is called the probability density function, p.d.f.. Since $\sigma(t)$ is, by definition, a non-decreasing function, $f(t) \geq 0$ for any real t.

Claim 3. The Nevanlinna functions are determined by the Riesz – Herglotz transform:

$$F(z) = az + b + \int_{-\infty}^{\infty} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) dg(t), \qquad (3)$$

where $\{a,b\} \in \mathbb{R}$, $a \geq 0$ and $g(t)$ is a non-decreasing bounded function (distribution) such that

$$\int_{-\infty}^{\infty} \frac{dg(t)}{1+t^2} < \infty .$$

Claim 4 *Notice that we can always choose the function* g(t) *so that b was equal to*

$$b = \int_{-\infty}^{\infty} \frac{tdg(t)}{1+t^2} ;$$

and that

$$a = 0.$$

Definition 5 (*The class of functions* $\Re_0$*): A function G*(z) ∈ $\Re_0$ *if G*(z) ∈ $\Re$ *and*

$$\lim_{z\to\infty} \frac{G(z)}{z} = 0 , \ \mathrm{Im}\, z > 0 , \tag{4}$$

so that for such functions from (3) we have:

$$G(z) = \int_{-\infty}^{\infty} \frac{dg(t)}{t-z} + ih , \ h > 0 , \tag{5}$$

where the non-negative parameter h does not depend on z, but might depend on other parameters, e.g., in Physics, on the wavenumber.

2.2 The classical Hamburger problem of moments

Definition 6 *The real numbers*

$$\mu_m = \int_{-\infty}^{\infty} t^m d\sigma(t) , \ m = 0,1,2,... \tag{6}$$

are the (power) moments of the distribution σ(t). If the distribution σ(t) is differentiable and f(t) = σ'(t) is symmetric, all odd-order moments (6) vanish.

Let us summarize some notions and results of the classical theory of moments [18-20].

The Hamburger problem is formulated in the following way.

Problem 7 *Given a set of real numbers* $\{\mu_0, \mu_1, \mu_2, ...\}$, *find all distributions* $\sigma(t)$ *such that*

$$\int_{-\infty}^{\infty} t^m d\sigma(t) = \mu_m , \ m = 0,1,2,... \tag{7}$$

The Hamburger moment problem is solvable, i.e., there exists at least one distribution (p.d.f.) which satisfies (7), if and only if the given set of numbers $\{\mu_m\}_{m=0}^{\infty}$ *is non-negative, i.e., if the Hankel matrix* $(\mu_{m+n})_{m,n=0}^{\infty} \geq 0$*. If the problem is solvable, it can have a unique solution (a determinate problem) or an infinite number of solutions (an indeterminate problem).*

Definition 8. *Notice that if σ(t < 0) ≡ const (i.e., if f(t < 0) ≡ 0), we have the Stieltjes moment problem, and if σ(t) ≡ const (f(t) ≡ 0) for t < a, t > b, a,b ∈* $\mathbb{R}$, *we deal with the Hausdorff problem finite interval moment problem.*

Theorem 9 *[21] A Hamburger moment problem (7) is solvable if*

$$\Delta_m = \det(\mu_{i+j})_{i,j=0}^{m} \geq 0 , \ m = 0,1,2,...$$

The problem has an infinite number of solutions if and only if

$$\Delta_m = \det(\mu_{i+j})_{i,j=0}^{m} > 0 , \ m = 0,1,2,...$$

The problem (7) is determinate if and only if

$$\Delta_0 > 0,...,\Delta_k > 0 , \ \Delta_{k+1} = \Delta_{k+2} = ... = 0 .$$

Claim 10. *The set of solutions of an indeterminate problem is in a one-to one correspondence with a certain subset of the class of Nevanlinna functions [18]; this correspondence is described by the Nevanlinna formula, see below.*

Claim 11. *A truncated Hamburger moment problem [18], i.e., a moment problem with a finite set of given numbers, i.e.,* $\{\mu_m\}_{m=0}^{2\nu}, \nu = 0,1,2$ *is solvable if the Hankel matrix* $(\mu_{m+n})_{m,n=0}^{\nu} > 0$, *[22], see also [23] and [24]. In the degenerate case of a singular Hankel matrix* $(\mu_{m+n})_{m,n=0}^{\nu}$ *the problem of moments (under some special conditions established in [25] and [23], [24]) has a unique solution described in [23], [24].*

Theorem 12 *[26, 21, 19] A sufficient condition that the Hamburger moment problem (6) be determinate is that (Carleman's criterion)*

$$\sum_{m=1}^{\infty} \mu_{2m}^{-1/2m} = \infty .$$

Example 13. *The p.d.f.*

$$f_\alpha(t;\gamma) = \frac{\alpha\gamma^{1/\alpha}}{2\Gamma\left(\frac{1}{\alpha}\right)} \exp\left(-\gamma|t|^\alpha\right), \alpha, \gamma > 0 \quad (8)$$

where $\Gamma(z)$ *is the Euler* Γ *function, has an infinite number of moments for any positive* α*:*

$$\mu_{2m}(\alpha;\gamma) = \int_{-\infty}^{\infty} t^{2m} f_\alpha(t)dt = \frac{\Gamma\left(\frac{2m+1}{\alpha}\right)}{\gamma^{2m/\alpha}\Gamma\left(\frac{1}{\alpha}\right)}, \quad (9)$$

$$\mu_{2m+1}(\alpha;\gamma) = 0 \, , m = 0,1,2,...$$

but the Hamburger moment problem for the set of numbers

$$\left\{1, 0, \frac{\Gamma\left(\frac{3}{\alpha}\right)}{\gamma^{2/\alpha}\Gamma\left(\frac{1}{\alpha}\right)}, 0, \frac{\Gamma\left(\frac{5}{\alpha}\right)}{\gamma^{4/\alpha}\Gamma\left(\frac{1}{\alpha}\right)}, 0, ...\right\}, \quad (10)$$

has, as it stems from the Carleman criterion, a unique solution, which is the p.d.f. (8), if $\alpha > 1$*, in particular the Gaussian density* $f_2(t; \frac{1}{2a^2})$, $a > 0$*, and an infinite number of solutions if* $\alpha \le 1$*. In this latter case, all solutions of the moment problem are described by the Nevanlinna formula ([19]), see below.*

Other examples of sets $\{\mu_m\}_{m=0}^{\infty}$ which generate indeterminate moment problems are provided in [20].

In (solvable) problems where we already have at least one p.d.f. with a set of moments, like the problems we are interested in here, the only question which arises is the one of uniqueness of the solution of the problem of reconstruction of a (one-dimensional) p.d.f. by its power moments, $\{\mu_m\}_{m=0}^{\nu}$.

2.3 Orthogonal polynomials and the Nevanlinna formula

Theorem 14. *(Nevanlinna) There is a one-to-one correspondence between all solutions of the Hamburger problem (7), or all complex Nevanlinna functions*

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{d\sigma(t)}{t-z}, \quad (11)$$

and all Nevanlinna functions $R(z) \in \Re_0$ *such that*

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{d\sigma(t)}{t-z} = \frac{E_{n+1}(z) + R(z)E_n(z)}{D_{n+1}(z) + R(z)D_n(z)} . \quad (12)$$

This last formula is called the **Nevanlinna formula.**

Definition 15 *Here* $\{D_l(z)\}_{l=0}^{\infty}$ *are orthonormalized polynomials with respect to the measure* $d\sigma$ *[20]:*

$$\int_{-\infty}^{\infty} D_n(t)D_m(t)d\sigma(t) = \delta_{nm} \, , n, m = 0,1,..., \quad (13)$$

and $E_n(z)$ *are their conjugate polynomials:*

$$E_n(z) = \int_{-\infty}^{\infty} \frac{D_n(z) - D_n(t)}{z-t} d\sigma(t) . \quad (14)$$

Precisely

$$D_0(t) = \frac{1}{\sqrt{\mu_0}}, \; \Delta_{-1} = 1, \; \Delta_0 = \mu_0 ,$$

$$D_l(t) = \frac{1}{\sqrt{\Delta_l \Delta_{l-1}}} \det \begin{bmatrix} \mu_0 & \cdots & \mu_{l-1} & 1 \\ \mu_1 & \cdots & \mu_l & t \\ \vdots & \vdots & \vdots & \vdots \\ \mu_l & \cdots & \mu_{2l-1} & t^l \end{bmatrix}, \quad (15)$$

$$\Delta_l = \det \begin{bmatrix} \mu_0 & \cdots & \mu_l \\ \vdots & \vdots & \vdots \\ \mu_l & \cdots & \mu_{2l} \end{bmatrix}, \; l = 1,2,... \quad (16)$$

Let us point out the properties of these orthonormalized polynomials:

Claim 16. *It can be easily seen that both sets of polynomials do not depend on the distribution we seek, they are determined by the moments only:*

$$D_0(z)=\frac{1}{\sqrt{\mu_0}},\ D_1(z)=\frac{1}{\sqrt{\mu_0}}\frac{z-a_0}{b_0},$$

$$D_2(z)=$$

$$=\frac{\left(\mu_0\mu_2-\mu_1^2\right)z^2+z\left(\mu_1\mu_2-\mu_3\mu_0\right)+\left(\mu_3\mu_1-\mu_2^2\right)}{\sqrt{\left(\mu_0\mu_2-\mu_1^2\right)\Delta_2}},$$

$$E_0(z)=0,\ E_1(z)=\frac{\sqrt{\mu_0}}{b_0},$$

$$E_2(z)=$$

$$=\frac{\mu_0\left(\mu_0\mu_2-\mu_1^2\right)z+\left(\mu_0\mu_2-\mu_1^2\right)\mu_1+\mu_0\left(\mu_1\mu_2-\mu_0\mu_3\right)}{\sqrt{\left(\mu_0\mu_2-\mu_1^2\right)\Delta_2}} \tag{17}$$

In addition:

1. The zeros of the polynomials $D_l(t)$ and $E_l(t)$, $l\in\mathbb{N}$, are all real;
2. The zeros of the polynomials $D_l(t)$ and $D_{l-1}(t)$, $l\in\mathbb{N}$, are all real and they alternate. The zeros of the polynomials $D_l(t)$ and $E_l(t)$, $l\in\mathbb{N}$, alternate;
3. The polynomials $D_l(t)$ and $E_l(t)$, $l\in\mathbb{N}$, can be expressed in terms of each other:

$$zD_l(z)=b_{l-1}D_{l-1}(z)+a_lD_l(z)+b_lD_{l+1}(z),\quad l=1,2,... \tag{18}$$

$$zE_l(z)=b_{l-1}E_{l-1}(z)+a_lE_l(z)+b_lE_{l+1}(z),\quad l=1,2,... \tag{19}$$

where

$$a_l=a_{l,l}=\int_{-\infty}^{\infty}tD_l(t)D_l(t)d\sigma(t),$$

$$b_l=a_{l,l+1}=\int_{-\infty}^{\infty}tD_l(t)D_{l+1}(t)d\sigma(t)=\frac{\sqrt{\Delta_{l-1}\Delta_{l+1}}}{\Delta_l},\quad l=1,2,...$$

4. They satisfy the Liouville-Ostrogradsky (or Schwarz-Christoffel) formula:

$$D_{l-1}(z)E_l(z)-D_l(z)E_{l-1}(z)=\frac{1}{b_{l-1}}=\frac{\Delta_{l-1}}{\sqrt{\Delta_{l-2}\Delta_l}},\quad l=2,3,... \tag{20}$$

Claim 17. *The latter relation permits to define these polynomials in the recurrent way. Indeed, since*

$$D_0(z)=\frac{1}{\sqrt{\mu_0}},\ D_1(z)=\frac{1}{\sqrt{\mu_0}}\frac{z-a_0}{b_0},$$

$$E_0(z)=0,\ E_1(z)=\frac{\sqrt{\mu_0}}{b_0},$$

we have that

$$D_2(z)=$$

$$=\frac{\left(\mu_0\mu_2-\mu_1^2\right)z^2+z\left(\mu_1\mu_2-\mu_3\mu_0\right)+\left(\mu_3\mu_1-\mu_2^2\right)}{\sqrt{\left(\mu_0\mu_2-\mu_1^2\right)\Delta_2}},$$

$$E_2(z)=$$

$$=\frac{\mu_0\left(\mu_0\mu_2-\mu_1^2\right)z+\left(\mu_0\mu_2-\mu_1^2\right)\mu_1+\mu_0\left(\mu_1\mu_2-\mu_0\mu_3\right)}{\sqrt{\left(\mu_0\mu_2-\mu_1^2\right)\Delta_2}}$$

and so on. This procedure can be easily programmed.

Claim 18. *It can be easily checked that the polynomials $D_\ell(z)$, $\ell = 0,1,2$ are all normalized to unity and mutually orthogonal.*

Claim 19. *The set of orthogonal (but not normalized) polynomials* $\{D_\ell(t)\}_{\ell=0}^{\infty}$ *can be constructed from the canonical basis of the Hilbert vector space of polynomials,*

$$\left\{1,t,t^2,...\right\},$$

but with the scalar product and the norm defined as

$$\langle f,g\rangle = \int_{-\infty}^{\infty} f(t)\overline{g(t)}d\sigma(t)\,,\ \ \|f\| = \sqrt{\langle f,f\rangle}\,,$$

by means of the standard Gram-Schmidt procedure. Then,

$$D_0(t)=1\,, D_1(t) = t-\frac{\mu_1}{\mu_0}\,,$$

$$D_2(t) = t^2 - t\frac{\mu_1\mu_2-\mu_0\mu_3}{\mu_1^2-\mu_0\mu_2}+\frac{\mu_2^2-\mu_3\mu_1}{\mu_1^2-\mu_0\mu_2}\,,$$

$$D_3(t) = t(t^2+At+B)\,,$$

$$E_0(t)=0\,, E_1(t)=\mu_0 \tag{21}$$

$$E_2(t) = \mu_0\left(t-\frac{\mu_1\mu_2-\mu_0\mu_3}{\mu_1^2-\mu_0\mu_2}\right)+\mu_1\,,$$

$$E_3(t) =$$

$$=\mu_0\left(t^2+t\left(A+\frac{\mu_1}{\mu_0}\right)+\left(\frac{\mu_2}{\mu_0}+A\frac{\mu_1}{\mu_0}+B\right)\right)$$

where

$$A =$$

$$=\frac{\mu_1\left(\mu_3^2+\mu_2\mu_4\right)-\mu_3\left(\mu_2^2+\mu_0\mu_4\right)-\mu_5\left(\mu_1^2-\mu_0\mu_2\right)}{\mu_2\left(\mu_2^2-\mu_0\mu_4\right)+\mu_3\left(\mu_0\mu_3-\mu_1\mu_2\right)+\mu_1\left(\mu_4\mu_1-\mu_2\mu_3\right)}$$

$$B =$$

$$=\frac{\mu_5\left(\mu_1\mu_2-\mu_0\mu_3\right)-\mu_3\left(\mu_1\mu_4-\mu_2\mu_3\right)-\mu_4\left(\mu_2^2-\mu_0\mu_4\right)}{\mu_2\left(\mu_2^2-\mu_0\mu_4\right)+\mu_3\left(\mu_0\mu_3-\mu_1\mu_2\right)+\mu_1\left(\mu_4\mu_1-\mu_2\mu_3\right)}$$

An important observation can be deduced from the expressions (15) and (21): both sets of orthogonal polynomials do not depend on the distribution we seek, they are determined by the moments only. In other words, these polynomials are known as soon as the moments are.

2.4 Canonical and degenerate solutions of a solvable truncated Hamburger moment problem

Claim 20. *It is clear that, at least, due to numerical and measurement problems, we never know a large number of moments. Besides, as we will see, in certain physically important problems, this number is limited by physical phenomena.*

To satisfy the moment conditions

$$\mu_m = \int_{-\infty}^{\infty} t^m d\sigma(t) = \int_{-\infty}^{\infty} t^m f(t)dt\,, \qquad m=0,1,2,...,2\nu\,, \nu = 0,1,2,...\,, \tag{22}$$

one can first consider a step-like distribution

$$d\sigma(t) = \sum_{j=0}^{2\nu} m_j\delta(t-t_j)dt \tag{23}$$

with the density which actually consists of $2\nu + 1$ point masses located at some distinct points of the real axis $\{t_j\}_{j=0}^{2\nu}$. This is the so called *canonical solution* of the problem. Then the assumption (23) can be substituted into the conditions (22) and the masses $\{m_j\}_{j=0}^{2\nu}$ can be obtained directly from the system with the determinant which is the Van der Monde determinant of an arbitrary set of distinct numbers $\{t_j\}_{j=0}^{2\nu}$:

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ t_0 & t_1 & \cdots & t_{2\nu} \\ \vdots & \vdots & \ddots & \vdots \\ t_0^{2\nu} & t_1^{2\nu} & \cdots & t_{2\nu}^{2\nu}\end{bmatrix}\begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_{2\nu}\end{bmatrix} = \begin{bmatrix}\mu_0 \\ \mu_1 \\ \vdots \\ \mu_{2\nu}\end{bmatrix} \tag{24}$$

In other words, we obtain an infinite number of canonical solutions parametrized by the latter set of points of the real axis.

Example 21. Gaussian distribution *$\exp(-t^2)$. Consider a truncated problem generated by the moments*

$$\mu_m = \int_{-\infty}^{\infty} t^m \exp\left(-t^2\right)dt\,,\ m = 0,1,2,...,2\nu\,,$$

$$\mu_0 = \sqrt{\pi}\,, \mu_1 = 0\,, \mu_2 = \frac{\sqrt{\pi}}{2}\,.$$

Then the system (24) becomes:

$$\begin{bmatrix} 1 & 1 & 1 \\ t_0 & t_1 & t_2 \\ t_0^2 & t_1^2 & t_2^2 \end{bmatrix}\begin{bmatrix} m_0 \\ m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} \sqrt{\pi} \\ 0 \\ \sqrt{\pi}/2 \end{bmatrix}$$

Its solution is just:

$$\begin{pmatrix} m_0 \\ m_1 \\ m_2 \end{pmatrix} = \frac{\sqrt{\pi}}{2}\begin{pmatrix} \dfrac{(2x_1x_2+1)}{(x_2-x_0)(x_1-x_0)} \\ \dfrac{(2x_0x_2+1)}{(x_2-x_1)(x_0-x_1)} \\ \dfrac{(2x_0x_1+1)}{(x_1-x_2)(x_0-x_2)} \end{pmatrix}.$$

Claim 22. *Nevertheless, for the moment set* $\{\mu_0, 0, \mu_2\}$*, there exists the following canonical solution of the moment problem where*

$$\int_{-\infty}^{\infty} t^m f(t)\,dt = \mu_m,\ m = 0,1,2,$$

$$f(t) = \frac{\mu_0}{2}\left[\delta(t-\xi) + \delta(t+\xi)\right],\ \xi^2 = \frac{\mu_2}{\mu_0}$$

Claim 23. *While, for the moment set* $\{\mu_0, 0, \mu_2, 0, \mu_4\}$*, there exists the following canonical solution of the moment problem*

$$\int_{-\infty}^{\infty} t^m f(t)\,dt = \mu_m,\ m = 0,1,2,3,4:,$$

$$f(t) =$$

$$= \mu_0\left\{\left(1 - \frac{\xi_1^2}{\xi_2^2}\right)\delta(t) + \frac{\xi_1^2}{2\xi_2^2}\left[\delta(t-\xi_2) + \delta(t+\xi_2)\right]\right\}$$

where

$$\xi_1^2 = \frac{\mu_2}{\mu_0},\ \xi_2^2 = \frac{\mu_4}{\mu_2}$$

This solution will be interpreted later, e.g., in Chapter 3.2 dedicated to the investigation of one-component plasmas. The positivity of the central feature intensity, $(1 - (\xi_1/\xi_2)^2)$ *follows from the Cauchy-Schwarz inequality.*

Example 24. ***Degenerate case.*** *Consider now a degenerate truncated problem generated by the moments*

$$\mu_0 = 1,\ \mu_1 = \sqrt{2},\ \mu_2 = 2 \qquad (25)$$

whose Hankel matrix

$$H_1 = \begin{bmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{bmatrix},$$

is obviously singular ($\det H_1 = 0$*). In this case the solution of the problem is unique, it can be found in the following way. Find the null-space basis of the matrix* H_1*, in our case it is a vector* $\begin{bmatrix} -\sqrt{2} \\ 1 \end{bmatrix} := \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix}$

with $\xi_1 \neq 0$*, construct the polynomial*

$$p(t) = \xi_1 t + \xi_0,$$

calculate its zeros (in our case we have only one zero $t_0 = \sqrt{2}$*), these are the locations* $\{t_i\}_{i=1}^{\nu}$ *of the masses in the degenerate solution*

$$d\sigma(t) = \sum_{i=0}^{2\nu} m_j \delta(t - t_i)\,dt$$

and determine the corresponding masses from the moment conditions (22). Particularly, for the moments (25) we have

$$d\sigma(t) = \delta\left(t - \sqrt{2}\right)dt$$

which automatically satisfies the conditions

$$\mu_0 = 1, \mu_1 = \sqrt{2}, \mu_2 = 2$$

Claim 25. *Certainly, in physical problems we are basically interested in noncanonical, continuous solutions Nevertheless, some physical interpretation* *of the canonical solutions will be discussed as well. To show how the moment method works in this case, let us consider dynamic properties of the intrinsically classical one – and two – component completely ionized hydrogen – like plasmas in thermal equilibrium.*

2.5. Non-canonical solutions of a truncated Hamburger problem. Application of the Nevanlinna formula

In physical problems we deal with further, we are interested in continuous solutions of truncated Hamburger problems generated by **positive** sets of power moments

$$\{\mu_0, \mu_1, \mu_2, ..., \mu_{2\nu-1}, \mu_{2\nu}\}, \ \nu = 0,1,2,...,$$

basically, with $\nu = 2$ and with the so called immaterial elements $\mu_{2\nu+1}$ and $\mu_{2\nu+2}$. Let us see how the Nevanlinna formula in this case provides a continuous, non-canonical, solution of the problem: construct the p.d.f. $f(t)$ such that

$$\mu_l = \int_{-\infty}^{\infty} t^l f(t)dt, \ l = 0,1,2,...,2\nu, \quad \nu = 0,1,2,..., \tag{26}$$

The Nevanlinna formula in this case takes the following form:

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{f(t)}{t-z}dt = -\frac{E_{\nu+1}(z) + R_\nu(z)E_\nu(z)}{D_{\nu+1}(z) + R_\nu(z)D_\nu(z)}, \tag{27}$$

Claim 26. *Observe that the Nevanlinna parameter function $Q_\nu(z) \in \mathfrak{R}_0$ effectively depends on the number of moments involved. Nevertheless, the asymptotic expansion of the Cauchy transform of the density in question will satisfy the moment conditions (26) independently of our choice of this parameter function.*

Proof. Indeed, along any ray within the upper half-plane *Imz > 0,*

$$\begin{aligned} &\varphi(z \to \infty) = \\ &= -\frac{1}{z}\int_{-\infty}^{\infty} \frac{f(x)}{1-\dfrac{x}{z}}dx \underset{z\to\infty}{\simeq} - \\ &-\frac{1}{z}\int_{-\infty}^{\infty} f(x)\left(\sum_{l=0}^{2\nu}\left(\frac{x}{z}\right)^l + O\left(\frac{1}{z}\right)^{2\nu+1}\right)dx = \\ &= -\sum_{l=0}^{2\nu}\frac{1}{z^{l+1}}\int_{-\infty}^{\infty} x^l f(x)dx + O\left(\frac{1}{z}\right)^{2\nu+2} = \\ &= -\sum_{l=0}^{2\nu}\frac{\mu_l}{z^{l+1}} + O\left(\frac{1}{z}\right)^{2\nu+2} \end{aligned} \tag{28}$$

In other words, the contribution related to the Nevanlinna parameter function $Q_\nu(z)$, due to the additional property (4), will appear in the asymptotic expansion (28) only in the correction of excessive order $2\nu + 2$. Now, by definition, on the real axis *Imz = 0,*

$$\begin{aligned} \varphi(t) &= \mathrm{Im}\left(\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\frac{f(s)ds}{s-t-i\eta}\right) = \\ &= \mathrm{Im}\left(P.V.\int_{-\infty}^{\infty}\frac{f(s)ds}{s-t} + \pi i f(t)\right) = \ , \\ &= \pi f(t) = -\mathrm{Im}\frac{E_{\nu+1}(t) + R_\nu(t)E_\nu(t)}{D_{\nu+1}(t) + R_\nu(t)D_\nu(t)} \end{aligned}$$

P.V standing for the principal value of the integral. Let

$$R(t) = \mathrm{Re}\,R(t) + i\,\mathrm{Im}\,R(t),$$
$$\overline{R(t)} = \mathrm{Re}\,R(t) - i\,\mathrm{Im}\,R(t)$$

and observe that, also by definitions (15) and (16), we have:

$$D_{\nu+1}(t) = \frac{1}{\sqrt{\Delta_{\nu+1}\Delta_\nu}} \det \begin{bmatrix} \mu_0 & \cdots & \mu_{\nu-1} & \mu_\nu & 1 \\ \mu_1 & \cdots & \mu_\nu & \mu_{\nu+1} & t \\ \vdots & \cdots & \vdots & \vdots & \vdots \\ \mu_{\nu-1} & \cdots & \mu_{2\nu-1} & \mu_{2\nu} & t^\nu \\ \mu_\nu & \cdots & \mu_{2\nu} & \mu_{2\nu+1} & t^{\nu+1} \end{bmatrix}$$

so that the algebraic minor, (subdeterminant) of the $D_{\nu+1}(t)$ polynomial leading term is just the Hankel determinant

$$\Delta_\nu = \det \begin{bmatrix} \mu_0 & \cdots & \mu_{\nu-1} & \mu_\nu \\ \mu_1 & \cdots & \mu_\nu & \mu_{\nu+1} \\ \vdots & \vdots & \vdots & \vdots \\ \mu_{\nu-1} & \cdots & \mu_{2\nu-1} & \mu_{2\nu} \end{bmatrix}, \quad (29)$$

Hence,

$$P_{\nu+1}(t) = \sqrt{\frac{\Delta_\nu}{\Delta_{\nu+1}}} P_{\nu+1}(t),$$
$$P_\nu(t) = \sqrt{\frac{\Delta_{\nu-1}}{\Delta_\nu}} P_\nu(t) \quad (30)$$

where $\{P_l(t)\}_{l=0}^{\nu+1}$ are orthogonal monic polynomials with respect to the measure density $f(t)$, see the Claim 19. Thus 1, due to the Liouville-Ostrogradsky equality (20), the "problem" is that the determinant $\Delta_{\nu+1}$ (see (29)) contains the "immaterial" moments $\mu_{2\nu+1}$ and $\mu_{2\nu+2}$, which we do not know. They might even diverge! This spurious contradiction is immediately resolved by taking into account the normalization of the orthonormalized polynomials $\{P_l(t)\}_{l=0}^{\nu+1}$: use instead the monic polynomials $\{P_l(t)\}_{l=0}^{2\nu}$:

$$f(t) = \frac{\Delta_\nu}{\pi\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}} \frac{\operatorname{Im} R_\nu(t)}{\left|P_{\nu+1}(t) + R_\nu(t)P_\nu(t)\right|^2} =$$
$$= \frac{\Delta_\nu}{\pi\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}} \frac{\operatorname{Im} R_\nu(t)}{\left|\sqrt{\frac{\Delta_\nu}{\Delta_{\nu+1}}} P_{\nu+1}(t) + R_\nu(t)\sqrt{\frac{\Delta_{\nu-1}}{\Delta_\nu}} P_\nu(t)\right|^2} = \quad (31)$$
$$= \frac{\Delta_\nu}{\pi\Delta_{\nu-1}} \frac{\operatorname{Im} Q_\nu(t)}{\left|P_{\nu+1}(t) + Q_\nu(t)P_\nu(t)\right|^2} > 0$$

where

$$Q_\nu(t) = R_\nu(t)\frac{\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}}{\Delta_\nu}$$

Notice that due to the positivity of the moment sequence (26), the Hankel determinants $\Delta_{\nu-1}$ and Δ_ν are all strictly positive.

Thus, the immaterial members of the moment sequence are eliminated due to the renormalization procedure. What matters for the physical applications is that the poles of the reconstructed density $f(z)$, $Imz < 0$ are the roots of the "polynomial" equation

$$P_{\nu+1}(z) + Q_\nu(z)P_\nu(z) = 0 \quad (32)$$

which "starts" from $z^{\nu+1}$, i.e., if, in accordance with the $\Re_0$-version of the Riesz-Herglotz formula (5), we approximate the Nevanlinna parameter function (NPF) $q_\nu(z)$ by its static value:

$$Q_\nu(z) = Q_\nu(z=0) = ih \quad (33)$$

equation (32) acquires the form of the genuine polynomial equation of the order $\nu+1$, which can be easily solved at least numerically. Nevertheless, our aim here is to study the possibilities of employment of frequency-dependent NPFs.

3 Solution of physical problems by the method of moments.

Here we will study the dynamic properties of dense one – and two-component plasmas in the context of the truncated Hamburger problem. We

[1] Remember that for any $z \in C$, *$Imz=(z-z^*)/2i$, where z^* is the complex conjugate of z.*

start with the calculation of power moments on the basis of the Kramers-Kronig relations and the Kubo linear theory.

3.1 The moments.

The physical characteristics of the system interfere, within the method of moments, basically through the sum rules. If we presume the existence of the Coulomb or Coulomb-like system inverse (longitudinal) dielectric function, $\varepsilon^{-1}(k,\omega)$ (IDF), the sum rules are effectively the power frequency moments of the (positive) even loss function $L(k,\omega) = -\mathrm{Im}\,\varepsilon^{-1}(k,\omega)/\omega$:

$$C_\nu(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^\nu L(k,\omega)d\omega, \quad \nu = 0,2,4. \tag{34}$$

Notice that the odd order moments vanish due to the symmetry of the loss function. Let us also introduce the characteristic frequencies

$$\omega_1^2(k) = \frac{C_2(k)}{C_0(k)}, \quad \omega_2^2(k) = \frac{C_4(k)}{C_2(k)} \tag{35}$$

In a classical plasma, due to the fluctuation-dissipation theorem (FDT), the dynamic structure factor (charge density-charge density)

$$S(q,\omega) = \frac{q^2 n_e}{3\pi\Gamma} B(\beta\hbar\omega) L(q,\omega), \tag{36}$$

where

$$B(w) = w(1-\exp(-w))^{-1} \underset{w\to 0}{\cong} 1 \tag{37}$$

is the Bose factor. Both dynamic functions, $L(q,\omega)$ and $S(q,\omega)$, behave at low frequencies and/or in classical systems in a similar way. Hence, the moments $\{C_0(q), 0, C_2, 0, C_4(q)\}$ are effectively proportional to the moments of the dynamic structure factor (DSF).

Since the IDF is a genuine response function [27] and thus satisfies, by virtue of the causality principle, the Kramers-Kronig relations,

$$\varepsilon^{-1}(k,z) = 1 + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\,\varepsilon^{-1}(k,\omega)}{\omega - z} d\omega, \quad \mathrm{Im}\, z > 0, \tag{38}$$

and since the imaginary part $\mathrm{Im}\epsilon^{-1}(q,\omega)$ is an odd function of frequency and thus vanishes at $\omega = 0$, we can write:

$$\varepsilon^{-1}(k,0) = 1 + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\,\varepsilon^{-1}(k,\omega)}{\omega} d\omega = 1 - C_0(q) \tag{39}$$

We conclude that

$$C_0(k) = 1 - \varepsilon^{-1}(k,0)$$

The above relations permit to study the asymptotic expansion of the IDF along any ray in the upper half-plane:

$$\varepsilon^{-1}(q,z) - \varepsilon^{-1}(q,0) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{L(q,\omega)d\omega}{1-\frac{\omega}{z}} \underset{z\to\infty}{\cong}$$
$$\underset{z\to\infty}{\cong} \frac{1}{\pi}\int_{-\infty}^{\infty}\left(1 + \frac{\omega}{z} + \left(\frac{\omega}{z}\right)^2 + \left(\frac{\omega}{z}\right)^3 + \left(\frac{\omega}{z}\right)^4 + \dots\right) L(q,\omega)d\omega = \tag{40}$$
$$= C_0(q) + \frac{C_2}{z^2} + \frac{C_4(q)}{z^4} + \dots$$

Thus,

$$\varepsilon^{-1}(q, z\to\infty) \cong 1.$$

Similarly, for the dielectric function itself, inverting the last formula,

$$\varepsilon^{-1}(q,z) \underset{z\to\infty}{\cong} 1 - \frac{\omega_p^2}{z^2} - \frac{\omega_p^2\left(\omega_2^2(q) - \omega_p^2\right)}{z^4} + \dots \tag{41}$$

It stems directly from the *f*-sum rule [27] that even if the interparticle interaction might be different from the bare Coulomb one and is described by an effective potential [15],

$$C_2 = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^2 L(k,\omega)d\omega \equiv \omega_p^2 \qquad (42)$$

where ω_p is the system plasma frequency.

It has been established [28,29] and further, within the Kubo linear-reaction theory and using the second-quantization technique [14], generalized for a multicomponent Coulomb system with the pairwise interaction energy Fourier transform,

$$W_{ab}(q) = \frac{4\pi e^2 a}{q^2}\zeta_{ab}(q), \qquad (43)$$
$$\zeta_{ab}(q) = \zeta_{ba}(q), \;\; a,b = e, i_1, i_2, ...,$$

that the fourth moment and, hence, the second characteristic frequency contains four contributions:

$$\omega_2^2(q) = \qquad (44)$$
$$= \omega_p^2\left[\zeta_{ee}(q) + K(q) + U(q) + H\right],$$

The kinetic contribution

$$K(q) = \frac{q^2}{\Gamma}\frac{F_{3/2}(\eta)}{D^{3/2}} + \frac{q^4}{12 r_s} \qquad (45)$$

and the coupling contributions are:

$$U(q) =$$
$$= \frac{1}{12\pi}\int_0^{\infty} p^2 (S_{ee}(p)-1)\left(Z_{ee}(p,q) - \frac{8\zeta_{ee}(p)}{3}\right)dp,$$
$$H = \frac{2\sqrt{Z}}{9\pi}\int_0^{\infty} p^2 S_{ei}(p)\zeta_{ei}(p)dp, \qquad (46)$$
$$Z_{ee}(p,q) = \int_{|p-q|}^{p+q} \zeta_{ee}(s)\left(p^2 - q^2 - s^2\right)^2 \frac{ds}{pq^3 s}$$

Here,

$$F_\mu(\eta) = \int_0^{\infty} \frac{t^\mu}{\exp(t-\eta)+1}dt$$

is the order-μ Fermi integral, and η is the dimensionless chemical potential of the electronic subsystem, which should be determined by the normalization condition

$$F_{1/2}(\eta) = \frac{2}{3}D^{3/2}.$$

Notice that the e–i contribution is q-independent. Terms of the order of the ratio m/M were neglected to obtain these simple expressions. To reiterate that we are able to evaluate the moments independently with a precision determined by the numerical scheme employed to compute the partial static structure factors, see the paper [17] for details. Notice also that in the hydrodynamic limiting case

$$\omega_2^2(q \to 0) \cong \omega_p^2\left(1 + H\right) \qquad (47)$$

while at short distances we recover the single-particle behavior:

$$\omega_2^2(q \to \infty) \cong \frac{\omega_p^2 q^4}{12 r_s} \qquad (48)$$

It is obvious that in one-component plasmas, classical or not, the electron-ion contribution $H = 0$. In the same way, higher order moments can be calculated, e.g. in model Coulomb systems with the effective potential (43) different from the bare Coulomb one. But in purely Coulomb systems containing species of different masses, the sixth and higher-order moments diverge [30]. This takes place because the corresponding explicit expressions contain uncompensated contributions like

$$\sum_q \left\langle n_{\mathrm{q}}^a n_{-\mathrm{q}}^a \right\rangle = \infty$$

The divergence of higher-order moments $C_{2l}(k)$ with $l > 2$ is directly related to the slow decay of the loss function as $|\omega| \to \infty$. If we presume that for

$$L(k, |\omega| \to \infty) \cong A(k)/|\omega|^\gamma$$

then, due to the divergence of the sixth moment and the convergence of the fourth one (44), we conclude that $5 < \gamma \le 7$.

In a completely ionized plasma for $\omega >>(\beta\hbar)^{-1}$ the microscopic acts of the electromagnetic field energy absorption become the processes inverse with respect to the bremsstrahlung during pair collisions of charged particles. As it was shown by L. Ginzburg ([31]) this circumstance permits to use the detailed equilibrium principle to express the imaginary part of the longitudinal dielectric function, $\mathrm{Im}\epsilon(k,\omega)$, of a completely ionized plasma, which is directly related to the plasma external dynamic conductivity $\sigma^{ext}(k,\omega)$ real part, in terms of the bremsstrahlung cross-section. A calculation similar to that of Ginzburg, but using the well-known expression for the bremsstrahlung differential cross-section for high values of energy transfer and $\omega \gg (\beta\hbar)^{-1}$ [32], lead to the following asymptotic form of $Im\epsilon(k,\omega)$ in a completely ionized (for simplicity, hydrogen-like) plasma [30]:

$$\begin{aligned}&\mathrm{Im}\,\varepsilon\left(k,\omega>>\left(\beta\hbar\right)^{-1}\right)\cong\\&\cong\frac{4\pi A_0}{\omega^{9/2}}\left(1-\frac{\omega_T}{\omega}+...\right)\end{aligned},\tag{49}$$

where

$$A_0=\frac{2^{5/2}\pi}{3}n_en_i\frac{Z^2e^6}{\left(\hbar m\right)^{3/2}},\quad \omega_T=\frac{3}{4\beta\hbar},$$

$n_i = Zn_e$. The main term of (49) was obtained by Perel' and Eliashberg [33]. One of our aims is to specify (49) taking into account the sum rules (34). Notice that even the main term of the plasma dielectric function asymptotic behavior (49) is still discussed in literature, producing sometimes even contradictory results [34].

3.2 Classical one-component plasmas.

The classical one-component plasma (OCP) might be considered a test-tube for the modelling of strongly interacting Coulomb systems [35], see also [36] and [37] for more recent reviews. OCP is often employed as a simplified version of real physical systems ranging from electrolytes and charged-stabilized colloids [38], laser-cooled ions in cryogenic traps [39] to dense astrophysical matter in white dwarfs and neutron stars [40]. Another modern and highly interesting pattern of the OCP is dusty plasmas with the pure Coulomb interparticle interaction potential substituted by the Yukawa effective potential [41].

The classical OCP is defined as a system of charged particles (ions) immersed in a uniform background of opposite charge. It is characterized by a unique dimensionless coupling parameter $\Gamma = \beta(Ze)^2/a$. Here, like before, β^{-1} stands for the temperature in energy units, Ze designates the ion charge, and $a = (3/4\pi n)^{1/3}$ is the Wigner-Seitz radius, n being the number density of charged particles. For $\Gamma > 1$ the interaction effects determine the physical properties of the OCP.

We successfully applied the method of moments complemented by some physical considerations in [17]. Precisely, the five-moment approximation $\{C_0(q), 0, C_2, 0, C_4(q)\}$ was applied to reconstruct the dynamic structure factor (36) and to study the properties of the collective modes in Coulomb and Yukawa model systems characterized by the diagonal form-factors in (43) equal to, respectively, $\zeta_C = 1$ and $\zeta_Y = q^2/(q^2+\kappa^2)$, where κ is the screening parameter of the Yukawa potential $(Z^2e^2/r)\exp(-\kappa r/a)$. With the simplification (33) and the symmetry of the loss function taken into account, the expression for the DSF can be written as

$$\begin{aligned}&\frac{\pi S(q,\omega)}{nS(q)}=\\&=\frac{\omega_1^2(\omega_2^2-\omega_1^2)h}{\omega^2(\omega^2-\omega_2^2)^2+h^2(\omega^2-\omega_1^2)^2}\end{aligned},\tag{50}$$

Since the loss function, and in a classical system, the DSF are even function of frequency, the r.h.s. of the previous expression depends only on the frequency squared. It implies that the first derivative of the DSF at $\omega^2 = 0$ vanishes only if

$$h=h_0(q)=\frac{\omega_2^2(q)}{\omega_1(q)\sqrt{2}}a\,,\tag{51}$$

The presence of an extremum of the loss function and, in classical systems, of the DSF at $\omega = 0$ follows from the canonical solution (23) with the point masses located at the points $\omega = 0$, $\omega = \omega_1$, and $\omega = \omega_2$ [42]:

$$\begin{aligned}&\frac{S_{\mathrm{can}}(q,\omega)}{nS(q)}=\left[1-\frac{\omega_1^2(q)}{\omega_2^2(q)}\right]\delta(\omega)+\\&+\frac{\omega_1^2(q)}{\omega_2^2(q)}\delta\left(\omega^2-\omega_2^2(q)\right)\end{aligned},$$

The validity of this result was confirmed numerically in [10] and also in [17] by comparison with numerical data on the dynamic characteristics of OCP's. It implies that, at least in classical OCPs, we can calculate the DSF and the collective mode characteristics entirely in terms of the static structure factor (SSF), $S(q)$, it makes it self-consistent. Indeed, due to the classical version of the FDT,

$$\frac{\omega_1^2(q)}{\omega_p^2} = \frac{q^2\omega_p^2}{3\Gamma S(q)}, \tag{52}$$

and the coupling-related

$$\frac{\omega_2^2(q)}{\omega_p^2} = \zeta(q) + \frac{q^2}{\Gamma} + \frac{1}{12\pi}\int_0^\infty p^2(S(p)-1)\Psi(p)dp, \tag{53}$$

where

$$\Psi(p) = \left(\int_{|p-q|}^{p+q} \frac{\zeta(s)\left(p^2-q^2-s^2\right)^2 ds}{pq^3 s} - \frac{8\zeta(p)}{3}\right),$$

is also determined by the SSF and the one-species form-factor, since in OCPS's H = 0. Numerical results obtained on the basis of the relations (50, 51, 52, 53) are presented in the following figures. The displayed quantitative agreement with the numerical simulation data the viability and robustness of the self-consistent moment approach.

3.2.1. The OCP numerical data.

As an example, I reproduce here our results published last year in [17]. To stress that here we employ no adjustment parameters whatsoever.

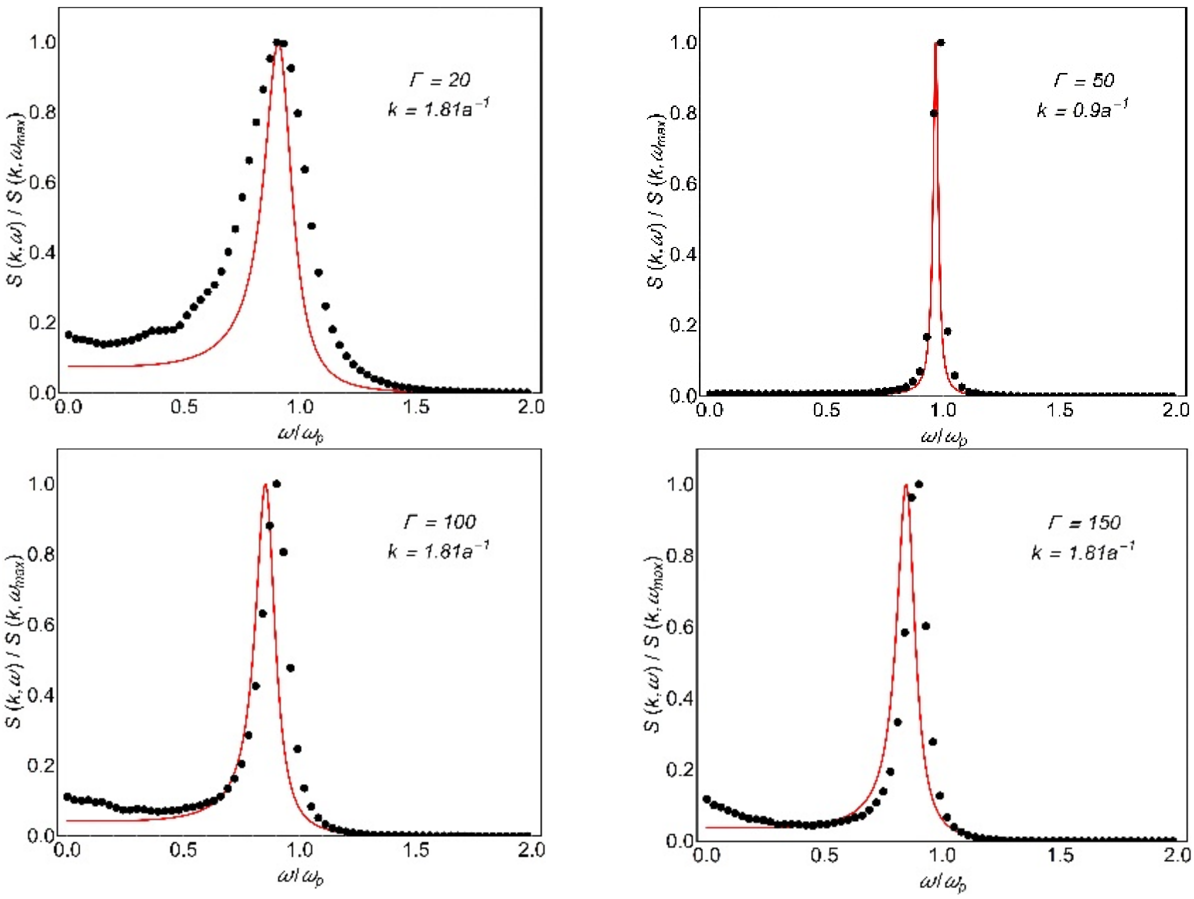

Figure 1 – Dynamic structure factor normalized to the shifted maxima values in strongly coupled COCPs, compared to the MD results [17], at various values of Γ and k

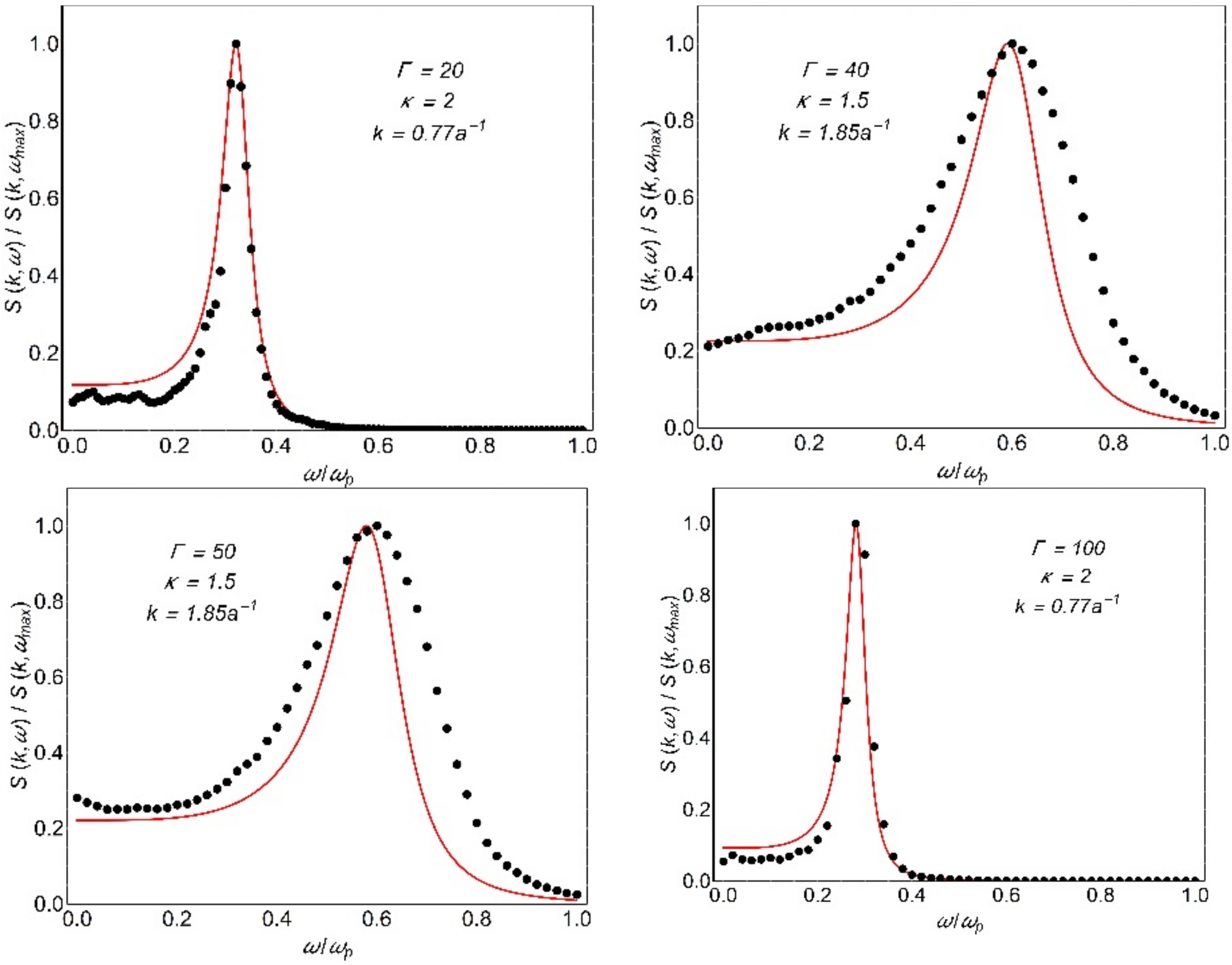

Figure 2 – As in Figure 1 but in strongly coupled YOCPs, compared to the MD results [17]

4 The search for the Nevanlinna parameter function

As we have seen in the previous Section, the self-consistent moment approach is quantitatively suitable for the description of dynamic properties of classical OCPs. It is shown in [43] how the method can be successfully extended to the partially or completely degenerate electron gases. Nevertheless, the simplification (33) effectively limits the applicability of the method in the low-coupling regime where the Landau collisionless damping is usually described within the RPA. In other words, we wish to choose a model expression for the NPF capable of incorporating the low-Γ RPA-like behavior into the moment scheme.

Here, we consider three different model expressions for the dynamic renormalized NPF $Q_2(\omega;q)$ both for classical and partially degenerate systems. Notice that in the physical context the variable t becomes frequency ω and we must take into account the spatial dispersion of the dynamic characteristics by introducing the (dimensionless) wavenumber variable q.

We start observing that the loss function effectively depends only on dimensionless variables

$$x = \frac{\omega^2}{\omega_p^2}, \quad x_j = \frac{\omega_j^2}{\omega_p^2}, \quad j = 1,2. \tag{54}$$

This implies that the dimensionless NPF can be written as

$$\frac{Q_2(\omega;q)}{\omega_p} = \sqrt{\frac{x}{x_0}} X\left(\frac{x}{x_0}\right) + iY\left(\frac{x}{x_0}\right), \tag{55}$$

where x_0 is the characteristic value of the new variable equal to $k^2v_{th}^2 = 2q^2/3\Gamma$ or $k^2v_F^2 = q^2v_F^2/a^2$, respectively, in the classical and quantum-mechanical cases, v_{th} and v_F being, certainly, the thermal and Fermi velocities. Indeed, then the frequency-dependent part of the r.h.s. of (31) can be written as a function of $y = x/x_0$ and from the condition of the loss function extremum at the point $y = 0$ we obtain:

$$h = \frac{x_2}{\sqrt{x_1}} \frac{1}{\sqrt{W_1(2W_1 - W_2x_1)} - W_0\sqrt{x_1}} , \qquad (56)$$

Where we have introduced the following values of the functions X, Y and of the derivative Y' at $y = 0$:

$$X_0 = hW_0,\ Y_0 = hW_1,\ Y_0^{'} = hW_2 .$$

Observe that if $Y_0 = h$; and $X_0 = Y_0' = 0$ so that $W_1 = 1$, $W_0 = 0$, $W_2 = 0$, we return to the "static" approximation,

$$h = \frac{x_2}{\sqrt{2x_1}} = h_0 .$$

4.1. Classical Coulomb OCPs.

Presume first that the NPF is the plasma dispersion function [44], i.e., put

$$\frac{Q_2(\omega;q)}{\omega_p} = \\ = \sqrt{\frac{x}{x_0}} X\left(\frac{x}{x_0}\right) + iY\left(\frac{x}{x_0}\right) = , \qquad (57a) \\ = \frac{h}{\sqrt{\pi}} Z\left(\frac{\omega + i0^+}{q\sqrt{2/(3\Gamma)}}\right)$$

where

$$Z(\zeta = \xi + i0^+) = \mathrm{i}\sqrt{\pi}\exp(-\xi^2) - 2F(\xi),$$
$$\xi = \frac{\omega}{q\sqrt{2/(3\Gamma)}} = \sqrt{\frac{x}{x_0}} \in \mathbb{R}$$

with

$$F\left(\frac{x}{x_0}\right) = \sqrt{\frac{x}{x_0}} \exp\left(-\frac{x}{x_0}\right) \int_0^1 \exp\left(\frac{xs^2}{x_0}\right) ds \qquad (58)$$

being the Dawson integral

$$Z(\xi + i0^+) = i\sqrt{\pi}\exp(-\xi^2) - 2F(\xi) . \qquad (59)$$

A simple variable substitution leads to the alternative representation of (58),

$$X(x) = -\frac{2h}{\sqrt{\pi}} \exp\left(-\frac{x}{x_0}\right) \int_0^1 \exp\left(\frac{xs^2}{x_0}\right) ds ,$$
$$Y(x) = h\exp\left(-\frac{x}{x_0}\right)$$

so that

$$X_0 = -\frac{2h}{\sqrt{\pi}},\ Y_0 = h,\ Y_0^{'} = -\frac{h}{x_0}$$

or

$$W_0 = -\frac{2}{\sqrt{\pi}}, W_1 = 1, W_2 = -\frac{1}{x_0}$$

Then, it stems from (56) that in this case

$$h_{RPA} = \frac{x_2\sqrt{x_0}}{\sqrt{x_1}} \frac{\pi\sqrt{x_1 + 2x_0} - 2\sqrt{\pi x_1 x_0}}{2\pi x_0 + \pi x_1 - 4x_0x_1}$$

Alternatively, we might introduce an adjustable parameter and redefine:

$$\frac{Q_2(\omega;q)}{\omega_p} = \sqrt{\frac{x}{x_0}} X\left(\frac{x}{x_0}\right) + iY\left(\frac{x}{x_0}\right) = \qquad (57b) \\ = \frac{ih}{\alpha + \frac{i(\alpha-1)}{\sqrt{\pi}} Z\left(\frac{\omega + i0^+}{q\sqrt{2/(3\Gamma)}}\right)} ,$$

Somewhat more cumbersome but straightforward calculations lead in this case to

$$h_{inv} =$$

$$= \frac{x_2}{\sqrt{x_1}} \frac{\sqrt{\pi x_0}}{\sqrt{2\pi x_0 - (1-\alpha)(\pi + 4(1-\alpha))x_1} - 2(1-\alpha)\sqrt{x_0 x_1}}$$

which tends to h_0 when $\alpha \to 1$. Notice that the parameter α, generally speaking, can be fixed by the Shannon-entropy maximization procedure [14].

4.2. Partly degenerate Coulomb OCPs.

There is a number of quantum-mechanical generalizations of the plasma dispersion function, see [45]. Consider, following D.B. Melrose and A. Mushtaq [46], the following generalization of (57a) (a misprint in the original paper is corrected)

$$Z(\zeta;\eta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{t \ln\left(\frac{t-\zeta}{t+\zeta}\right)}{\exp\left(t^2\right) + \exp\left(\eta\right)} dt = \tag{60}$$

$$= \frac{2}{\sqrt{\pi}} \int_{-\infty}^\infty \frac{t \ln\left(t-\zeta\right)}{\exp\left(t^2\right) + \exp\left(\eta\right)} dt = \tag{61}$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^\infty \frac{\ln\left(1+\exp(\eta - t^2)\right)}{\exp\left(\eta\right)} \frac{dt}{t-\zeta}$$

where $\xi = (\omega + i0^+)/(qv_{\text{eff}}/a)$ with, perhaps, $v_{\text{eff}} = v_F$. As usually, η is the dimensionless chemical potential. This function satisfies the following classical limiting property:

$$Z(\zeta;\eta \to -\infty) \cong Z(\zeta) \ ,$$

By definition, with x defined as in (54),

$$\operatorname{Im} Z(x;\eta) = \sqrt{\pi} \frac{\ln\left(1+\exp\left(\eta - \frac{x}{x_0}\right)\right)}{\exp(\eta)} \underset{\eta\to-\infty}{\cong} \tag{62}$$

$$\underset{\eta\to-\infty}{\cong} \sqrt{\pi} \exp\left(-\frac{x}{x_0}\right)$$

and

$$\operatorname{Re} Z(x;\eta) = \frac{2}{\sqrt{\pi}} P.V. \int_0^\infty \frac{t \ln\left|\frac{t-\sqrt{x/x_0}}{t+\sqrt{x/x_0}}\right|}{\exp\left(t^2\right) + \exp\left(\eta\right)} dt$$

Observing that

$$\frac{t \ln\left|\frac{t-\sqrt{x/x_0}}{t+\sqrt{x/x_0}}\right|}{\exp\left(t^2\right) + \exp\left(\eta\right)} = -\frac{2}{e^\eta + e^{t^2}} \sqrt{x/x_0} + O\left(x^{3/2}\right)$$

one obtains that

$$\frac{\operatorname{Re} Z(x;\eta)}{\sqrt{\pi}} = \frac{2}{\pi} P.V. \int_0^\infty \frac{t \ln\left|\frac{t-\sqrt{x/x_0}}{t+\sqrt{x/x_0}}\right|}{\exp\left(t^2\right) + \exp\left(\eta\right)} dt \underset{x\downarrow 0}{\cong}$$

$$\underset{x\downarrow 0}{\cong} \sqrt{x/x_0}\,\Xi(x)$$

and that

$$\Xi(0) = \Xi_0 = -\frac{4}{\pi} \int_0^\infty \frac{dt}{\exp\left(t^2\right) + \exp\left(\eta\right)} =$$

$$= -\frac{2e^{-\eta}}{\pi} \int_0^\infty \frac{s^{-1/2} ds}{\exp\left(s-\eta\right) + 1} = -\frac{2e^{-\eta}}{\pi} F_{-1/2}(\eta).$$

Now, from (62),

$$\Upsilon_0 = \frac{\operatorname{Im} Z(0;\eta)}{\sqrt{\pi}} = \frac{\ln\left(1+\exp\left(\eta\right)\right)}{\exp(\eta)},$$

$$\Upsilon_0^{'} = -\frac{1}{x_0(e^\eta + 1)} \ .$$

So, if one introduces the low-frequency NPF for partially degenerate plasmas as

$$\frac{Q_2(\omega;q)}{\omega_p} = h_{qm} \left(\sqrt{\frac{x}{x_0}}\Xi(x) + i\Upsilon(x)\right), \tag{63}$$

then,

$$w_0 = \Xi_0 = -\frac{2e^{-\eta}}{\pi}\int_0^{\infty}\frac{s^{-1/2}ds}{\exp(s-\eta)+1},$$

$$w_1 = \Upsilon_0 = \frac{\ln(1+\exp(\eta))}{\exp(\eta)},$$

$$w_2 = \Upsilon_0' = -\frac{1}{x_0(e^{\eta}+1)},$$

$$h_{qm} = \frac{x_2}{\sqrt{x_1}}\frac{1}{\sqrt{w_1(2w_1 - w_2 x_1)} - w_0\sqrt{x_1}}.$$

In other words, this new NPF equals

$$\frac{Q_2(\omega;q)}{\omega_p} = \frac{h_{qm}}{\sqrt{\pi}}\left(\operatorname{Re} Z(x;\eta) + i \operatorname{Im} Z(x;\eta)\right), \quad (64)$$

where the function $Z(x;\eta)$ is determined in (60) and (61). The formula for the DSF function is, as before,

$$\frac{\pi S(q,\omega)}{nS(q)} = B(\beta\hbar\omega)\frac{\omega_1^2(\omega_2^2-\omega_1^2)\operatorname{Im} Q_2(t)}{\left|D_3(t)+Q_2(t)D_2(t)\right|}, \quad (65)$$

The numerical data with respect to the above frequency-dependent NPFs is presented in the next Sect. The completely degenerate case is to be considered elsewhere.

4.3. Numerical data on the dynamic NPFs
4.3.1. Classical plasmas.

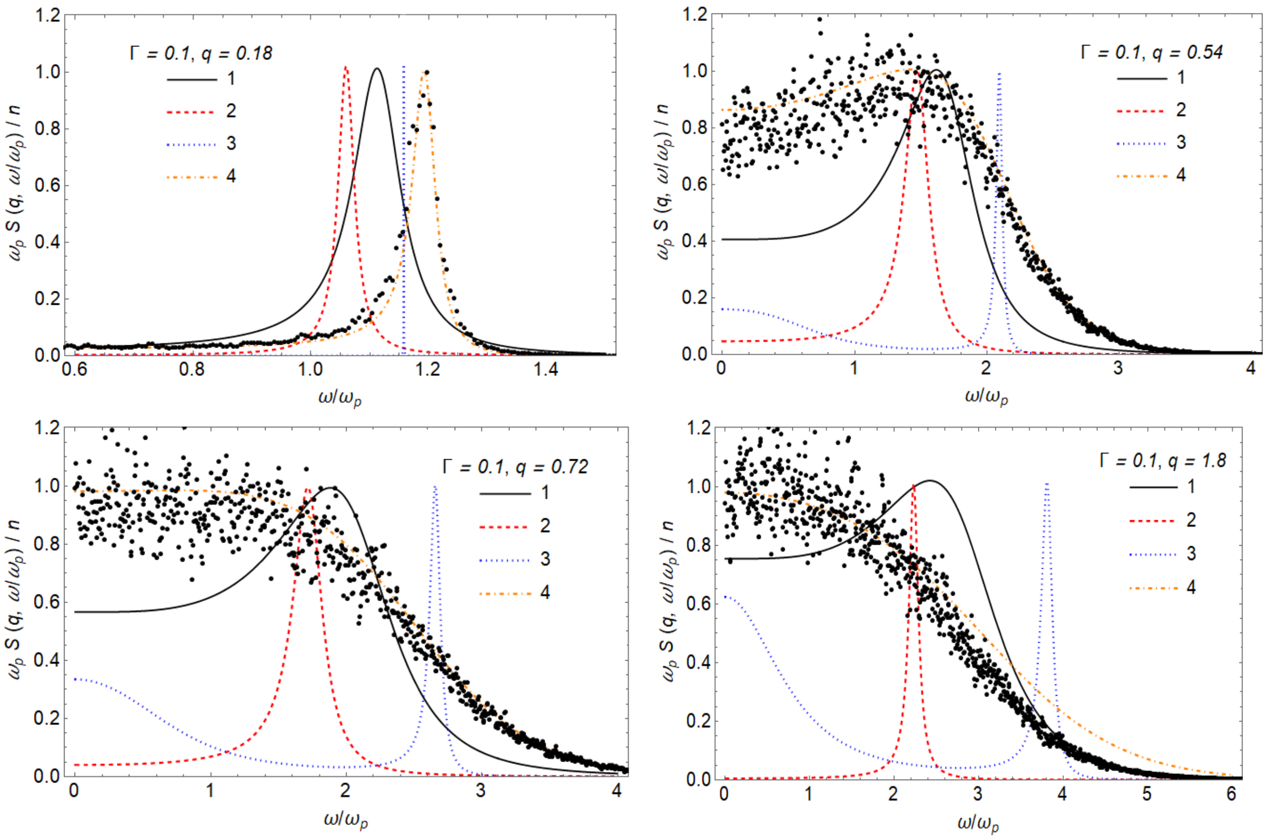

Figure 3 – Dynamic structure factor fot the COCP presenting the method of moments (MM) data vs. the MD data (dots). 1 – MM with $\frac{Q(q)}{\omega_p} = ih_0$, 2 – MM with $\frac{Q(q)}{\omega_p}$ from (57b), with $\alpha = 0.5$, 3 – MM with $\frac{Q(q)}{\omega_p}$ from (57a), 4 – RPA theory

4.3.2. Partly degenerate plasmas.

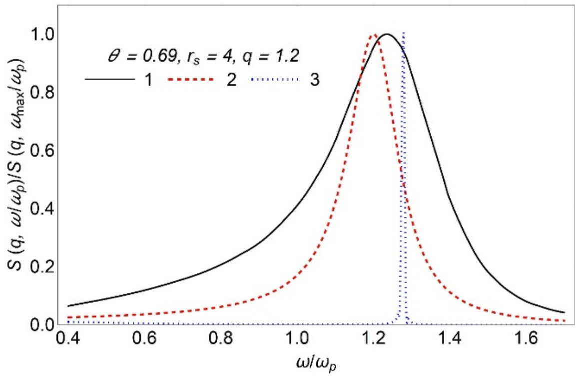

Figure 4 – Dynamic structure factor for partly degenerate OCPs (electron gas), MM data vs. data of [47].

1 – [47], 2 – MM with $\frac{Q(q)}{\omega_p} = ih_0$, 3 – MM with $\frac{Q_2(\omega;q)}{\omega_p}$ from (64)

5 Conclusions

A thorough review of the self-consistent method of moments is presented. Ways are discussed of qualitative improvement of the method consisting in the employment of different dynamic models of the Nevanlinna parameter function (NPF) analogous to the dynamic local-field correction function [12]. The latter is used to extend the realm of applicability of the random-phase approximation (RPA). Though the self-consistent method of moments with a static NPF (56) has proven to work very well in warm dense matter, our preliminary results demonstrate that the suggested model NPFs provide a satisfactory agreement with the simulation data in low-density Coulomb plasmas. Further steps along this path are planned to be taken, especially in the case of partly and completely degenerate systems. Finally, we stress that no adjustment parameters are used in our calculations.

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