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INVESTIGATION OF DYNAMIC PROPERTIES OF NON-IDEAL ONE COMPONENT PLASMAS BY THE METHOD OF MOMENTS

PhD Thesis

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CERTIFICA que la presente memoria **Investigation of dynamic properties of non-ideal one-component plasmas by the method of moments** ha sido realizada bajo mi co-dirección en el Departamento de Matemática Aplicada de la Universidad Politécnica de Valencia, por ABDIADIL ASKARULY y constituye su tesis para optar al grado de Doctor en Ciencias Matemáticas.

Y para que así conste, en cumplimiento con la legislación vigente, presentamos ante el Departamento de Matemática Aplicada de la Universidad Politécnica de Valencia, la referida Tesis Doctoral, firmando el presente certificado.

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INVESTIGATION OF DYNAMIC PROPERTIES OF NON-IDEAL ONE COMPONENT PLASMAS BY THE METHOD OF MOMENTS

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This thesis is dedicated to the memory of my sister, Aliya Kortykbayeva Askarkizi, who always supported me and was proud of me.

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CONTENTS

INTRODUCTION

General characteristics of the work

Dynamic characteristics of strongly coupled one-component plasmas are studied within the moment approach with local constraints by an algorithm similar to that of Schur. Some simulations of two-component plasmas are analyzed using sum rules and other exact relations.

Main part

It became clear by the end of the last millennium that due to the scientific and, especially, technological progress there has appeared a strong necessity in increasing production of electrical power. On the other hand the natural deposits of oil, gas and coal currently used in power plants will be rapidly depleting in the very near future. Therefore, in addition to nuclear fission reactors the search for alternative energy sources has been under way for past decades. One of the promising solutions to this problem could be a thermonuclear reactor based on fusion of light nuclei.

Since the late fifties of the past century an intensive research was started throughout the world to construct a fusion plant prototype with the magnetic confinement of plasmas. Later on an alternative approach emerged, the so-called inertial confinement fusion in which the thermonuclear reactions occur in deuterium and tritium targets due to the pressure compression created by evaporating outer shells. In such installations plasmas under extreme conditions are produced by powerful either laser or ion beams.

That is why the European Union adopted the special programme (HEDgeHOB - high energy density matter generated by heavy ion beams, http://hedgehob.physik.tu-darmstadt.de) which is aimed at theoretical and experimental studies of the properties of dense strongly coupled plasmas. At the same time the laser inertial fusion is currently advocated in the U.S. at the Lawrence Livermore National Laboratory which is called the National Ignition Facility (https:// lasers.llnl.gov/).

It has to be mentioned that besides installations for controlled nuclear fusion non-ideal or strongly coupled plasmas, i.e. plasmas in which the average interaction energy between charged particles is of the order of magnitude or even larger than their average kinetic energies of thermal motion, are also encountered in various astrophysical objects.

Researches in the field of plasma physics were initiated in the early twenties of the XXth century whereas dense Coulomb systems appeared in focus some fifty years later. Experimental investigations of dense plasmas remain quite complicated and expensive; therefore a number of theoretical methods were put forward to analyze their equilibrium and non-equilibrium properties. Among them is the pseudopotential theory of equilibrium systems in which particles interactions are described by effective potentials. A standard physical picture is also of wide use implying applications of modern methods of quantum statistical mechanics of many-body systems.

It is noteworthy that to describe the properties of dense Coulomb systems various models are utilized including a one-component plasma (OCP), a two-component plasma, etc.

On the other hand, one evidences a very wide spread of computer simulation techniques, such as molecular dynamics (MD) and Monte Carlo (MC). In those simulations all interparticle interactions are assumed to be known *a priori*. Then, one writes down the equations of motion or the transition probability from one particular state to another and the macroscopic characteristics are simply determined by averaging over corresponding microscopic states. Results of numerical simulations are considered the most reliable, since they are based on first principles and essentially deprived of far-reaching physical assumptions. A very special place is taken by the particle-in-cell (PIC) simulations designed for studying the dynamics of a continuous media.

Since dense Coulomb systems possess no perturbation parameters we apply, in the present work, the method of moments which is based on sun rules and other exact relations and is intrinsically non-perturbative.

One of the main problems of modern plasma physics is to obtain an analytic expression for the dielectric function determining the screening effects, the dispersion relations and other dynamic characteristics, such as the conductivity, the reflectivity, etc. The dielectric function can be derived from the linear-response theory [1], using the methods of the kinetic theory or hydrodynamics [2] and by means of the perturbation expansion of the Kubo formula [3]. On the other hand, the dielectric function can be deduced on the basis of the method of moments [4]. All methods mentioned above are mostly applicable in a limited range of plasma parameters where some perturbation expansions are applicable. On the contrary, the method of moments [5, 6] imposes no such restrictions on the plasma parameters thereby reconstructing any Nevanlinna class function by its convergent power moments. In physics those functions play a special role and are called response functions which are due to the causality principle and satisfy the Kramers-Kronig relations. A simple example is the plasma inverse dielectric function.

Another important dynamic characteristic is the dynamic structure factor which is related, via the fluctuation-dissipation theorem, to the imaginary part of the inverse dielectric function and can be extracted from experimental data [7]. Thus, from both the practical and mathematical points of view, the study of the dynamic structure factor is of great significance.

There exist several approaches to the investigation of the dynamic structure factor. Beyond experimental and theoretical methods one has to mention simulation techniques based on the first principles of mechanics and statistical physics. It is curious that the results of the pioneering work [8] remain in a good agreement with the most recent data of [9].

In the present thesis, the one-component plasma dynamic structure factor is modeled by the first three terms of its asymptotic expansion at high frequencies and its values at a few interpolation points on the real axis. This makes the dynamic structure factor a non-rational function whose extension onto the upper half-plane of the complex frequency is holomorphic with a non-negative imaginary part and with a continuous extension to the real axis. In the Schur-like algorithm [10] a free parameter of the non-rational model function is obtained from the

Shannon entropy maximization procedure. The results automatically satisfy not only the sum rules (the power moments) and other exact relations but, also, interpolate between the chosen frequencies. Quite a good agreement is obtained with the available simulation data on the plasma dynamic properties. The method permits to take into account the energy dissipation processes so that the results of the alternative theoretical approaches are included into the moment scheme and are to be complemented as well. Of course, such an algorithm can be used in a much broader setting.

Additionally, the classical molecular dynamic simulation data on the charge-charge dynamic structure factor of two-component plasmas modeled in [11] and [12] are analyzed and verified using the sum rules and other exact relations. The convergent power moments of the imaginary part of the model system dielectric function are expressed in terms of its partial static structure factors computed by the method of hypernetted chains using the Deutsch and other effective potentials. The high-frequency asymptotic behavior of the dielectric function is specified to include the effects of inverse bremsstrahlung.

Finally, we apply the above described approach to the modeling of optical properties of moderately coupled plasmas. On the basis of the Hölder inequalities, the monotonicity of the real part of the long-wavelength dynamic conductivity, predicted by the classical Drude-Lorentz model, is studied.

The work is terminated by a short comparison between the method of moments and a classical method of continuous fractions (as applied to the investigation of dynamic properties of physical systems), which is, due to Stieltjes, mathematically equivalent to the moment one.

Objectives:

1. To apply the mathematical method of moments, particularly with local constraints, to the investigation of dynamic properties of dense Coulomb systems.
2. To analyze the non-monotonicity of the dynamic electrical conductivity of non-ideal plasmas.

Dissertation structure

In the Introduction the applicability of the chosen research topic, the aims, the methods and the way for reaching the goals are generally presented.

The first section presents a background discussion introducing the model and methods that form a core of the second section of the dissertation. Then the results on dynamic characteristics of one-component plasmas such as dynamic structure factors, the mode spectrum and the decrement of damping are presented.

The second section is devoted to the description of the calculation of the dynamic structure factor for two-component plasmas based on the knowledge of the static limits and the interaction potential for different values of the plasma parameters.

The third section deals with some additional results on the characteristics of two-component plasmas and the relation of the classical method of continuous fractions to the method of moments is outlined. The thesis is ended by the Conclusions of the work and the Bibliography – the list of used references.

1 APPLICATION OF THE METHOD OF MOMENTS TO A SPECIFIC PHYSICAL SYSTEM

1.1 One-component plasma model

The classical one-component plasma (OCP) might be considered as a test-tube for the modeling of strongly interacting Coulomb systems [13], see also [9, 14] for more recent reviews. OCP is often employed as a simplified version of real physical systems ranging from electrolytes and charged-stabilized colloids [15], laser-cooled ions in cryogenic traps [16] to dense astrophysical matter in white dwarfs and neutron stars [17]. Another modern and highly interesting pattern of the OCP is a dusty plasma with the pure Coulomb interparticle interaction potential substituted by the Yukawa effective potential [18].

The classical OCP is defined as a system of charged particles (ions) immersed in a uniform background of the opposite charge. It is characterized by a unique dimensionless coupling parameter

$$\Gamma = \frac{\beta (Ze)^2}{a}. \tag{1.1}$$

Here 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 with n being the number density of charged particles. For $\Gamma \gtrsim 1$ the interaction effects determine the physical properties of the OCP.

The OCP static properties like the pair correlation function $g(r)$, the static structure factor (SSF), $S(k)$, and the static local-field correction, $G(k)$, can be extracted from computer simulations, see [9, 14]. Moreover, molecular dynamics (MD) as well as other simulations provide invaluable information on the dynamic structure factor (DSF), $S(k,\omega)$, and some other dynamic characteristics.

Here, the OCP dynamic properties are studied within the moment approach based on sum rules and other exact relations, see [19, 20] and references therein and comparison is made with the simulation data of Hansen *et al.* [8] and of Wierling *et al.* [9].

Consider five convergent sum rules which are frequency power moments of the system DSF,

$$S_v(k) = \frac{1}{n} \int_{-\infty}^{\infty} \omega^v S(k,\omega) d\omega, \quad v = 0,1,2,3,4. \tag{1.2}$$

All odd-order moments vanish since the DSF is an even function of frequency in a statistically classical system.

The method of moments is, generally speaking, capable of handling an arbitrary number of convergent sum rules. In two-component plasmas, though, all higher-order frequency moments diverge which can be attributed to and understood [4] from the exact asymptotic expansion of the imaginary part of the dielectric function [21]. There is no such clear theoretical result for the model system to be dealt with here and, thus, it is simply impossible to presume that the three first even order moments Eq. (1.2) are the only convergent frequency sum rules of even order. However, the ambiguity of higher-order frequency moments [22], related to our scarce knowledge of the triplet and, presumably, higher-order correlation functions, remains insuperable nowadays and can only impede our understanding of the physical processes to be described below.

It is well known [6] that the analytic prolongation of the positive function of frequency, DSF, onto the upper half-plane $\mathrm{Im} z > 0$, is constructed by means of the Cauchy integral formula,

$$S(k,z) = \frac{1}{n} \int_{-\infty}^{\infty} \frac{S(k,\omega)}{\omega - z} d\omega, \tag{1.3}$$

and admits the asymptotic expansion:

$$S(k,z) \cong -\frac{S_0(k)}{z} - \frac{S_2(k)}{z^3} - \frac{S_4(k)}{z^5} - o\left(\frac{1}{z^5}\right), \qquad \mathrm{Im} z \geq 0. \tag{1.4}$$

The zero-order moment is, obviously, the SSF, $S_0(k) = S(k)$, while the second moment is the f-sum rule,

$$S_2(k) = \omega_0^2(k) = \omega_p^2\left(\frac{k^2}{k_D^2}\right) = \omega_p^2\left(\frac{q^2}{3\Gamma}\right), \qquad (1.5)$$

and the fourth moment equals

$$S_4(k) = \omega_p^2\omega_0^2(k)\left\{1 + \frac{3k^2}{k_D^2} + U(k)\right\}, \qquad (1.6)$$

$$= \omega_p^2\omega_0^2(q)\left\{1 + \frac{q^2}{\Gamma} + U(q)\right\}. \qquad (1.7)$$

Here $q = ka$, $\omega_p = \sqrt{4\pi n(Ze)^2/m}$ refers to the plasma frequency, and $k_D = \sqrt{4\pi n e^2 Z^2 \beta}$ is the Debye wavelength with m being the ion mass, and

$$U(q) = \frac{1}{4\pi^2 n}\int_0^\infty [S(k') - 1]\, f(k';k) k'^2\, dk', \qquad (1.8)$$

$$= \frac{1}{3\pi}\int_0^\infty [S(p) - 1]\, f(p;q) p^2\, dp,$$

where

$$f(p;q) = \frac{5}{6} - \frac{p^2}{2q^2} + \left(\frac{p^3}{4q^3} - \frac{p}{2q} + \frac{q}{4p}\right) ln\left|\frac{q+p}{q-p}\right|, \tag{1.9}$$

$$q = ka,$$

$$p = k'a. \tag{1.10}$$

The last contribution to the fourth moment is due to the ion-ion interactions in the OCP, while the second term represents the Vlasov correction to the ideal-gas dispersion relation of the plasmon mode $\omega_L = \omega_p$.

As in [23] the following limits hold

$$U(k \to \infty) = \frac{2}{3}(\mathrm{g}(0) - 1) = -\frac{2}{3}, \tag{1.11}$$

$$U(k \to 0) \cong \frac{2}{15}\frac{\langle \phi(k) \rangle}{\phi(k)}, \tag{1.12}$$

where, by virtue of the Parseval theorem,

$$\langle \phi(k) \rangle = \int \phi(k)\,[S(k)-1]\frac{dk}{(2\pi)^3 n} = \int \phi(r)\,[\mathrm{g}(\mathrm{r})-1]dr, \qquad (1.13)$$

is the average interaction energy between two ions with

$$\phi(k) = \frac{4\pi(Ze)^2}{k^2}, \quad \phi(r) = \frac{(Ze)^2}{r}. \qquad (1.14)$$

The Nevanlinna formula of the classical theory of moments [5, 6] expresses the response function [19],

$$S(k,z) = -\frac{1}{n}\frac{E_3(z;k) + Q(k,z)E_2(z,k)}{D_3(z;k) + Q(k,z)D_2(z,k)}, \qquad (1.15)$$

in terms of a Nevanlinna class function $Q = Q(k,z)$, analytic in the upper half-plane $\mathrm{Im}z > 0$ with a positive imaginary part $\mathrm{Im}(Q(k,\omega + i\eta) > 0$, $\eta > 0$. The function $Q(k,z)$ should additionally satisfy the limiting condition:

$$\frac{Q(k,z)}{z} \underset{z\uparrow\infty}{\longrightarrow} 0, \quad \mathrm{Im}z > 0. \qquad (1.16)$$

Such a function admits the integral representation [5, 6]

$$Q(k,z) = \frac{i}{\tau(k)} + 2z\int_0^\infty \frac{du(t)}{t^2 - z^2}, \tag{1.17}$$

with $\tau(k) > 0$ and a non-decreasing bounded function $u(t)$ such that

$$\int_{-\infty}^{\infty} \frac{du(t)}{1+t^2} < \infty. \tag{1.18}$$

Furthermore, the polynomials $D_j(z;k)$, $j = 0,1,2,3$, are orthogonal with respect to the measure $S(k,\omega)$ together with their conjugate counterparts $E_j(z;k)$, $j = 0,1,2,3$ determined as

$$E_j(z;k) = \int_{-\infty}^{\infty} \frac{D_j(\omega,k) - D_j(z;k)}{\omega - z} S(k,\omega)d\omega, \tag{1.19}$$

These polynomials have only real coefficients and alternating zeros [5, 6]. A rather routine renormalization casts these polynomials as

$$D_0(z;k) = 1, \quad D_1(z;k) = z,$$

$$D_2(z;k) = z^2 - \omega_1^2(k), \qquad D_3(z;k) = z^3 - z\omega_2^2(k),$$

$$E_0(z;k) \equiv 0, \quad E_1(z;k) = S_0(k), \tag{1.20}$$

$$E_2(z;k) = S_0 z, \quad E_3(z;k) = S_0(k)[z^2 + \omega_1^2 - \omega_2^2].$$

The frequencies $\omega_1(k)$ and $\omega_2(k)$ in Eq. (1.20) are defined by the respective ratios of the moments $S_\upsilon(\nu)$ [19] and, thus, are determined by the system static characteristics:

$$\omega_1^2 = \omega_1^2(k) = \frac{S_2(k)}{S_0(k)}, \tag{1.21}$$

$$\omega_2^2 = \omega_2^2(k) = \frac{S_4(k)}{S_2(k)}. \tag{1.22}$$

The DSF is therefore found from Eq. (1.3) as

$$S(k,\omega) = \frac{n}{\pi} \lim_{\eta \downarrow 0} \operatorname{Im} S(k, \omega + i\eta) = \\ = \frac{n}{\pi} \frac{S(k)\omega_1^2(\omega_2^2 - \omega_1^2)\operatorname{Im}Q}{[\omega(\omega^2 - \omega_2^2) + \operatorname{Re}Q(\omega^2 - \omega^2)]^2 + [\operatorname{Im}Q]^2(\omega^2 - \omega_1^2)^2}. \tag{1.23}$$

Here we approximate the Nevanlinna interpolation function $Q = Q(k,\omega)$ by its static value $i\tau^{-1}(k) = Q(k,0)$, where the "relaxation time" is selected to reproduce an exact static value of the dynamic structure factor in Eq. (1.23):

$$\tau(k) = \frac{\pi S(k,0)}{nS(k)} \frac{\omega_1^2(k)}{\omega_p^2 \Delta(k)}. \tag{1.24}$$

Alternatives in determination of the relaxation time were discussed in [24, 25]. Note that

$$\Delta(k) = \frac{\omega_2^2(k) - \omega_1^2(k)}{\omega_2^2} > 0, \tag{1.25}$$

due to the Cauchy-Schwarz inequality. It is important that the DSF, Eq. (1.23), by virtue of Eq. (1.16), obeys the correct asymptotic expansion (1.4) and, hence, satisfies the sum rules (1.2) by construction, regardless of the form of the Nevanlinna parameter function $Q(k,\omega)$. On the other hand, this means that the asymptotic expansion (1.4) holds for any adequate choice of the function $Q(k,\omega)$.

Within the approximation described above we adopt

$$\frac{S(k,\omega)}{S(k,0)} = \frac{\omega_1^4}{[\omega^2 - \omega_1^2(k)]^2 + \left[\left(\omega^2 - \omega_2^2(k)\right)\omega\tau(k)\right]^2}, \tag{1.26}$$

The static characteristics, i.e. $S(k,0)$, $S(k)$ together with the moments $S_0(k)$, $S_2(k)$ and $S_4(k)$, which, in turn, determine the characteristic frequencies $\omega_1(k)$, $\omega_2(k)$, and $\tau^{-1}(k)$, are to be calculated independently, e.g., in the hypernetted chain (HNC) approximation or to be taken directly from the MD simulation data on the DSF. Note that the DSF Eq. (1.26) contains an exact static value, $S(k,0)$.

In a classical system and due to the fluctuation-dissipation theorem (FDT),

$$S(k,\omega) = \frac{L(k,\omega)}{\pi\beta\phi(k)}, \tag{1.27}$$

so that the moments in Eq. (1.2) are proportional, for a given value of the wave number, to the corresponding moments of the loss function

$$L(k,\omega) = -\frac{\mathrm{Im}\varepsilon^{-1}(k,\omega)}{\omega}, \tag{1.28}$$

in the following way:

$$S_v(k) = \frac{k^2}{k_D^2} C_v(k), \quad v = 0,2,4, \tag{1.29}$$

where

$$C_v(k) = \frac{1}{\pi} \int_{-\infty}^{\infty} \omega^v L(k,\omega)\, d\omega, \quad v = 0,2,4, \tag{1.30}$$

and $\varepsilon^{-1}(k,\omega)$ stands for the plasma inverse dielectric function (IDF) which is a genuine response (Nevanlinna) function of frequency.

Since the DSF has previously been constructed on the basis of the Nevanlinna formula [5, 6], we, thus, obtain for the IDF [19]:

$$\varepsilon^{-1}(k,z) = 1 + \frac{\omega_p^2(z+Q)}{z(z^2-\omega_2^2)+Q(z^2-\omega_1^2)}, \quad z = \omega + i0^+, \tag{1.31}$$

where the Nevanlinna parameter function $Q = Q(k,z)$ coincides with that in Eq. (1.15) due to relation (1.27).

1.2 Method of moments with local constraints

Consider the mixed Löwner-Nevanlinna problem [5, 6, 22, 26-28], see also Ref. [29] for the matrix version of the problem.

Problem 1. Given a set of real numbers $(c_0, \ldots, c_{2n})$*, a finite set of points* $(t_1, \ldots, t_p)$ *on the real axis, and a set of complex numbers* $(\omega_1, \ldots, \omega_p)$ *with non-negative imaginary parts, find a positive function* $f(t), t \in R$ *such that*

$$\int_{-\infty}^{\infty} t^k f(t) dt = c_k, \quad k = 0,1, \ldots, 2n, \tag{1.32}$$

and

$$w_s = \lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\infty} \frac{f(t)dt}{t - t_s - i\varepsilon}, \quad s = 1, \ldots, p. \tag{1.33}$$

The Problem 1 is a mixture of the truncated Hamburger moment problem [5, 26, 27] with the Löwner-type interpolation problem in the class of Nevanlinna functions [28].

We describe and test numerically an algorithm for finding of non-rational solutions to this problem. We are particularly interested in the possibility to solve the problem when only a very small number of moments and constraints (data at the interpolation nodes) are known.

The mixed problem solution

Assume that the set of moments is positively definite so that the truncated Hamburger moment problem is solvable [5, 26, 27], and that there exists an infinite set of non-negative measures $g(t)$ on the real axis such that

$$\int_{-\infty}^{\infty} t^k \, dg(t) = c_k, \quad k = 0,1,\dots,2n. \tag{1.34}$$

Then, the formula,

$$-\int_{-\infty}^{\infty} \frac{dg(t)}{t-z} = \frac{E_{n+1}(z) + \zeta(z) E_n(z)}{D_{n+1}(z) + \zeta(z) D_n(z)}, \quad \mathrm{Im} z > 0, \tag{1.35}$$

$$n = 0,1,2,\dots,$$

according to Nevanlinna's theorem [5], establishes a one-to-one correspondence between the set of all measures $g(t)$ satisfying (1.34) and the Nevanlinna functions $\zeta(z) \in \mathbb{R}$, i.e., functions which are analytic in the upper half-plane $\mathrm{Im} z > 0$, continuous on its closure $\mathrm{Im} z = 0$ with a positive imaginary part at $\mathrm{Im} z \geq 0$ and such that $\lim_{z\to\infty} \zeta(z)/z = 0$, $\mathrm{Im} z > 0$.

The polynomials $\{D_k\}_0^{n+1}$ form the orthogonal system with respect to each g-measure satisfying (1.34) and can be found by the Gram-Schmidt procedure applied to the basis $\{1, t, t^2, \ldots, t^{n+1}\}$, while $\{E_k\}_0^{n+1}$ is the corresponding set of conjugate polynomials [5]. Notice that the zeros of each orthogonal polynomial $D_k(z)$ are real and, by virtue of the Schwarz-Christoffel identity, the zeros of $D_{k-1}(z)$ alternate with the zeros of $D_k(z)$ as well as with the zeros of $E_{k-1}(z)$.

To meet the constraints (1.33) it is enough now to substitute into the right hand side of (1.35) any function $\zeta\ z$ which satisfies the following conditions:

$$\xi_s = \zeta(t_s) = -\frac{w_s D_{n+1}(t_s) + E_{n+1}(t_s)}{w_s D_n(t_s) + E_n(t_s)}, \quad s = 1, \ldots, p. \tag{1.36}$$

Note that $\mathrm{Im}\xi_s > 0$. Thus, Problem 1 reduces to Problem 2.

Problem 2. Given a finite number of distinct points $(t_1, \ldots, t_p)$ *of the real axis and a set of complex numbers* $(\omega_1, \ldots, \omega_p)$ *with positive imaginary parts, find the set of functions* $\zeta(z) \in \mathbb{R}$ *that are continuous in the closed upper half-plane and satisfy conditions (1.36).*

Each Nevanlinna function $\zeta(z)$ in the upper half-plane admits the Caley representation,

$$\zeta(z) = i\frac{1+\theta(z)}{1-\theta(z)}, \tag{1.37}$$

where

$$\theta(z) = i\frac{\zeta(z)-i}{\zeta(z)+i}, \tag{1.38}$$

is a holomorphic function (in the upper half-plane) with contractive values, i.e. $|\theta(z)| \le 1$, $\mathrm{Im} z > 0$. Therefore, Problem 2 is equivalent to the following problem for contractive functions.

Let $\mathcal{H}$ be the set of all contractive functions which are holomorphic in the upper half-plane and continuous on its closure.

Problem 3. Given a finite number of distinct points $t_1, \dots, t_p$ of the real axis and a set of points $\lambda_1, \dots, \lambda_p$,

$$\lambda_s = \frac{\xi_s - i}{\xi_s + i}, \quad |\lambda_s| \le 1, \quad s = 1, \dots, p, \tag{1.39}$$

find a set of functions $\theta \in \mathcal{H}$ such that

$$\theta(t_s) = \lambda_s, \quad s = 1, \dots, p. \tag{1.40}$$

Problem 3 is a limiting case of the Nevanlinna-Pick problem [5, 6] with interpolation nodes on the real axis. Its solvability for any interpolation data $\lambda_1, \dots, \lambda_p$ inside the unit circle was actually proven in Ref. [30]. The point is that the associated Pick matrix is automatically positively definite for any given contractive interpolation values as soon as the interpolation nodes are close enough to the axis; this guarantees that the approximate Nevanlinna-Pick problem is solvable if the interpolation nodes are close enough to the real axis. Then, the Vitali-Montel theorem is applied to take the limit of the interpolation nodes approaching the real axis. This also implies that the Nevanlinna-Pick problem is solvable even if some or all $|\lambda_s| = 1$.

We describe below an algorithm of solving Problem 3 when all $|\lambda_s| < 1$, which is a simple modification of the Schur algorithm. An alternative algorithm, similar to the Lagrange method of the interpolation theory, can be applied if some or even all $|\lambda_s| = 1$ [27].

1.3 Schur algorithm and its application

Note that a function $\theta \in \mathcal{H}$ satisfies the condition $\theta(t_1) = \lambda_1$, $|\lambda_1| < 1$, if and only if it admits the representation,

$$\theta(z) = \frac{\phi(z) + \lambda_1}{\lambda_1 \phi(z) + 1}, \tag{1.41}$$

where $\phi \in \mathcal{H}$ and $\phi(t_1) = 0$. In case of the Nevanlinna-Pick problem, i.e., when t_1 belongs to the upper half-plane, the function $\phi(z)$ admits the representation:

$$\phi(z) = \frac{z - t_1}{z - \bar{t}_1} \chi(z), \tag{1.42}$$

where $\chi(z)$ is an arbitrary contractive function in the upper half-plane. There is no such simple form for the contractive function $\phi(z)$ when $t_1 \in \mathbb{C}$.

Here we carry out the reconstruction procedure using the non-rational functions, as suggested in Ref. [27]:

$$\phi(z) = \theta_1(z) exp\left\{\frac{\alpha}{\pi i} \int_{t_1-1}^{t_1+1} \frac{1+tz}{t-z} ln|t-t_1| \frac{dt}{t^2+1}\right\}, \tag{1.43}$$

$$= \theta_1(z) u_1(z),$$

with a unique free parameter $\alpha \in 0,1$. Here θ_1 is any function from $\mathcal{H}$ such that

$$\theta_1(t_s) = \lambda_s' = \frac{1}{u_1(t_s)} \frac{\lambda_s - \lambda_1}{1 - \overline{\lambda_1}\lambda_s}, \quad s = 2, \dots, p. \tag{1.44}$$

Such a choice of $\theta_1(z)$ guarantees that conditions (1.40) are all verified. Hence, Problem 3, initially formulated for p interpolation nodes on the real axis and strictly contractive values of the functions to be found at these nodes, reduces to the same problem but with $p - 1$ interpolation nodes and modified values at these nodes given by (1.44). Repeating the above procedure $p - 1$ times with a suitable choice of the parameter α and modifying the values of emerging contractive functions at the remaining points $\mathrm{t}_{s+1}, \dots, \mathrm{t}_{\mathrm{p}}$ according to (1.44), permits to obtain a solution to Problem 3. Note that contrary to the Nevanlinna-Pick problem with nodes in the open upper half-plane, Problem 3 is always solvable if the values of the function to be reconstructed are contractive at the interpolation nodes.

Let $\theta_{s-1} \in \mathcal{H}$ be a contractive function emerging after $s - 1$ steps in the course of solving Problem 3 by the above described method, and let $\lambda_s^{(s-1)} = \theta_{s-1}(t_s)$, $\lambda_1^{(0)} = \lambda_1$. It follows from the above stated arguments that should the initial parameters $\lambda_1, \dots, \lambda_p$ be strictly contractive, there exists a set of solutions to Problem 3 described by the formula,

$$\theta(z) = \frac{a(z)\mu(z) + b(z)}{c(z)\mu(z) + d(z)}, \tag{1.45}$$

where the matrix elements of linear fractional transformation (1.45) are non-rational functions constructed as described above and $\mu(z)$ runs the subset of all functions from $\mathcal{H}$ satisfying the condition $\mu(t_p) = \lambda_p^{(p-1)}$. This matrix can be calculated as

$$\begin{pmatrix} \mathrm{a}(z) & b(z) \\ \mathrm{c}(z) & d(z) \end{pmatrix} = \prod_{s=1}^{p-1} \begin{pmatrix} \dfrac{u_s(z)}{\lambda_s^{(s-1)} u_s(z)} & \begin{matrix} \lambda_s^{(s-1)} \\ 1 \end{matrix} \end{pmatrix}, \tag{1.46}$$

where the indices s in the right-hand-side matrix factors increase from left to right.

Observe that the simplest choice for the function $\mu(z)$ in (1.45) is just to assume $\mu(z) \equiv \lambda_p^{(p-1)}$. Hence, if initial parameters $\lambda_1, \dots, \lambda_p$ in Problem 3 are strictly contractive, then, among the solutions to this problem there are non-rational functions of the kind we consider.

1.4 Dynamic structure factors

Since in physical applications we usually try to reconstruct certain non-negative densities, the solvability of the moment problem is not an issue. In each case the absolutely continuous non-negative measure with this density is just one of the solutions to the moment problem.

To apply the Schur-like algorithm described above, one has to know not only the values of some power moments of the distribution density $f(t)$ under investigation,

$$c_k = \int_{-\infty}^{\infty} t^k f(t)\,dt, \quad k = 0,1,\dots,2n, \quad n = 1,2\dots, \tag{2.47}$$

but also the values of the Nevanlinna function at the set of points$(t_1,\dots,t_p)$:

$$w_s = \varphi(t_s) = P.V.\int_{-\infty}^{\infty} \frac{f(t)dt}{t-t_s} + i\pi f(t_s). \tag{1.48}$$

In all cases considered below we use only three non-zero moments, $n = 2$, with three interpolation nodes, $p = 3$; the latter principal value integrals have been computed numerically and the orthogonal polynomials are calculated directly as

$$D_0(z) = 1, \quad D_1(z) = z, \quad D_2(z) = z^2 - \omega_1^2,$$

$$D_3(z) = z(z^2 - \omega_2^2), \qquad E_0(z) \equiv 0, \quad E_1(z) = c_0, \tag{1.49}$$

$$E_2(z) = c_0 z, \quad E_3(z) = c_0(z^2 - \omega_2^2 + \omega_1^2),$$

where $\omega_1^2 = c_2/c_0$, $\omega_2^2 = c_4/c_2$.

To find the free parameter $\alpha \in (0,1)$ of the auxiliary function

$$u_s(z) = exp\left\{\frac{\alpha}{\pi i}\int_{t_s-1}^{t_s+1} \frac{1+tz}{t-z} ln|t-t_s| \frac{dt}{t^2+1}\right\}, \tag{1.50}$$

$s = 1,2,3,$

we make use of the Shannon entropy [31],

$$\sigma(\alpha) = -\int_{-\infty}^{+\infty} F(\alpha,t) ln\big(F(\alpha,t)\big) dt, \tag{1.51}$$

maximization procedure [32], where the density $F(\alpha,t)$ is reconstructed in the above described algorithm and represents the imaginary part (divided by π) of the model function obtained in the Schur-algorithm procedure. The density $F(\alpha,t)$ has no real poles and is positive over the whole real axis, hence it is quite easy to solve the maximization procedure equation: $d\sigma(\alpha)/d\alpha = 0$.

To check the quality of the reconstruction technique proposed above, we carry out an extensive study of the present approach with application to the simulation data of [9]. In particular, we apply the Nevanlinna theorem to the OCP dynamic structure factor (DSF), $S(k,\omega)$, which is expressed in terms of the Nevanlinna parameter function $\zeta(\omega,k)$, reconstructed by the above algorithm, as

$$S(k,\omega) = \frac{n}{\pi}\frac{S(k)\omega_1^2(\omega_2^2-\omega_1^2)\mathrm{Im}\zeta}{[\omega(\omega^2-\omega_2^2)+\mathrm{Re}\zeta(\omega^2-\omega_1^2)]^2+[\mathrm{Im}\zeta]^2(\omega^2-\omega_1^2)^2}. \qquad (1.52)$$

Here

$$S(k) = c_0(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} S(k,\omega)d\omega, \qquad (1.53)$$

stands for the static structure factor. Notice that with the space dispersion taken into account, the moments,

$$c_j = \frac{1}{n} \int_{-\infty}^{\infty} \omega^j S(k,\omega) d\omega, \quad j = 0,2,4, \tag{1.54}$$

and the frequencies $\omega_j = \omega_j(k) = \sqrt{c_{2j}(k)/c_{2(j-1)}(k)}$, $j = 1,2,$ have been calculated directly from the numerical data on the dynamic structure factor [9]. The latter is an even function of frequency and the moments $c_1(k)$ and $c_3(k)$ simply vanish.

The numerical results on the dynamic structure factor have been compared to the simulation data of [9] and are summarized in Figures 1.1-1.5. In all figures the squares correspond to the data of [9] with ω_p being the plasma frequency, $q = k \cdot a$ and k is a value of wave number. In the figures we observe good agreement between the data of the numerical experiments and the calculations performed in the dissertation by the method of moments with local constrains. And we see that the maximum shifts to higher frequencies with increasing wave number (Figures 1.1 and 1.2).

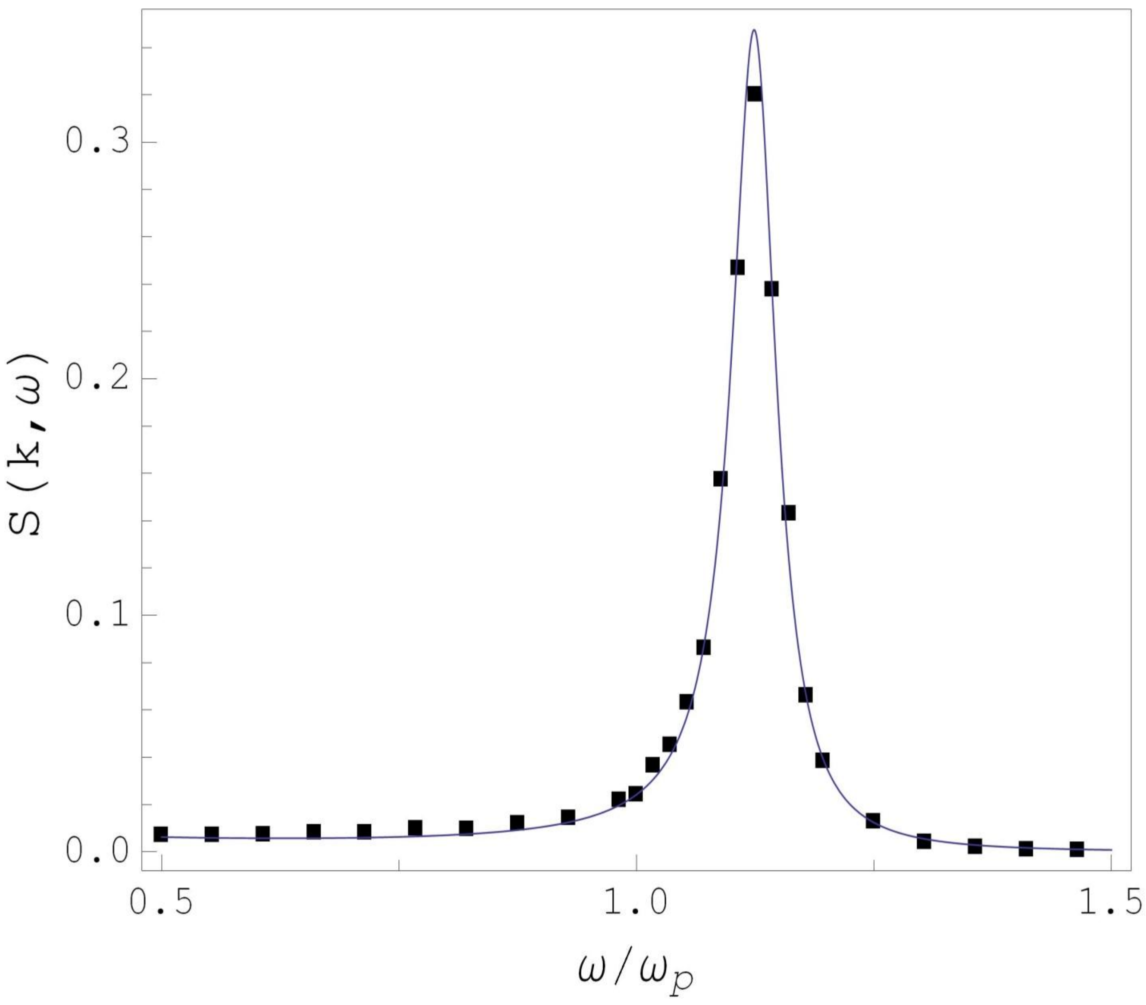


Figure 1.1 – The OCP normalized dynamic structure factor in comparison with the simulation data of [9] (boxes) at Γ = 0.993 and q = 0.6187.

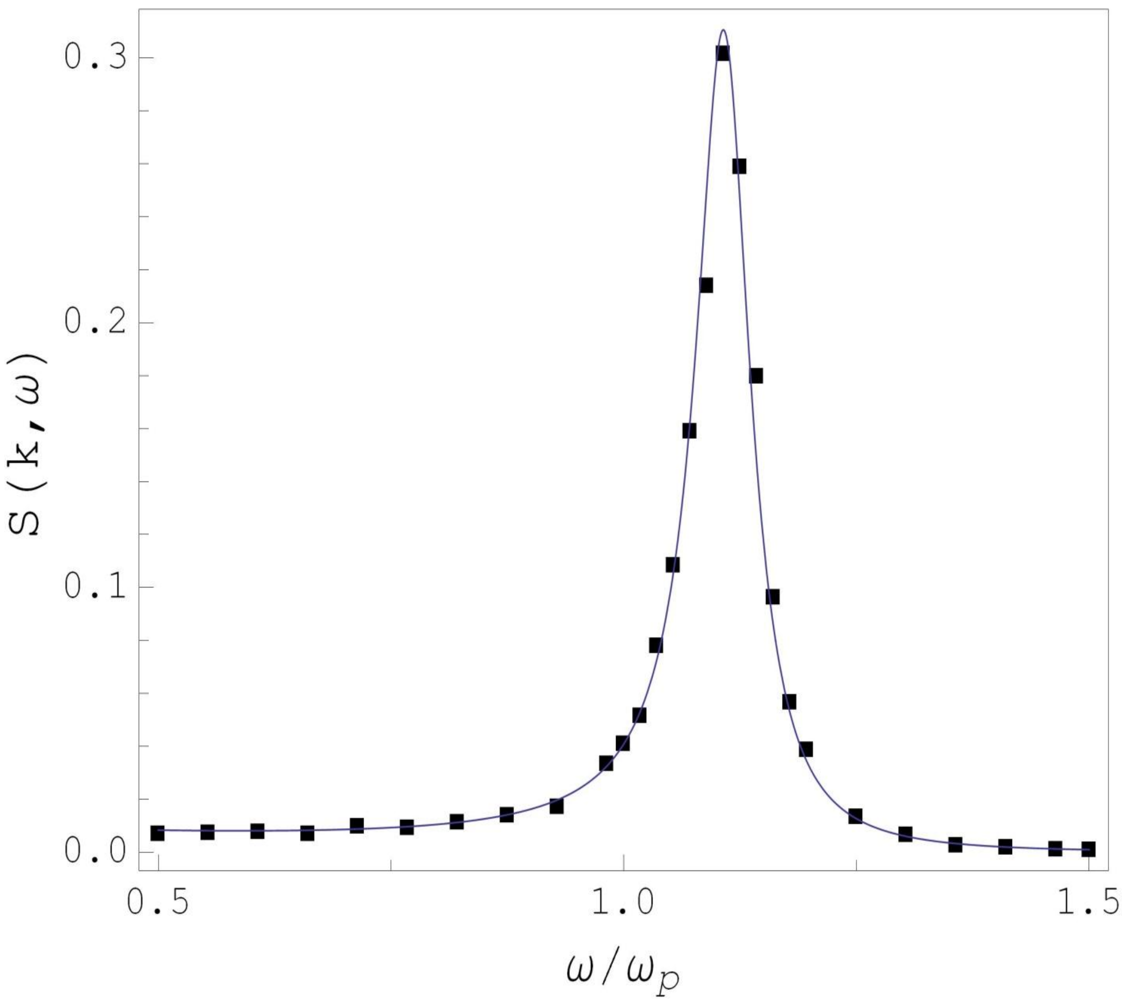


Figure 1.2 – The OCP normalized dynamic structure factor in comparison with the simulation data of [9] (boxes) at Γ = 1 and q = 0.49109.

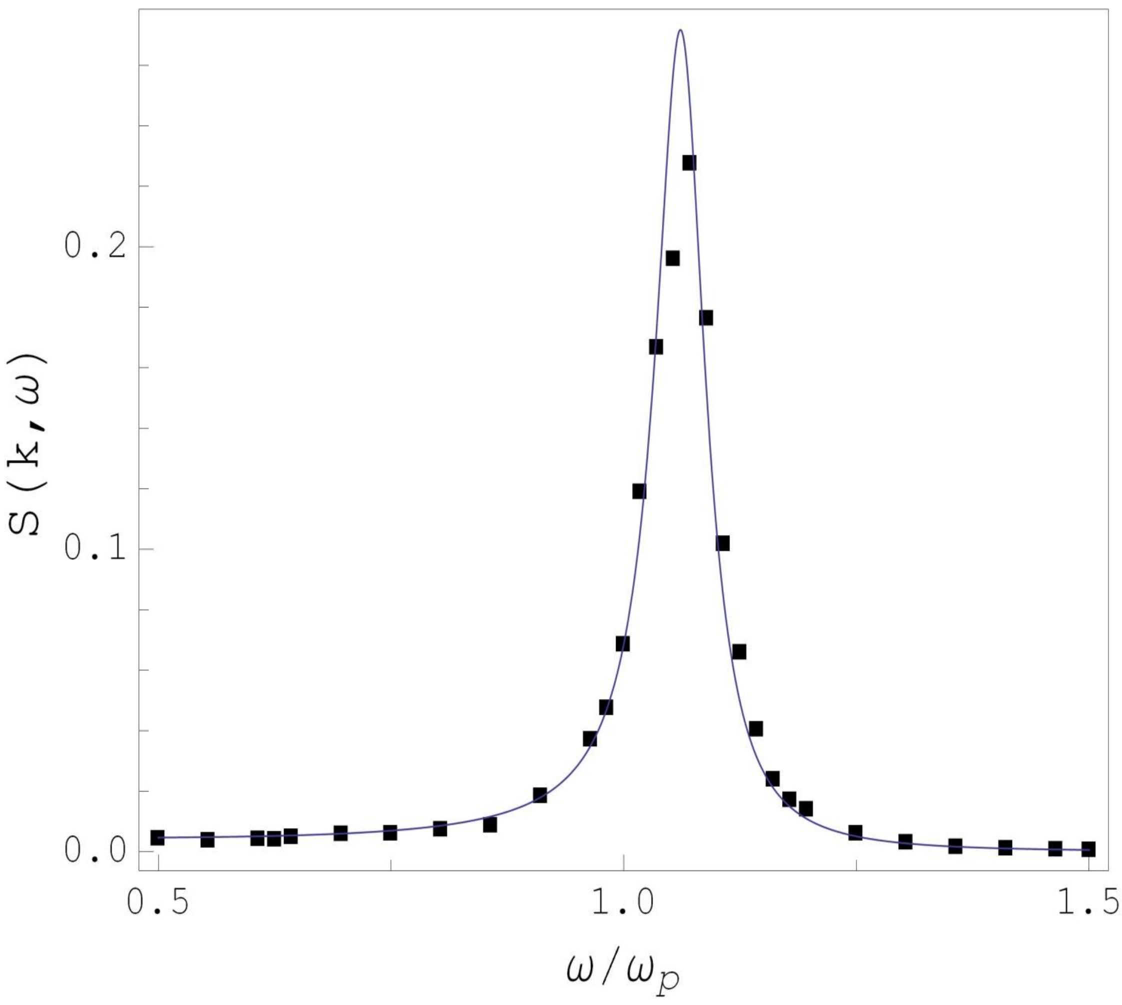


Figure 1.3 – The OCP normalized dynamic structure factor in comparison with the simulation data of [9] (boxes) at Γ = 2 and q = 0.60145.

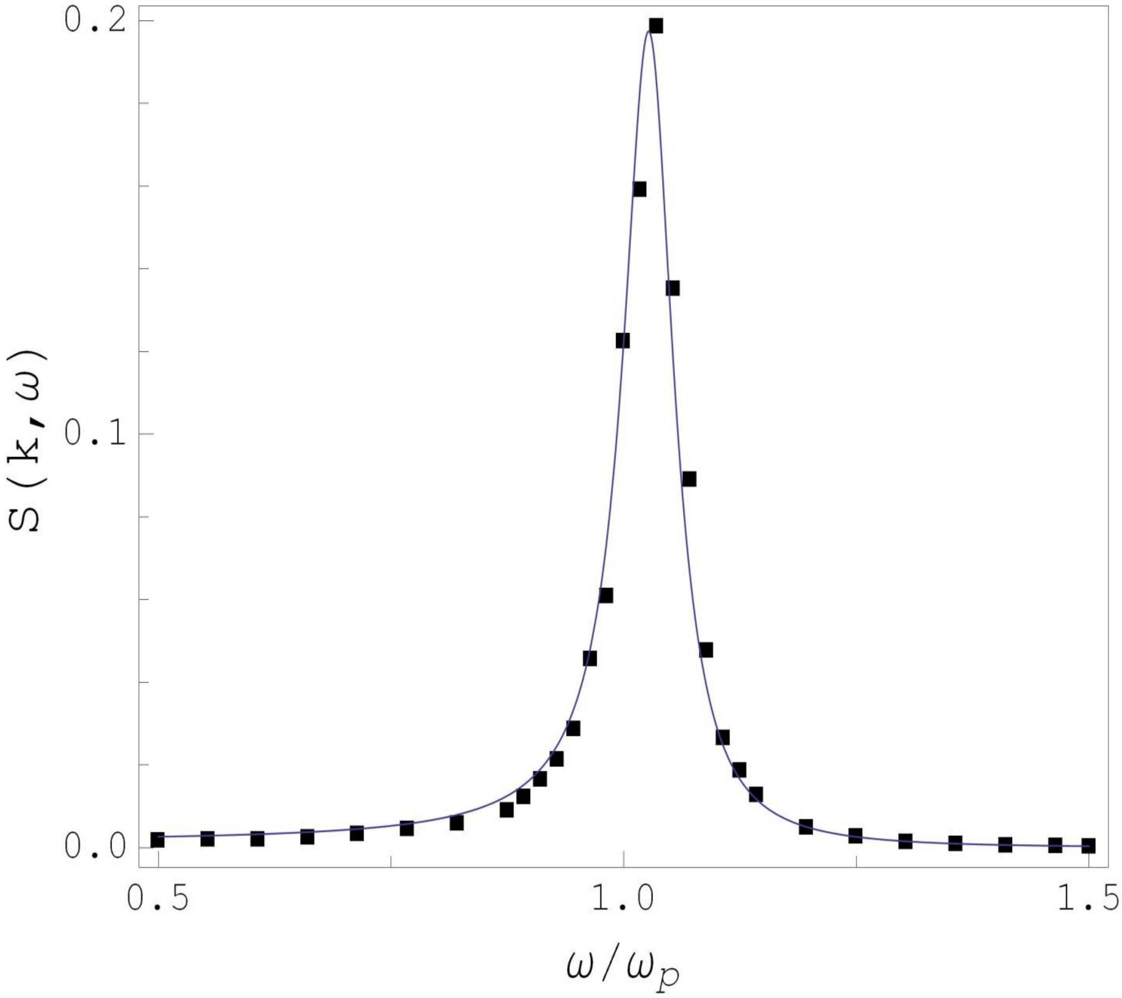


Figure 1.4 – The OCP normalized dynamic structure factor in comparison with the simulation data of [9] (boxes) at Γ = 4 and q = 0.6945.

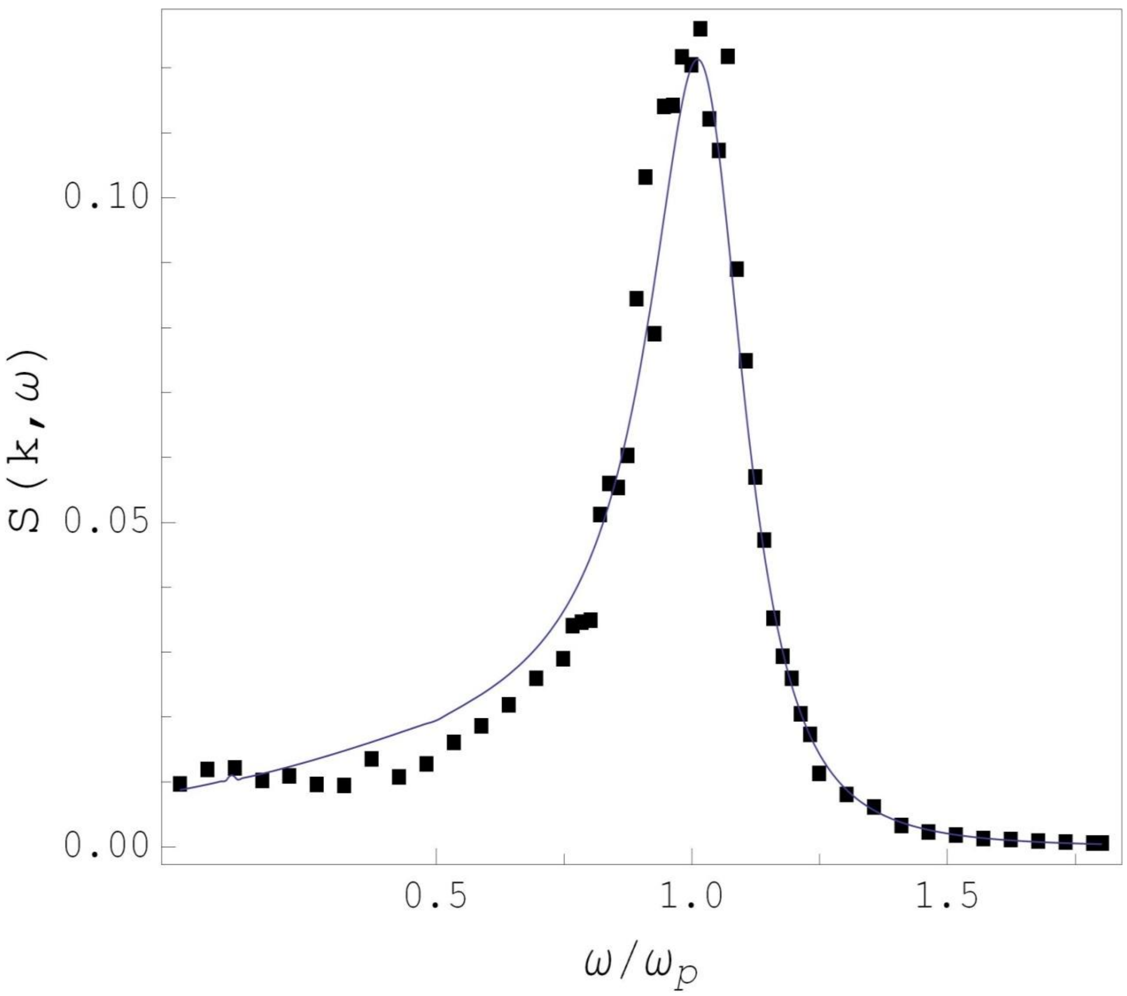


Figure 1.5 – The OCP normalized dynamic structure factor in comparison with the simulation data of [9] (boxes) at Γ = 8 and q = 1.389.

1.5 Spectrum and decrement of damping

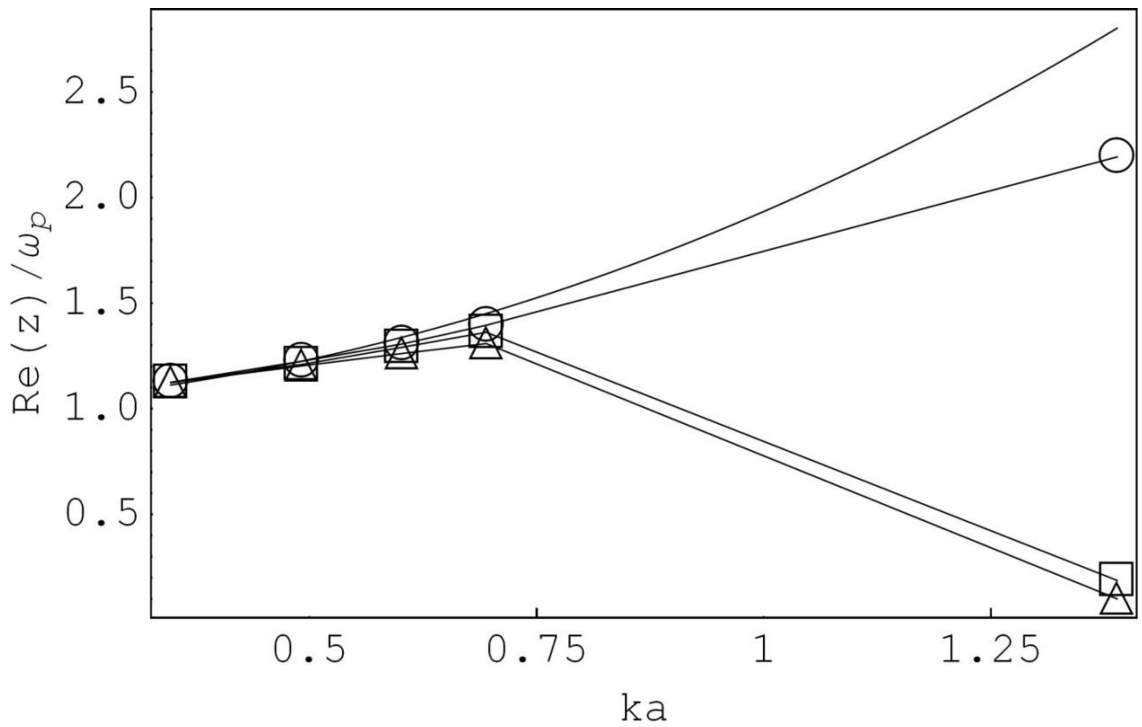
To study the characteristics of the plasmon mode we use the data for the Nevanlinna parameter function $\zeta(z;k)$ to solve the dispersion equation

$$z\left(z^2-\omega_2^2(k)\right)+\zeta(z;k)\left(z^2-\omega_1^2(k)\right)=0. \tag{1.55}$$

If the parameter function $\zeta(z;k)$ vanishes, the dispersion reduces to the frequency $\omega_2(k)$. These results are presented in Figures 1.6-1.10 together with our data on the frequency $\omega_2(k)$ and the interpolation dispersion relation of [2]. It is seen how the unsystematic behavior of the fourth moment is corrected by the present approach to obtain a very satisfactory agreement with the simulation data. Finally, we mention that the short-time asymptotic behavior of the dynamic structure factor is qualitatively quite similar to that obtained in [9] where the recurrence relation method was used. Certainly, the ω^{-6} asymptotic behavior of the DSF observed in [9] follows directly from (1.52) as long as the imaginary part of the Nevanlinna parameter function $\zeta(\omega;k)$ is a positive constant.

The solution of the dispersion equation (1.53) produces also the decrement of damping of the plasmon mode and the results are displayed in Figure 1.11.

We can conclude that the algorithm proposed gives a quantitative agreement between the simulation data on the plasma dynamic characteristics and their non-rational counterparts reconstructed by a few integral characteristics, i.e., the power moments together with the local constraints.



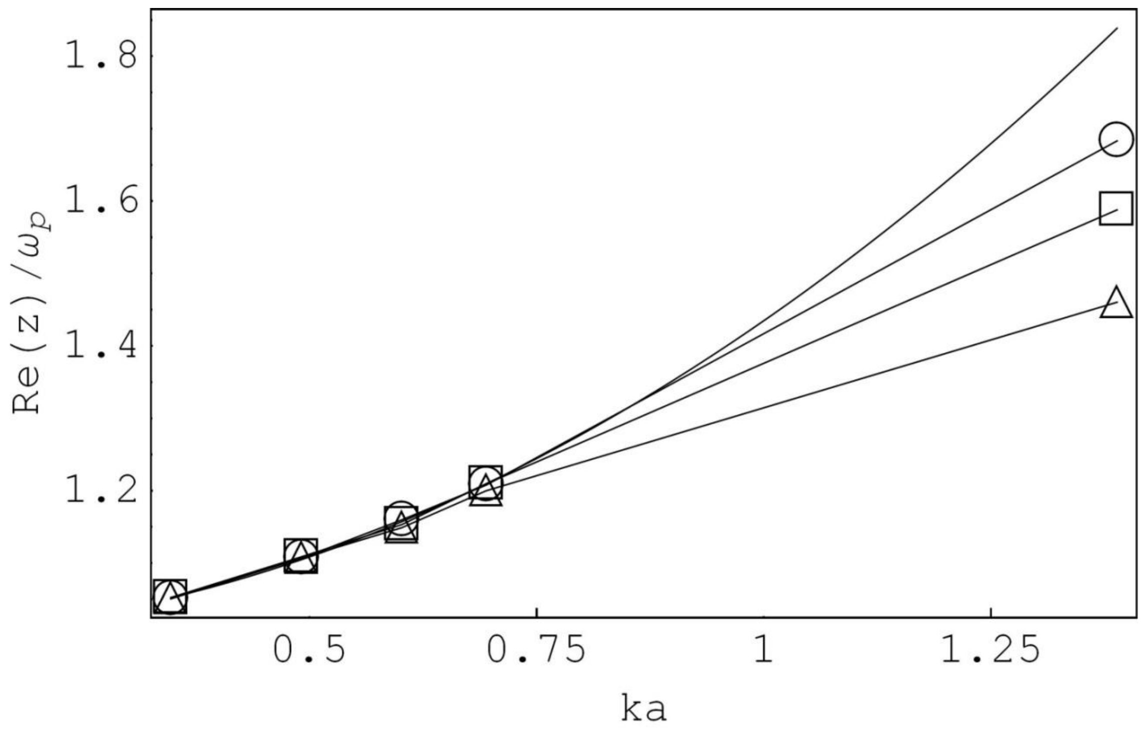
represent the positions of the maxima of the DSF

stand for the solutions of the dispersion equation (1.55)

correspond to $\omega_2(k)/\omega_p$

calculated by the interpolation formulas of [33]

Figure 1.6 – The plasmon dispersion relation, i.e., the real part of the solution of the dispersion equation (1.55) vs. ka at Γ = 0.993.



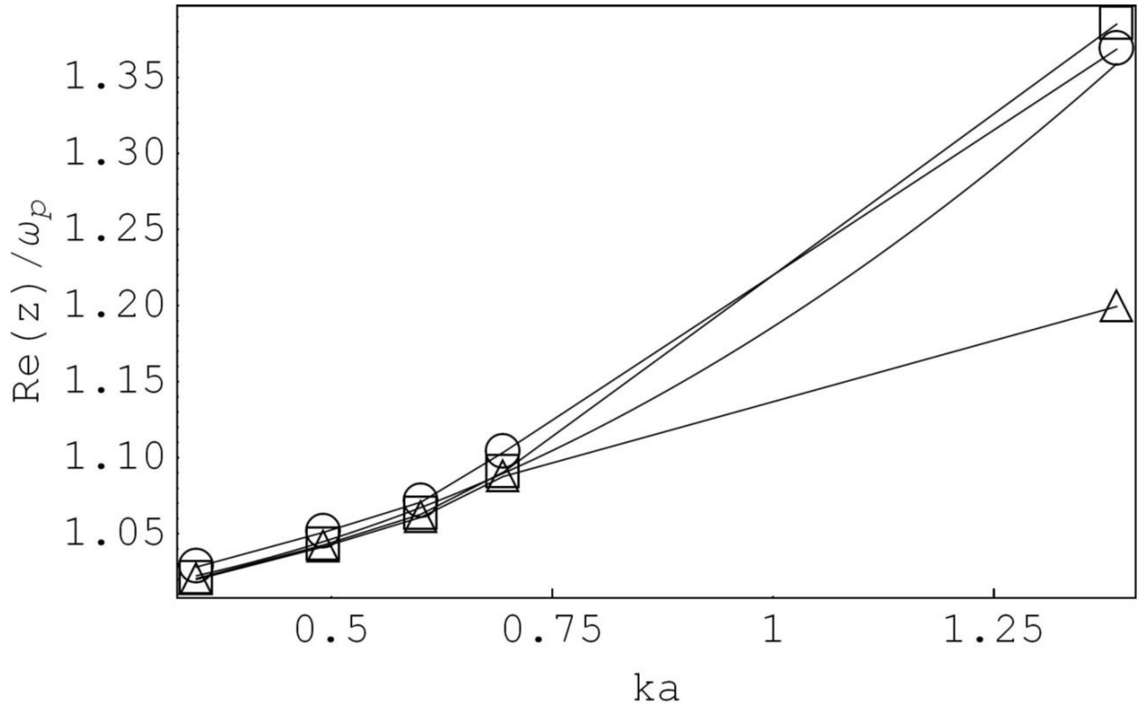
represent the positions of the maxima of the DSF

stand for the solutions of the dispersion equation (1.55)

correspond to $\omega_2(k)/\omega_p$

calculated by the interpolation formulas of [33]

Figure 1.7 – The plasmon dispersion relation, i.e., the real part of the solution of the dispersion equation (1.55) vs. ka at Γ = 1.



△ represent the positions of the maxima of the DSF

□ stand for the solutions of the dispersion equation (1.55)

○ correspond to $\omega_2(k)/\omega_p$

— calculated by the interpolation formulas of [33]

Figure 1.8 – The plasmon dispersion relation, i.e., the real part of the solution of the dispersion equation (1.55) vs. ka at Γ = 2.

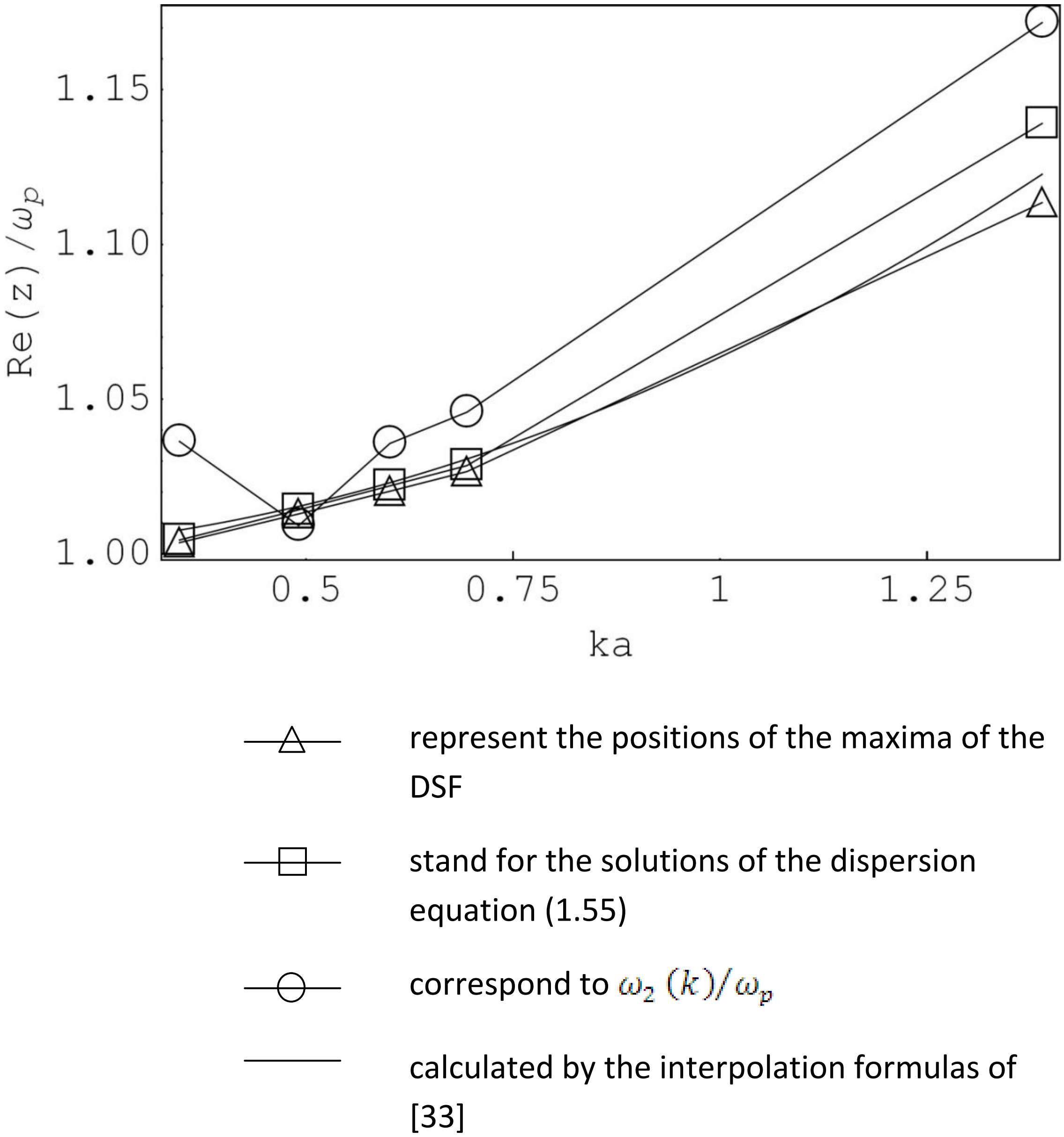
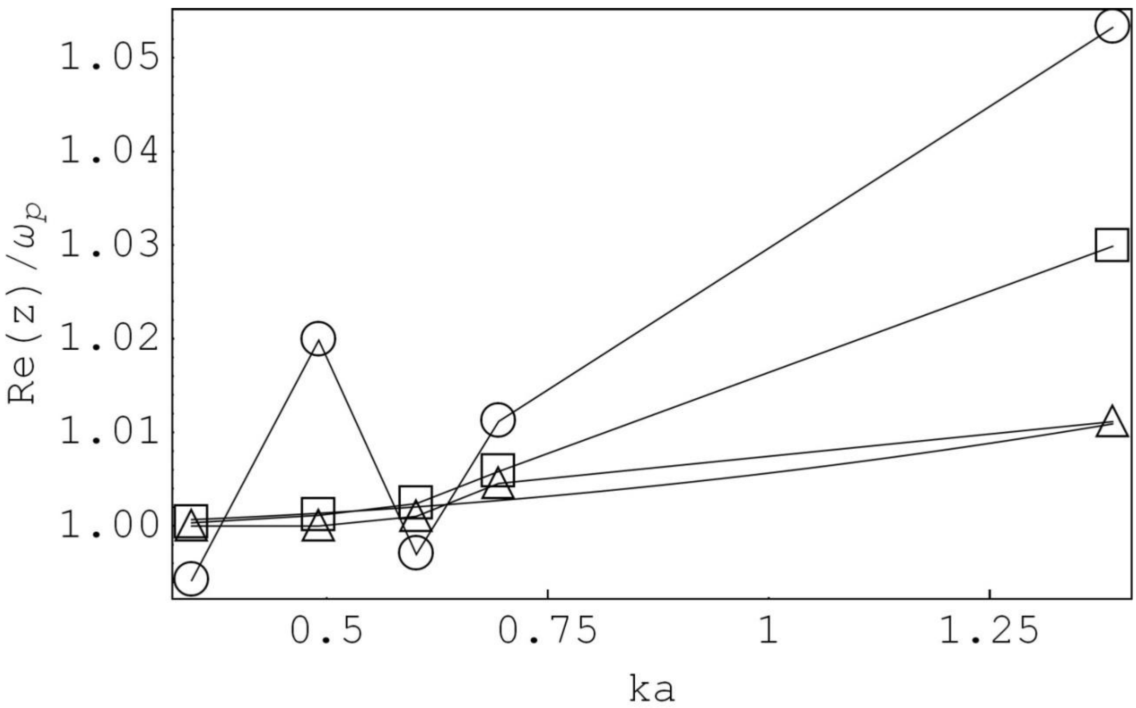


Figure 1.9 – The plasmon dispersion relation, i.e., the real part of the solution of the dispersion equation (1.55) vs. ka at Γ = 4.



△ represent the positions of the maxima of the DSF

□ stand for the solutions of the dispersion equation (1.55)

○ correspond to $\omega_2(k)/\omega_p$

— calculated by the interpolation formulas of [33]

Figure 1.10 – The plasmon dispersion relation, i.e., the real part of the solution of the dispersion equation (1.55) vs. ka at Γ = 8.

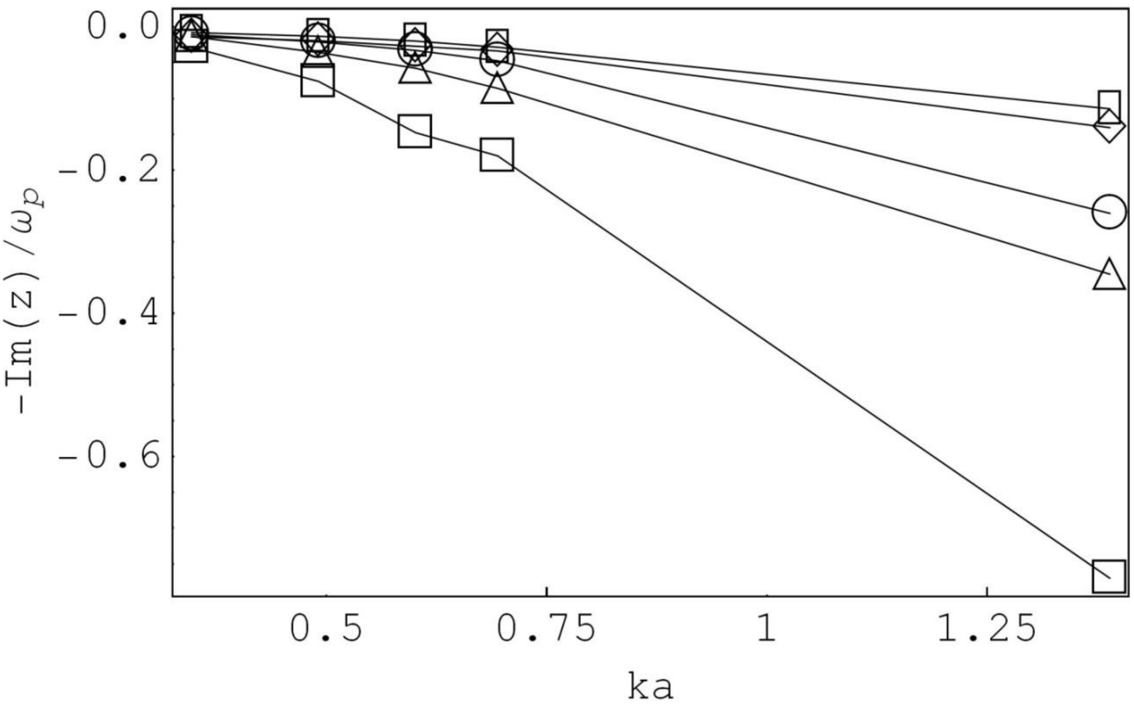


Figure 1.11 – The plasmon mode damping decrement, i.e., the imaginary part of the solution of the dispersion equation (1.55) vs. ka for Γ = 0.5 (squares), Γ = 1.0 (triangles), Γ = 2.0 (circles), Γ = 4.0 (diamonds), and Γ = 8.0 (rectangles).

Notice that alternative approaches like the QLCA or the continued-fraction method do not predict the damping of the plasmon modes.

2 APPLICATION OF THE CLASSICAL METHOD OF MOMENTS TO THE INVESTIGATION OF DYNAMICAL PROPERTIES OF A PHYSICAL SYSTEM

2.1 Nevanlinna parameter function

In contrast to one component plasma, a two-component plasma is described by two parameters: the dimensionless coupling parameter mentioned above and the dimensionless density parameter,

$$r_s = \frac{a}{a_0} = \frac{ame^2}{\hbar^2}, \tag{2.1}$$

where a_0 is the Bohr radius.

The Deutsch pseudopotential is taken as an interaction potential, which is finite at small interparticle distances because of the diffraction effects and coincides with the Coulomb potential at large distances,

$$\varphi_{ab}(r) = Z_a Z_b \frac{e^2}{r}\left[1 - exp\left(-\frac{r}{\lambda_{ab}}\right)\right], \quad a, b = e, i, \tag{2.2}$$

$$\lambda_{ab} = \sqrt{\frac{\beta\hbar^2}{2\pi\mu_{ab}}}, \qquad \mu_{ab} = (m_a^{-1} + m_b^{-1})^{-1},$$

where μ_{ab} is the reduced mass of an *a*-*b* pair, m_a designates the species *a* mass, and $\hbar$ $\hbar$ is the Planck constant. The fact that the potentials (2.2) remain finite as $r \to 0$, is a consequence of the uncertainty principle and prevents the Coulomb collapse. In the temperature range of interest $a \gg \lambda_{ii}$, with a being the "ion-sphere" radius. Thus the effective ion-ion interaction is virtually identical to the bare Coulomb one at all separations.

Static correlation functions that are used to compute the dynamic characteristics of two-component plasmas are calculated by the method of hypernetted chain equations [34]. Precisely, the pair correlation function,

$$h_{ab}(r) = g_{ab}(r) - 1 \tag{2.3}$$

can be derived from the direct correlation function $c_{ab}(r)$ by Ornstein-Zernicke relation [34],

$$h_{ab}(r) = c_{ab}(r) + \sum_d n_d \int d\boldsymbol{r}' h_{ad}(|\boldsymbol{r} - \boldsymbol{r}'|)\, c_{db}(r'). \tag{2.4}$$

On the other hand, the radial distribution function is

$$g_{ab}(r) = exp[-\beta\varphi_{ab}(r) + h_{ab}(r) - c_{ab}(r)]. \quad (2.5)$$

Equations (2.3) – (2.5) form a closed loop set of equations and can be solved numerically to required precision.

Below the scheme is presented for calculation of dynamic structure factor on the basis of the method of moments. The power moments are

$$C_0(k) = \frac{k_D^2}{k^2} S_{zz}(k), \quad (2.6)$$

$$C_2(k) = \omega_p^2, \quad (2.7)$$

$$C_4(k) = \omega_p^4[1 + W(k)]. \quad (2.8)$$

Notice that the moment $C_0(k)$ is expressed, by virtue of the FDT, in terms of the static structure factors, the second moment is actually the f-sum rule, and does not depend on interactions in the system. The fourth moment contains various contributions:

$$W(k) = K(k) + U(k) + H. \qquad (2.9)$$

The first contribution proceeds from the kinetic term of the system Hamiltonian. In a classical limit it coincides with the Vlasov term in the dispersion equation:

$$K(k) = 3\frac{k^2}{k_D^2}. \qquad (2.10)$$

In our case it has the following form [35]:

$$K(k) = 3\frac{k^2}{k_D^2} + \sqrt{\frac{\pi}{18}}\frac{\lambda_T^3}{\lambda_L}k^2 + \frac{\lambda_T^2 k^4}{2k_D^2}, \qquad (2.11)$$

including both thermal and quantal contributions.

The last two terms in the fourth moment follow from contributions that are responsible for interaction in the system Hamiltonian and, therefore, depend on the interaction potential used,

$$U(k) = \frac{1}{2\pi^2 n}\int_0^\infty p^2 (S_{ee}(p) - 1) f(p,k) dp, \tag{2.12}$$

$$H = \frac{k_{ei}^2}{6\pi^2 n}\int_0^\infty \frac{p^2 S_{ei}(p)}{p^2 + k_{ei}^2} dp, \tag{2.13}$$

where

$$f(\mathrm{p},\mathrm{k}) = \frac{\mathrm{k}_{\mathrm{ee}}^2}{4\mathrm{k}^2} + \frac{(\mathrm{k}^2 - \mathrm{p}^2)^2}{8\mathrm{pk}^3}\ln\left|\frac{\mathrm{p}+\mathrm{k}}{\mathrm{p}-\mathrm{k}}\right| - $$
$$- \frac{(\mathrm{p}^2 - \mathrm{k}_{\mathrm{ee}}^2 - \mathrm{k}^2)^2}{16\mathrm{pk}^3}\ln\frac{(\mathrm{p}+\mathrm{k})^2 + \mathrm{k}_{\mathrm{ee}}^2}{(\mathrm{p}-\mathrm{k})^2 + \mathrm{k}_{\mathrm{ee}}^2} - \frac{\mathrm{k}_{\mathrm{ee}}^2/3}{\mathrm{p}^2 + \mathrm{k}_{\mathrm{ee}}^2}. \tag{2.14}$$

Consider the following characteristic frequencies,

$$\omega_1(k) = \sqrt{\frac{C_2}{C_1}}, \tag{2.15}$$

$$\omega_2(k) = \sqrt{\frac{C_4}{C_2}}. \tag{2.16}$$

These frequencies were estimated by the method of hypernetted chain equations.

To specify the Nevanlinna parameter function $Q(k,z)$ and, hence, the non-canonical solution given by the Nevanlinna formula for the IDF,

$$\epsilon^{-1}(k,z) = 1 + \frac{\omega_p^2 (z+Q)}{z(z-\omega_2^2) + Q(z-\omega_1^2)}, \tag{2.17}$$

we have to reconsider the details of energy absorption in the system without violating the sum rules.

Precisely, we might try to satisfy the well-known Perel'-Eliashberg classical asymptotic relation for the imaginary part of the dielectric function. The latter result can be summarized in the following way.

In a completely ionized plasma for $\omega \gg (\beta\hbar)^{-1}$, 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 [36], this circumstance permits to use the detailed equilibrium principle to express the imaginary part of the dielectric function, $\mathrm{Im}\epsilon(k,\omega)$ of a completely ionized plasma in terms of the bremsstrahlung cross section and leads to the following asymptotic form of $\mathrm{Im}\epsilon(k,\omega)$ in a completely ionized (for simplicity, hydrogen-like) plasma obtained by Perel' and Eliashberg in [21] and amended later in [37, 38]:

$$\mathrm{Im}\epsilon(k,\omega \gg (\beta\hbar)^{-1}) \cong \frac{4\pi A}{\omega^{9/2}}\left(1-\frac{\omega_T}{\omega}\right), \tag{2.18}$$

$$B(k) = \frac{4\pi A}{\omega_p^2(\omega_2^2-\omega_1^2)},$$

where

$$A = \frac{2^{5/2}\pi}{3} n_e n_i \frac{Z^2 e^6}{(\hbar m_e)^{3/2}}, \qquad n_i = Z n_e, \quad \omega_T = \frac{3}{4\beta\hbar}. \tag{2.19}$$

This result also implies that higher even order frequency moments, $C_{2v}(k)$, $v \geq 3$, diverge.

To take into account all convergent sum rules (power frequency moments) and the exact asymptotic relation [21] we apply the Nevanlinna formula with the following model expression for the Nevanlinna parameter function on the real axis [39]:

$$Q(k,\omega) = B(k)\sqrt{|\omega|}\left(\frac{\omega}{|\omega|} + i\right) - \frac{h(k)\omega_p}{\omega + i\omega_p} \equiv \tag{2.20}$$

$$\equiv Q_1(k,\omega) + iQ_2(k,\omega).$$

where

$$B(k) = \frac{4\pi A}{\omega_p^2(\omega_2^2 - \omega_1^2)}. \tag{2.21}$$

2.2 Dynamic structure factors

Using the Nevanlinna parameter function $Q(\mathrm{k},z)$ of (2.20), one can calculate the dynamic structure factor,

$$S_{zz}(k,\omega) = \frac{\omega_p^2}{\pi\beta\varphi(k)} \frac{[\omega_2^2(k) - \omega_1^2(k)]Q_2(k,\omega)}{|\omega[\omega^2 - \omega_2^2(k)] + Q(k,\omega)[\omega^2 - \omega_1^2(k)]|^2}, \tag{2.22}$$

with $\varphi(k) = 4\pi e^2/k^2$.

The accuracy of obtained results is checked by the sum rules,

$$S_v(k) = \frac{1}{n\omega_p^v} \int_{-\infty}^{\infty} \omega^v S_{zz}(k,\omega) d\omega. \tag{2.23}$$

Particularly, for v = 0,

$$S(k) = \frac{1}{n} \int_{-\infty}^{\infty} S_{zz}(k,\omega) d\omega. \tag{2.24}$$

The results on the charge-charge dynamic structure factor are presented in Figures 2.1-2.4 below. In the figures we can see that the obtained results for dynamic structure factors, that were calculated via the static values from NHC scheme and using the method of moments with dynamic Nevanlinna function, agree with corresponding MD data of [40] quantitatively and in figure 2.2 qualitatively. It is also seen that the DSF calculated using classical expression for kinetic term (2.10) agrees better with the experimental data than when the quantal case (2.11) is used. And finally we observe that the asymptotic tales of the modeled points of [40] cross the calculated ones but in some case they do not, as in figure 2.2.

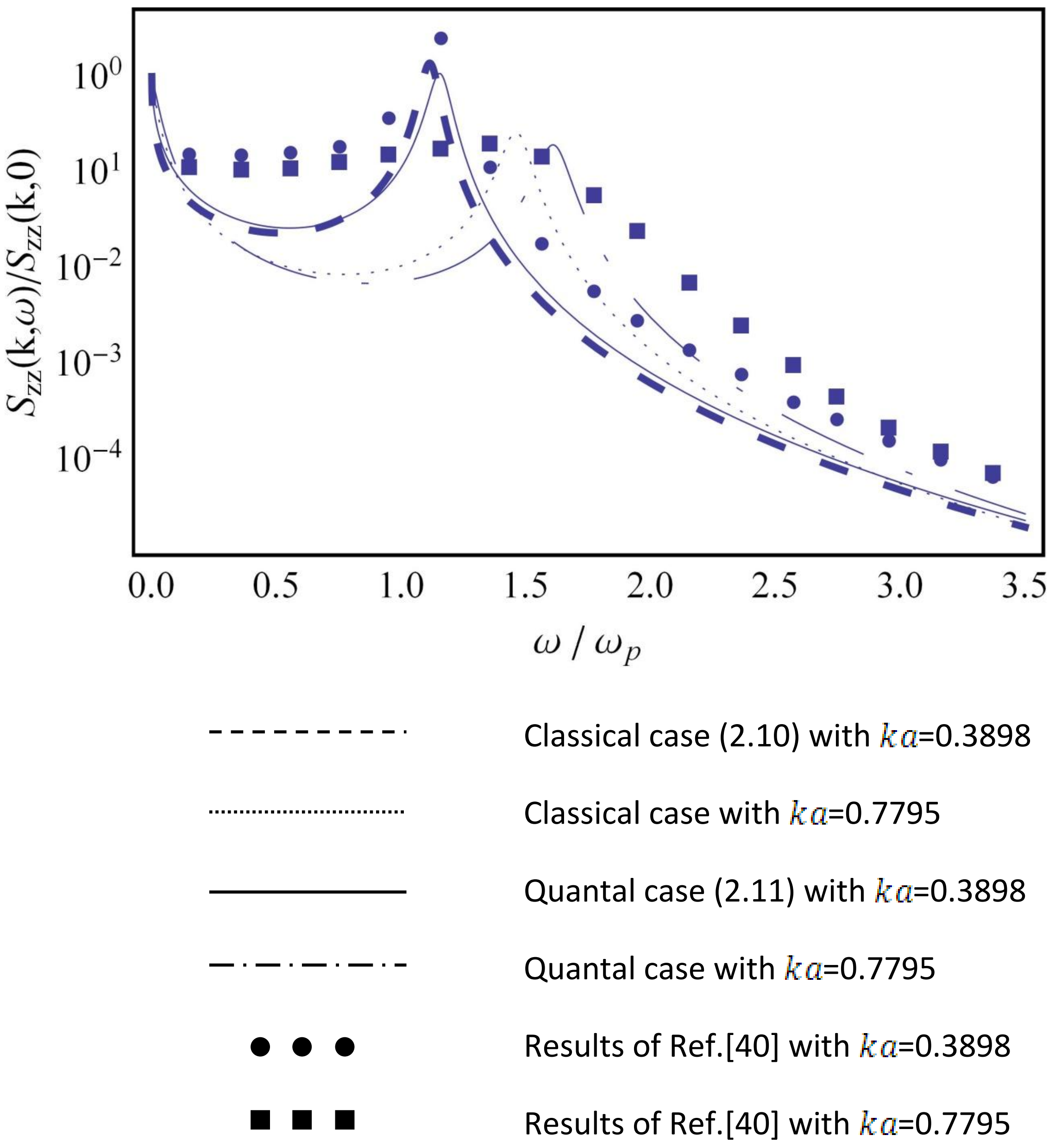


Figure 2.1 – Normalized charge-charge dynamic structure factor vs. frequency at Γ = 0.5 and λ_{ep} = 0.4.

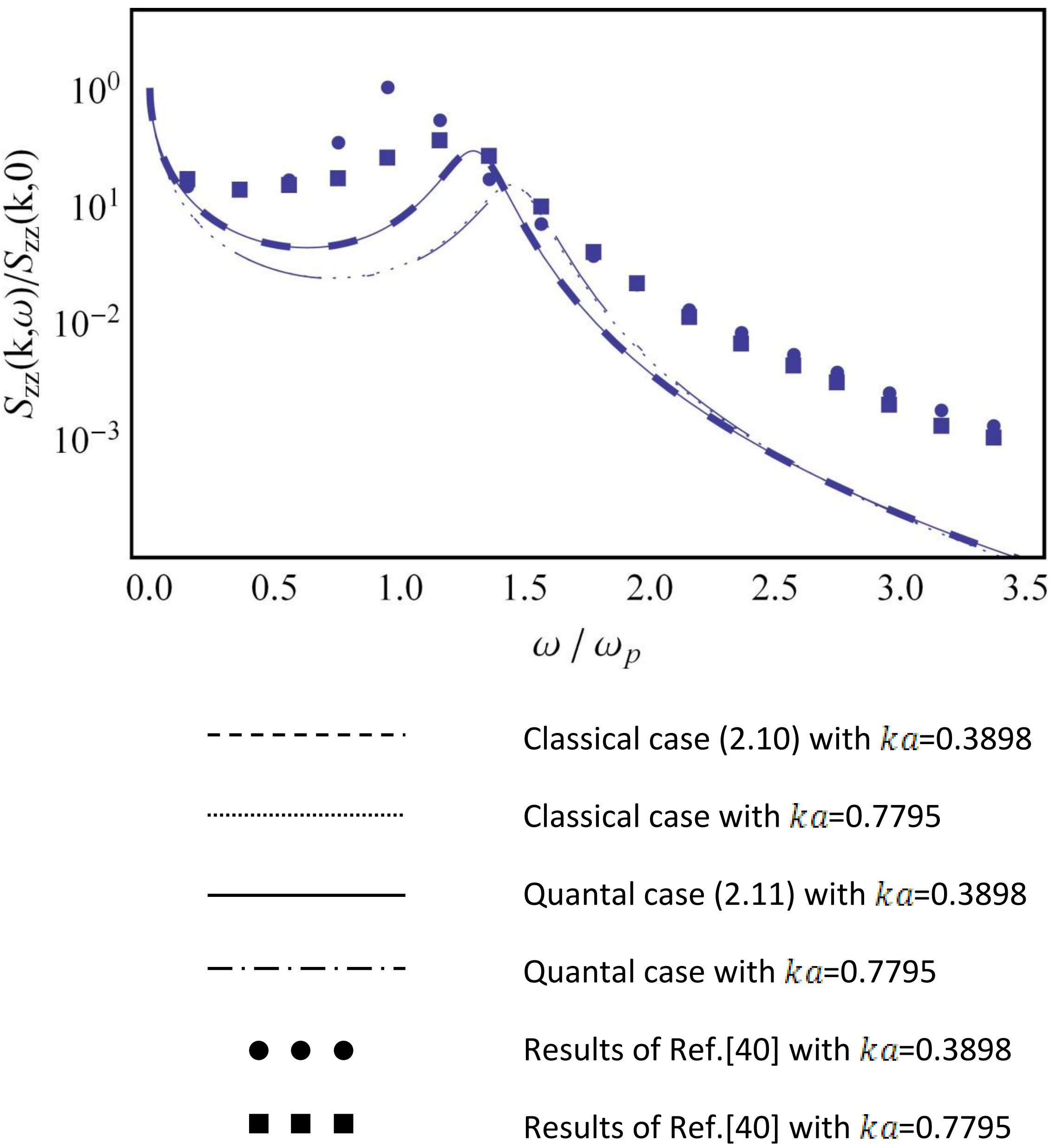


Figure 2.2 – Normalized charge-charge dynamic structure factor vs. frequency at $\Gamma = 1$ and $\lambda_{ep} = 0.2$.

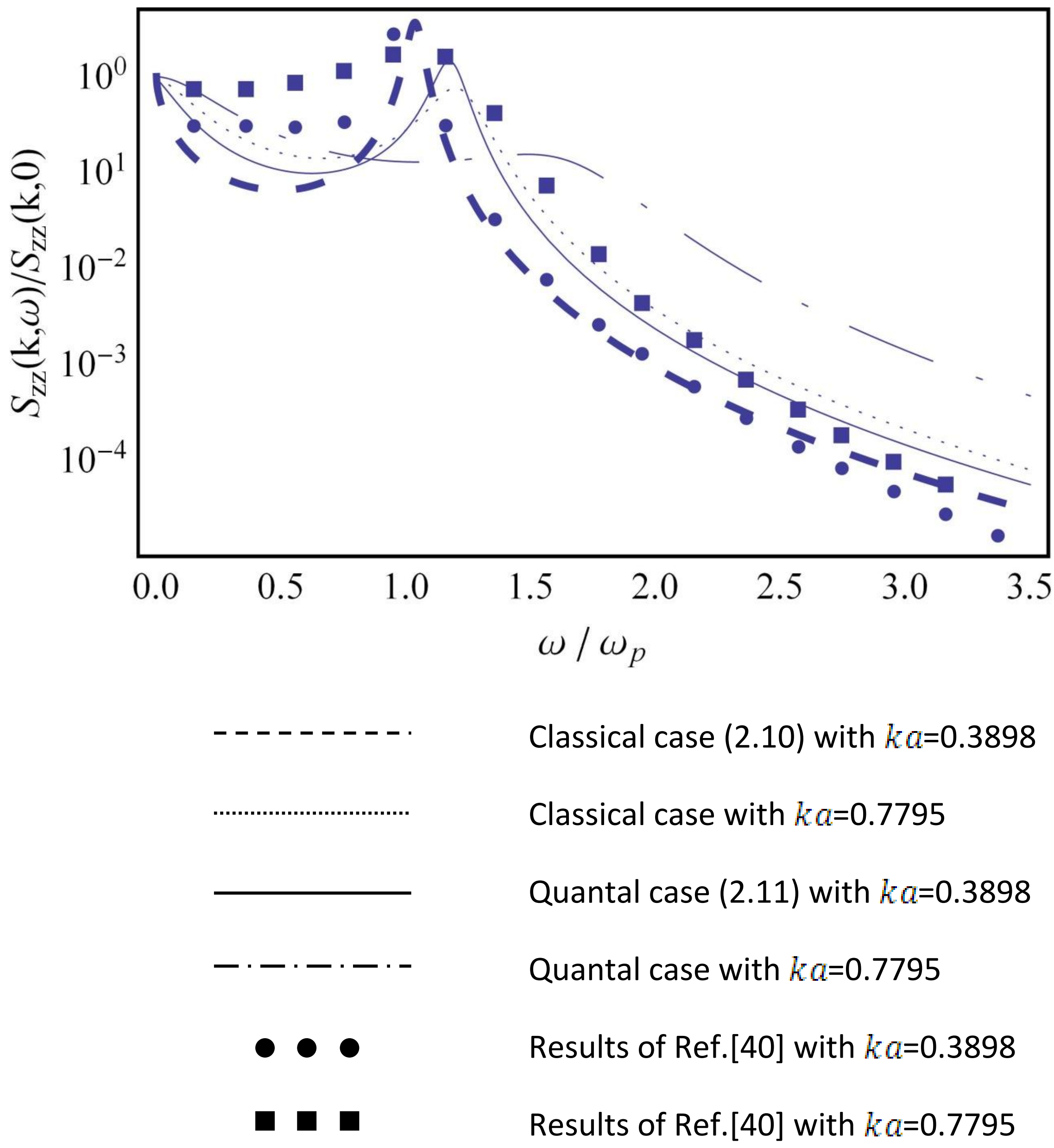
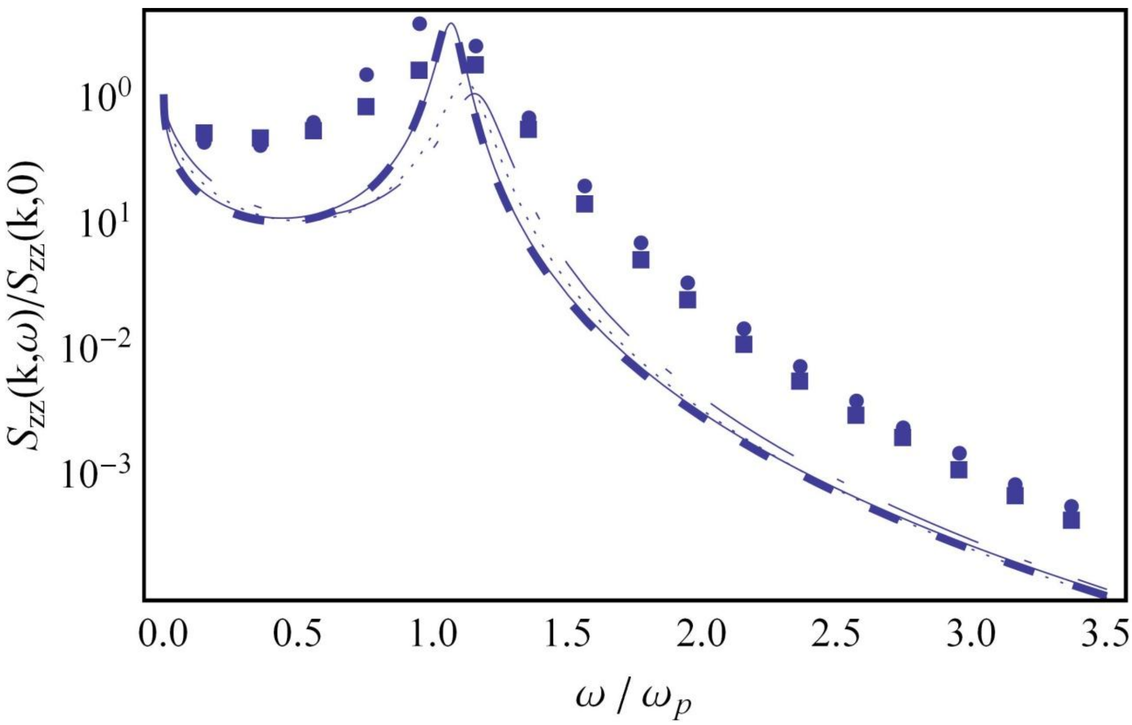


Figure 2.3 – Normalized charge-charge dynamic structure factor vs. frequency at Γ = 1 and λ_{ep} = 0.8.



Classical case (2.10) with ka=0.3898

Classical case with ka=0.7795

Quantal case (2.11) with ka=0.3898

Quantal case with ka=0.7795

Results of Ref.[40] with ka=0.3898

Results of Ref.[40] with ka=0.7795

Figure 2.4 – Normalized charge-charge dynamic structure factor vs. frequency at Γ = 2 and λ_{ep} = 0.4.

3 SOME ADDITIONAL RESULTS

3.1 Non-monotonic behavior of the dynamic conductivity of hydrogen and aluminum plasmas

External conductivity [41]

To characterize the optical properties of plasmas one should, in the first place, distinguish the long wavelength limiting values $(k \to 0)$ of the external $\sigma^{\mathrm{ext}}(\mathrm{k}, \omega)$ and internal $\sigma^{\mathrm{int}}(\mathrm{k}, \omega)$ conductivities, the former being a genuine response (Nevanlinna) function describing the system reaction to the external, not the Maxwellian harmonic field [19, 37, 38].

If a certain number of frequency power moments of the real part of the external conductivity is known, then the Riesz-Herglotz representation [5, 42] can be generalized in such a way that $\sigma^{ext}(\omega) \equiv \sigma^{int}(0, \omega)$ becomes a fractional-linear transformation of the Cauchy-type integrals. This new representation is obtained here on the basis of the Nevanlinna formula of the classical theory of moments.

Consider the even function [38],

$$\eta(\omega) = \mathrm{Re}\sigma^{ext}(\omega)/\omega^2. \tag{3.1}$$

Additional information on this function is contained in the "negative" sum rule [19],

$$C_0 = \int_{-\infty}^{\infty} \eta(\omega) d\omega = \frac{1}{4}, \quad (3.2)$$

and the second

$$C_2 = \int_{-\infty}^{\infty} \omega^2 \eta(\omega) d\omega = \frac{\omega_p^2}{4}, \quad (3.3)$$

and the fourth order

$$C_4 = \int_{-\infty}^{\infty} \omega^4 \eta(\omega) d\omega = \frac{\omega_p^2}{4} \left(\Omega^2 + \omega_p^2 \right), \quad (3.4)$$

frequency moments, $\omega_p = \sqrt{4\pi n_e e^2 / m}$ being the plasma frequency; the odd order moments are all equal to zero, higher even order moments diverge. An explicit expression for the frequency Ω is related to static correlations in a plasma, and is model-dependent [37, 38, 42]. In particular, it was shown [37] that in a completely ionized hydrogen-like plasma, the moment (3.4) depends on the probability to encounter an electron and an ion at the same spatial point:

$$\Omega^2 = \frac{\omega_p^2}{3}\left(g_{ei}(0) - 1\right) \equiv \omega_p^2 H. \tag{3.5}$$

The parameter H was first evaluated in the modified RPA in [37], this result was recently generalized in [43]:

$$H = \frac{4}{3} Z r_s \sqrt{\Gamma}\left[3Z\Gamma^2 + 4r_s + 4\Gamma\sqrt{3(1+Z)r_s}\right]^{-1/2}. \tag{3.6}$$

The truncated Hamburger moment problem [18] consists in the construction of a Nevanlinna class function, i.e., a function with a positive imaginary part which is analytic in the closed upper half-plane $\mathrm{Im}z \geq 0$, by its first $2n$ +1 power moments. In our case $n \leq 2$.

Introduce the set of orthonormalized polynomials $\{D_v(\omega)\}$, v=0,1,…,2n, over the measure $\eta(\omega)$:

$$\int_{-\infty}^{\infty} D_v(\omega) D_\mu(\omega) \eta(\omega) d\omega = \delta_{v\mu}\,, \quad v, \mu = 0,1,\ldots,2n. \tag{3.7}$$

These polynomials and their conjugate counterparts,

$$\varepsilon_v(\omega) = \lim_{\eta \downarrow 0} \int_{-\infty}^{\infty} \frac{D_v(\omega') - D_\mu(z)}{\omega' - \omega - i\eta} \eta(\omega) d\omega, \quad v = 0,1, \dots, 2n, \tag{3.8}$$

are determined in the process of the Gramm-Schmidt orthogonalization procedure of the first five elements of the canonical basis $\{1, \omega, \omega^2, \dots\}$.

Let M_n be the set of all non-decreasing functions of bounded variation $s(\omega)$, such that

$$\int_{-\infty}^{\infty} \omega^v s(\omega) d\omega = \int_{-\infty}^{\infty} \omega^v \eta(\omega) d\omega = C_v, \quad v = 0,1, \dots, 2n. \tag{3.9}$$

The Nevanlinna theorem [44], see also [45], states that there exists a one-to-one correspondence between the set M_n of all solutions of the moment problem and the Nevanlinna functions $q(z)$, $\mathrm{Im} z \geq 0$ with the following additional property:

$$\lim_{z \to \infty} \frac{q(z)}{z} = 0, \quad \mathrm{Im} z > 0, \tag{3.10}$$

the Riesz-Herglotz representation for these functions $q(z)$ is simplified into

$$q(z) = \int_{-\infty}^{\infty} \frac{dg(\omega)}{\omega - z}, \tag{3.11}$$

with $g(\omega)$ being a non-decreasing function such that

$$\int_{-\infty}^{\infty} \frac{dg(\omega)}{\omega_0^2 + \omega^2} < \infty, \quad \omega_0^2 > 0. \tag{3.12}$$

This correspondence is established by the Nevanlinna formula,

$$\int_{-\infty}^{\infty} \frac{ds(\omega)}{z - \omega} = \frac{\varepsilon_{v+1}(z) + q(z)\varepsilon_v(z)}{D_{v+1}(z) + q(z)D_v(z)}. \tag{3.13}$$

In particular, among the functions (3.11) there is a unique function $q(\omega)$ which, for a given v, would yield:

$$\int_{-\infty}^{\infty} \frac{\eta(\omega)d\omega}{z-\omega} = \frac{\varepsilon_{v+1}(z) + \tilde{q}(z)\varepsilon_v(z)}{D_{v+1}(z) + \tilde{q}(z)D_v(z)}. \tag{3.14}$$

Hence, for the external electrical conductivity (at k = 0) we have:

$$\sigma^{ext}(z) = \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{Re\sigma^{ext}(\omega)}{z-\omega}d\omega = \frac{z}{4\pi i} + \frac{iz^2}{\pi}\frac{\varepsilon_3 + \widetilde{q_2}\varepsilon_2}{D_3 + \widetilde{q_2}D_2}. \tag{3.15}$$

In what follows, instead of the orthonormalized polynomials $\{D_v\}$ and $\{\varepsilon_v\}$ it turns out more convenient to use the polynomials $\{D_v\}$ and $\{\varepsilon_v\}$ by normalizing their higher order coefficients to unity or C_0, respectively. Their employment in the Nevanlinna formula (3.15) is equivalent to the multiplication of an unknown parameter function $\tilde{q}$ by a positive factor. These polynomials,

$$D_0(z) = 1, \quad D_1(z) = z, \quad D_2(z) = z^2 - \omega_1^2$$

$$D_3(z) = z^3 - z\omega_2^2, \quad E_0(z) \equiv 0, \quad E_1(z) = c_0, \tag{3.16}$$

$$E_2(z) = c_0 z, \quad E_3(z) = c_0(z^2 - \omega_2^2 + \omega_1^2)$$

satisfy the Christoffel identity [5, 6],

$$E_3 D_2 - D_3 E_2 = \frac{C_4 - C_2^2}{C_0} \geq 0, \tag{3.17}$$

their zeros are all real and alternate [5].

We have put in (3.16):

$$\omega_1^2 = \frac{C_2}{C_0} = \omega_p^2, \quad \omega_2^2 = \frac{C_4}{C_2} = \Omega^2 + \omega_p^2. \tag{3.18}$$

Thus (3.15) can be reduced to

$$\sigma^{ext}(z) = \frac{iz}{4\pi} \frac{\omega_p^2 \big(z + q(z)\big)}{z(z^2 - \omega_2^2) + q(z)(z^2 - \omega_1^2)}. \tag{3.19}$$

The asymptotic expansion of (3.19) as $z \to \infty$ in the upper half-plane is determined by the moments,

$$\sigma^{ext}(z \to \infty) \cong \frac{i\omega_p^2}{4\pi z} + \frac{i\omega_p^2 \omega_2^2}{4\pi z^3} + \cdots, \quad \mathrm{Im} z > 0, \tag{3.20}$$

independently of the specific form of the Nevanlinna parameter function $q(z)$, though that of the l.h.s. of (3.14) is simply

$$\int_{-\infty}^{\infty} \frac{\eta(\omega)d\omega}{z-\omega} \cong \frac{C_0}{z} + \frac{C_2}{z^3} + \frac{C_4}{z^5} + \cdots, \qquad z \to \infty, \qquad \mathrm{Im} z > 0. \tag{3.21}$$

Internal conductivity

The internal and external conductivities are closely related by the expression

$$\sigma^{int}(z) = \frac{\sigma^{ext}(z)}{1 - \frac{4\pi i}{z}\sigma^{ext}(z)}. \tag{3.22}$$

In particular, if $\sigma^{ext}(z)$ is given by formula (3.19), then

$$\sigma^{int}(z) = \frac{i}{4\pi} \frac{\omega_p^2\big(z + q(z)\big)}{z^2 - \Omega^2 + zq(z)}. \tag{3.23}$$

Due to the causality principle and the parity of $\mathrm{Re}\sigma^{ext}(\omega)$ [37], the function $\sigma^{int}(z)$ is analytic in the upper closed half-plane $\mathrm{Im}z > 0$. Provided the static conductivity,

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

is finite and

$$\sigma^{int}(z\to\infty) \cong \frac{i\omega_p^2}{4\pi z} + \frac{i\omega_p^2\Omega^2}{4\pi z^3} + \cdots \tag{3.24}$$

in the open upper half-plane $\mathrm{Im}z > 0$. According to the Akhiezer theorem [6], this is equivalent to say that the non-negative, even function $\mathrm{Re}\sigma(\omega)$ possesses two non-zero, convergent power moments [19, 37]:

$$m_0 = \int_{-\infty}^{\infty} \mathrm{Re}\sigma^{int}(\omega)d\omega = \frac{\omega_p^2}{4}, \tag{3.25}$$

$$m_2 = \int_{-\infty}^{\infty} \omega^2\mathrm{Re}\sigma^{int}(\omega)d\omega = \frac{\omega_p^2\Omega^2}{4}. \tag{3.26}$$

Monotonicity

Though the power moments are only integral characteristics of the system, knowledge of even a finite number of them can provide the possibility to make meaningful conclusions on the local properties of the response function in question.

As an example, consider a non-monotonous behavior of the internal conductivity. Intervals of negative differential conductivity can be observed on the Ohm-second characteristics of dense plasmas both in computer simulations and theory.

The stereotype opinion about a monotonous decrease of $\mathrm{Re}\sigma^{int}(\omega)$ at $\omega \to \infty$ is based on the Drude-Lorentz approximation,

$$\mathrm{Re}\sigma^{int}(\omega) \approx \frac{\sigma_0}{1+(\omega\tau)^2}, \tag{3.27}$$

(with $\tau = 4\pi\sigma_0/\omega_p^2$) which is well justified for many metals up to the ionic excitation frequency.

Suppose the static conductivity σ_0 and the values of the moments m_0 and m_2 are known. Then it is possible to prove the following general result with respect to the non-monotonicity of $\mathrm{Re}\sigma^{int}(\omega)$.

Given the static conductivity σ_0 and the moment m_0 and m_2, if the real part of the system internal conductivity $\mathrm{Re}\sigma^{int}(\omega)$ is a monotonously decreasing function of frequency, then

$$\sigma_0^2 \geq \frac{1}{12}\frac{m_0^3}{m^2} = \frac{\omega_p^4}{192\Omega^2} = \frac{\omega_p^2}{192H} = \frac{\omega_p^2}{64h_{ei}(0)}. \tag{3.28}$$

In classical plasmas with the Coulomb collapse, formally $h_{ei}(0) = \infty$ and inequality (3.28) is satisfied automatically. In a real hydrogen-like plasma, though, $0 < h_{ei}(0) < \infty$, and

$$\sigma_0 \geq \frac{\omega_p}{8\sqrt{h_{ei}(0)}}. \tag{3.29}$$

Violation of (3.28) implies the non-monotonicity of the function $\mathrm{Re}\sigma(0,\omega)$. In liquid metals with high static conductivity (3.28) is satisfied. In highly ionized non-ideal plasmas the static electrical conductivity might be smaller than the plasma frequency, so that the inequality (3.29) might be violated, and then $\mathrm{Re}\sigma(\omega)$. demonstrates a non-monotonous behavior.

Nevanlinna parameter function *q*

In general, there is no immediate phenomenological method in sight to determine the Nevanlinna parameter function $q(z)$. The simplest is to put it equal to zero, i.e. $q(z) = i0^+$. However, a direct relation between $q(z)$ and the conductivity or the dielectric function, permits to evaluate it in a somewhat more precise and physically interesting way. Presume that $q(z) = q(0) = \mathrm{i}h$ with $h > 0$. In order to determine the value of this positive parameter we can assume that $\sigma_0 > 0$ exists, together with the continuity of $\sigma(z)$ and $q(z)$ at $z = 0$, to get

$$h = \tau \Omega^2. \tag{3.30}$$

In this case, the long wavelength limit of the internal conductivity is of the form:

$$\sigma^{int}(z) = \frac{i\omega_p^2}{4\pi} \frac{z + i\tau\Omega^2}{z^2 - \Omega^2(1 - iz\tau)}. \tag{3.31}$$

Consider the properties of the long wavelength expression for the internal dynamic conductivity (3.31) on the real axis $z = \omega$ [37]. In the first place, by definition and construction,

$$\sigma_0 = \lim_{\eta \downarrow 0} \sigma^{int}(z = i\eta). \tag{3.32}$$

Secondly, if $\tau\Omega \leq \sqrt{2}$, the real part of (3.31) on the real axis,

$$\mathrm{Re}\sigma^{int}(\omega) = \frac{\sigma_0 \Omega^4}{(\omega^2 - \Omega^2)^2 + \omega^2 \tau^2 \Omega^4}, \tag{3.33}$$

possesses two symmetric maxima shifted to

$$\omega_{max} = \pm\Omega \sqrt{1 - \frac{\tau^2 \Omega^2}{2}}. \tag{3.34}$$

But if $\tau\Omega > \sqrt{2}$, (3.33) is a monotonous function similar to the real part of the Drude-Lorentz model conductivity.

To take into account all convergent sum rules (power frequency moments) and the exact asymptotic relation (2.18), we can apply the Nevanlinna theorem with the following model expression for the Nevanlinna parameter function on the real axis:

$$q(\omega) = B\sqrt{|\omega|}\left(\frac{\omega}{|\omega|} + i\right) + ih, \tag{3.35}$$

with

$$B = \frac{4\pi A}{\omega_p^2 \Omega^2}. \tag{3.36}$$

Notice that

$$B\sqrt{\omega_p} = \frac{\sqrt{2}}{3^{5/4}} \frac{r_s^{3/4} \omega_p^2}{\Omega^2}, \tag{3.37}$$

so that

$$\frac{q(\omega)}{\omega_p} = \frac{\sqrt{2}}{3^{5/4}} \frac{r_s^{3/4} \omega_p^2}{\Omega^2} \sqrt{\left|\frac{\omega}{\omega_p}\right| \left(\frac{\omega}{|\omega|} + i\right)} + ih. \tag{3.38}$$

Observe that this expression for the Nevanlinna parameter function, as above, also implies that higher even order frequency moments, m_{2j}, $j > 2$, diverge.

The application of this model extension for the Nevanlinna function was discussed for different systems in [46] and [4]. For further study of dynamic properties of cold plasmas in comparison with the simulation and experimental data, see [45].

Dynamic conductivity of model two-component plasmas

Two-component plasmas (TCPs) constitute the simplest model that simulates the physical properties of real plasmas. In particular, dense hydrogen plasmas $(Z = 1)$ were studied by molecular dynamics (MD) simulations of Hansen and McDonald [11]. Whereas in MD simulations charged particles are assumed to evolve according to the classical mechanics laws of motion, TCP statistical properties unravel its genuine quantum mechanical nature. In particular, the effects of quantum delocalization preventing the system collapse are accounted for by the employment of the Deutsch pair effective potential [47] which mimics quantum-diffraction effects,

$$\varphi_{ab}(r) = Z_a Z_b \frac{e^2}{r}\left(1 - exp(-k_{ab} r)\right), \quad a, b = e, i, \tag{3.39}$$

$$k_{ab} = \sqrt{\frac{2\pi\mu_{ab}}{\beta\hbar^2}}, \qquad \mu_{ab} = (m_a^{-1} + m_b^{-1})^{-1}, \tag{3.40}$$

where μ_{ab} is the reduced mass of an *a*-*b* pair and the exchange or symmetry contribution is excluded. Unlike the bare Coulomb potential, potential (3.39) remains finite at the origin $r \to 0$, as a consequence of the uncertainty principle. Once more, in the temperature range of interest $a \gg \lambda_{ii}$, a being the "ion-sphere" radius; hence the effective ion-ion interaction is virtually identical to the bare Coulomb at all separations.

The difference of the effective potential (3.39) from the bare Coulomb potential manifests itself in the value of the moment (3.26), which takes the form:

$$M_2 = \frac{\omega_p^2 \tilde{\Omega}^2}{4} = \frac{\omega_p^4}{4}\tilde{H} \tag{3.41}$$

with

$$\widetilde{H} = \frac{k_{ei}^2}{6\pi^2 n} \int_0^\infty \frac{p^2 S_{ei}(p)}{p^2 + k_{ei}^2} dp. \tag{3.42}$$

The model partial static structure factor $S_{ei}(k)$ was computed in [11], and more recently in [48], using the hypernetted-chain (HNC) approximation with the Deutsch effective potential. In Table we present our data on the interaction parameter $\widetilde{H}$ (Eq. (3.42)) as obtained in [48]. For the sake of completeness, in the same Table we reproduce the values (taken from [11]) of the relaxation time τ, which determines the plasma static conductivity.

Table 1 The static characteristics of the model plasma under the conditions of [11]: the relaxation time (Table III of [11]) and the parameter $\widetilde{H}$ calculated in the HNC approximation (see [48]).

Γ=0.5, r_s=0.4	Γ =0.5, r_s=1	Γ =2, r_s=1
$\tau\omega_p$ =45.239	$\tau\omega_p$ =27.018	$\tau\omega_p$ =13.823
$\widetilde{H}$=0.080265	$\widetilde{H}$=0.202421	$\widetilde{H}$=0.137148
$\tau\omega_p\sqrt{\widetilde{H}}$ =12.817	$\tau\omega_p\sqrt{\widetilde{H}}$ =12.156	$\tau\omega_p\sqrt{\widetilde{H}}$ =5.1191

Upon specification of the characteristic frequency Ω and the static conductivity, we need to choose the form of the Nevanlinna parameter function which closes the algorithm of calculation of the system dynamic conductivity up. For all three thermodynamic conditions studied here, we observe a very similar behavior of the conductivity for any of the two model functions $q(z)$ derived previously, i.e. either expression (3.35) or its static value. In fact, both can hardly be distinguished here from the known Drude-Lorentz model,

$$\sigma_{DL}(0,z) = \frac{\sigma_0}{1 - iz\tau}, \tag{3.43}$$

which indicates that the model plasma studied in [11] is a highly conducting non-ideal system. This metallic character can be further confirmed by checking that the condition (3.28) is very well satisfied for the values in Table 1. Similar results were obtained recently for real systems in [49].

The following Fig. 3.1 shows the dynamic conductivity (3.22) with q given by (3.35) compared to the Drude-Lorentz model (3.43). It is important to note that, although the latter seems to be applicable here, the dynamic conductivity model (3.22) is a generalization of the former, as it possesses a convergent second order power moment (3.26), which shows up in its asymptotic behavior. This additional convergent second order power moment is related to the satisfaction of the known third order frequency sum rule for the structure factor, which has been widely acknowledged to apply in completely ionized plasmas.

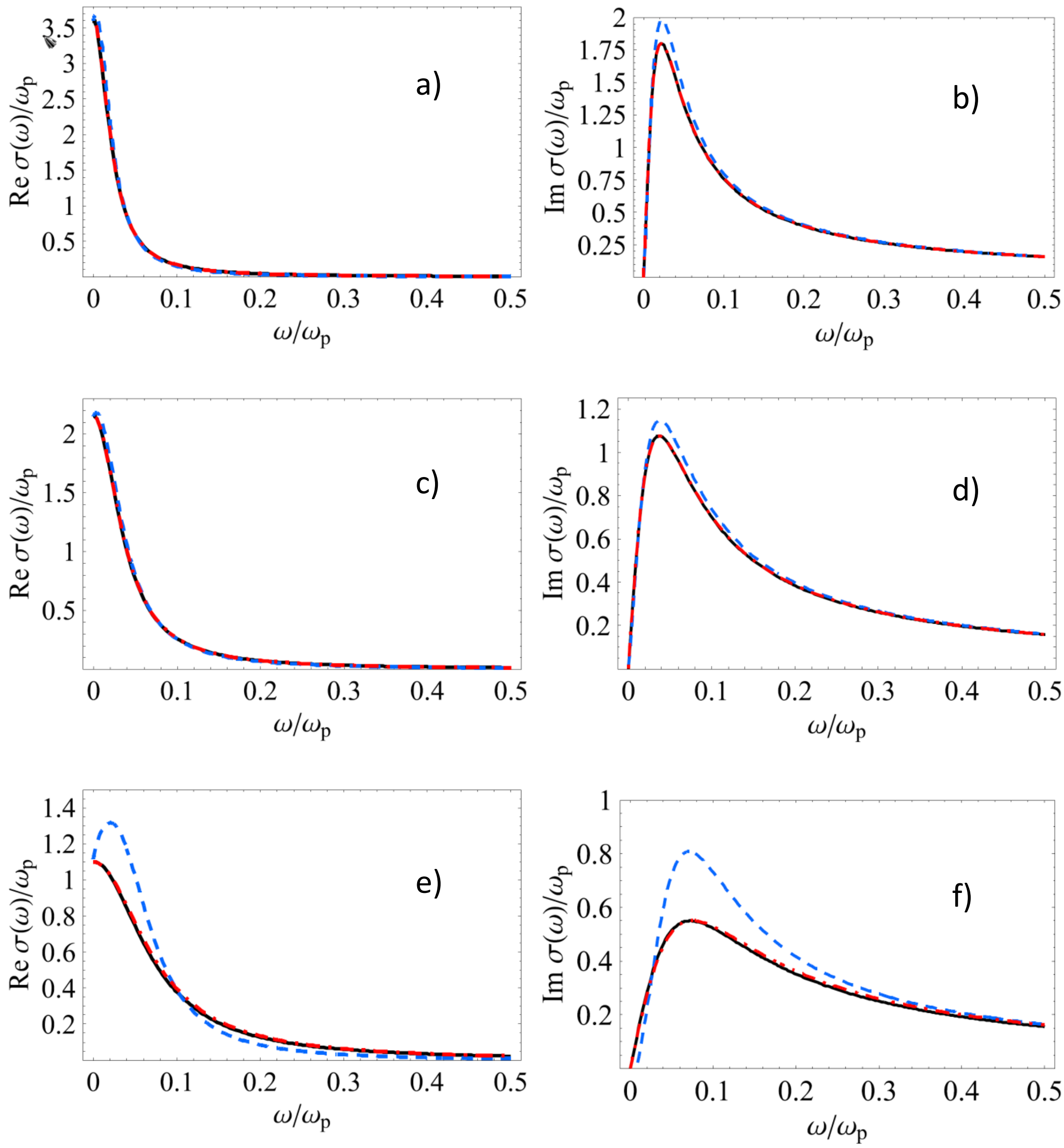


Figure 3.1 Real and imaginary parts of the internal dynamic conductivity for a TCP at the thermodynamic conditions simulated in [11]: (a) and (b) Γ =0.5, r_s=0.4; (c) and (d) Γ =0.5, r_s=1; (e) and (f) Γ =2, r_s=1. Three different models are used for σ: Drude-Lorentz formula (3.43) (solid line), two-moment model (3.23) with q given by (3.35) (dashed line), and its static value (dash-dot). The relevant parameters are taken from Table 1.

Dynamic conductivity of aluminum plasmas

More recently aluminum plasmas were studied by means of Quantum Molecular Dynamics simulations (QMD) in Ref. [45]. This simulation technique uses Density Functional Theory (DFT) to treat the electronic subsystem through the package VASP. The ionic subsystem is simulated by means of pseudopotential consistent with an assumed ionization model. Thus, the Kohn-Sham electronic wave functions and eigenenergies are computed for some fixed ionic configuration. Those results are then used as inputs for the Kubo-Greenwood formula, instead of the many-electron eigenstates [50]. This makes it possible to deal with partially ionized plasmas in an approximate manner.

Under those conditions, our two-moment model (3.23) is still applicable, but some comments are in order. First, as the f-sum rule is extended to the total electronic density, we cannot differentiate between electrons which are ’free’ or ’bound’, according to what it is obtained through this numerical approach. Second, we extend the validity of the existence of a third-frequency sum rule, although its value obviously depends on the properties of the system to be simulated. Then, for the reconstruction of the spectra obtained in Ref. [45], the values of the moments m_0 and m_2 are to be calculated from the computed spectra. In particular, we must understand here that the plasma frequency computed from the simulations is an effective one, accounting for the total electronic density.

We report in Table 2 the values of the quantity $192\sigma_0^2\omega_p^{-2}H$ for some of the thermodynamic conditions simulated in [51]. As we have seen, the monotonicity of $\sigma(\omega)$ implies (3.28) that this quantity should not be smaller than 1. We can identify that this inequality is violated when the density is 0.5 $\mathrm{g\cdot cm^{-3}}$, what allows us to predict the departure from the Drude-Lorentz model (3.43).

Table 2 Values of the quantity $192\sigma_0^2\omega_p^{-2}H$ for aluminum plasmas at different thermodynamic conditions, as obtained in [51] through the QMD simulations

	1.4 $\mathrm{g\cdot cm^{-3}}$	1.0 $\mathrm{g\cdot cm^{-3}}$	0.5 $\mathrm{g\cdot cm^{-3}}$
10 kK	3.88999	1.81524	0.27307
25 kK	3.12871	2.14840	0.63521

We can indeed confirm this prediction in Figure 3.2, where some of the simulation results of Ref. [51] for the dynamic conductivity are plotted. It is clear how the plasma goes from a highly conducting metallic phase at high densities, to the non-conducting one at lower densities.

In Figure 3.2 we also show our results on the dynamic conductivity obtained with $\sigma(z)$ as given by (3.31), which yields the best approximation to the simulation data here. We can clearly identify the maxima shown by this model at the values given by (3.34), which appear for $\tau\Omega \leq 2$. This is applicable for the cases with the density equal to 1.0 $\mathrm{g \cdot cm^{-3}}$ and 0.5 $\mathrm{g \cdot cm^{-3}}$.

Another parameterized model [52] for the dynamic conductivity was employed in [51] to describe these simulation results. The expression in [52] accounts for memory effects in the current-current autocorrelation function in a simplified manner. In fact, our model parameter Nevanlinna function $q(\omega)$ can be seen to play exactly this role [53]. Beyond the suitability of the different models to fit the simulation spectra at the given interval, there are important mathematical differences between our expression and the one of Ref. [52]. More particularly, the latter does not satisfy the convergent power moment m_2 in (4.26), just as the Drude-Lorentz model does, and, therefore, cannot lead to the correct asymptotic behavior in (3.24).

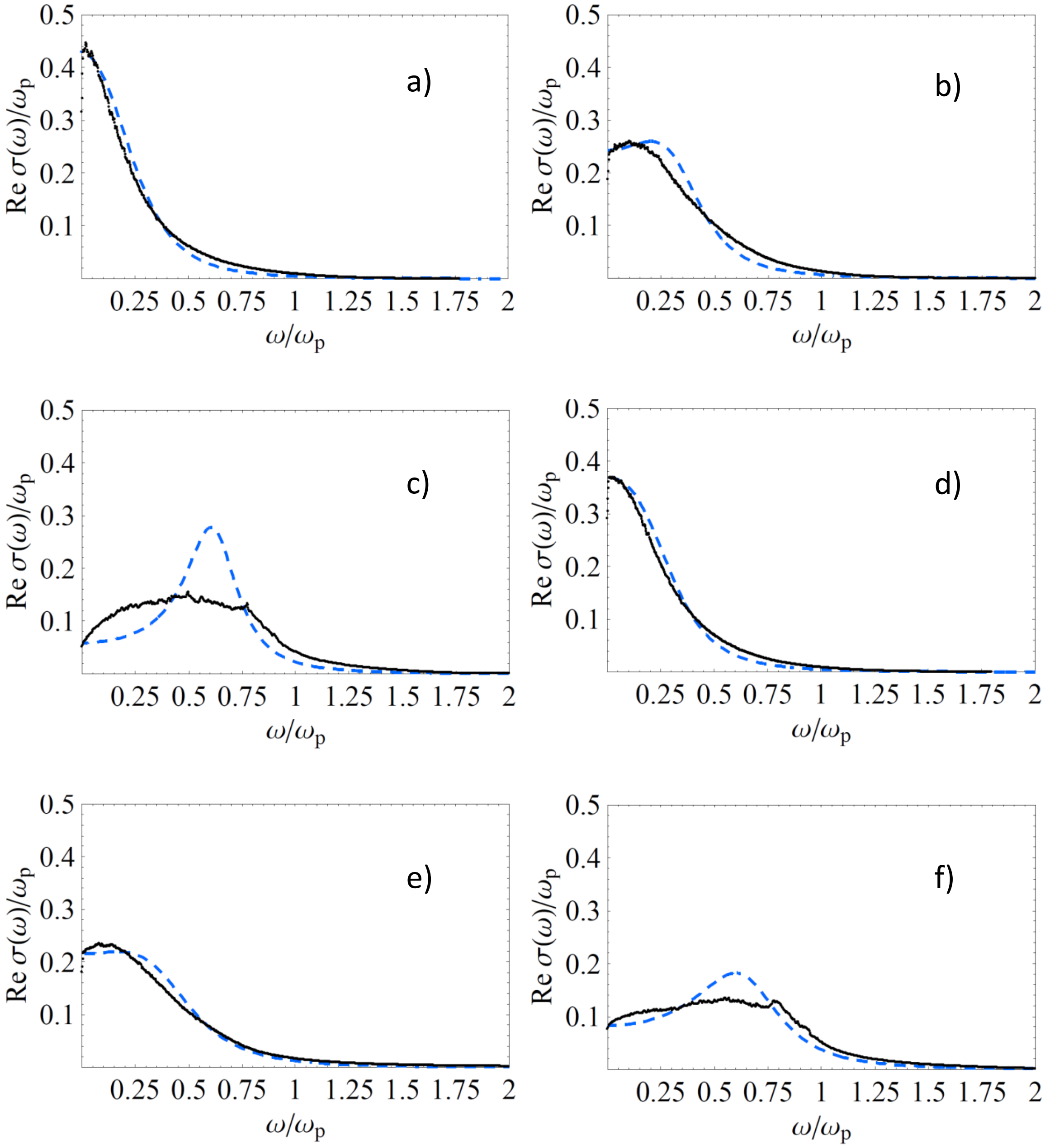


Figure 3.2 Real part of the internal dynamic conductivity for aluminum plasmas as simulated in Ref. [51]: (a) 10 kK, 1.4 $g \cdot cm^{-3}$; (b) 10 kK, 1.0 $g \cdot cm^{-3}$; (c) 10 kK, 0.5 $g \cdot cm^{-3}$; (d) 25 kK, 1.4 $g \cdot cm^{-3}$; (e) 25 kK, 1.0 $g \cdot cm^{-3}$; (f) 25 kK, 0.5 $g \cdot cm^{-3}$.

3.2 Comparison with the classical method of continuous fractions

There is another good approximation for calculation of dynamic properties of dense plasmas which is called the method of continued fractions [53-55]. The approach is based on recurrence relations within the dielectric response theory. One of the main quantities of this theory is a response function. Taking into account the dynamic local field correction $G(k,\omega)$, it has the form

$$\chi(k,\omega) = \frac{\chi^0(k,\omega)}{1 - v(k)[1 - G(k,\omega)]\chi^0(k,\omega)}, \qquad (3.44)$$

where

$$\chi^0(k,\omega) = -\frac{n}{k_B T} W(x) \qquad (3.45)$$

is the response function for the system of non-interacting particles, i.e., in the random-phase approximation. In the expression for $\chi^0(k,\omega)$,

$$W(x) = 1 - x\exp\left[-\frac{1}{2}x^2\right]\int_0^x dy\, exp\left(\frac{y^2}{2}\right) + \qquad (3.46)$$

$$+ix\left(\frac{\pi}{2}\right)^{1/2} exp\left(-\frac{x^2}{2}\right),$$

In equation (3.46) the notation $x = \frac{\omega}{k}\left(\frac{m}{k_B T}\right)^{1/2}$ is used.

According to [55] let us present here the essence of the method of continuous fractions. Let A be a dynamical variable whose time evolution is required to understand the dynamics of a system under consideration. The time evolution $A(t)$ may be expressed in terms of orthogonal bases $\{f_v, v = 0,1,2,\ldots,D-1\}$ spanning, a D-dimensional dynamical Hilbert space, i.e.,

$$A(t) = \sum_{v=0}^{D-1} a_v(t) f_v. \tag{3.47}$$

The inner product of this Hilbert space is defined as $(X,Y) = \langle XY^* \rangle$, where $\langle \quad \rangle$ and the asterisk mean the classical ensemble average and complex conjugate, respectively, and X, Y are elements of the Hilbert space.

If we set $f_0 = A$ and apply the orthogonalization process, the following recurrence relation [53, 55] for f_v can be obtained:

$$f_{v+1} = \dot{f}_v + \Delta_v f_{v-1}, \tag{3.48}$$

where $\Delta_v = (f_v, f_v)/(f_{v-1}, f_{v-1})$, $f_{-1} \equiv 0$, and $\dot{f}_v = \{H, f_v\}_{PB}$, H is the Hamiltonian. Here $\{,\}_{PB}$ represents the Poisson bracket. Another recurrence relation [53] for the coefficients $a_v(t)$ of equation (3.45) can be obtained by substituting (3.48) into (3.45), i.e.,

$$\Delta_{v+1} a_{v+1}(t) = -\dot{a}_v(t) + a_{v-1}(t), \tag{3.49}$$

where $a_{-1}(t) \equiv 0$. The Laplace transform of equation (3.49) is written as

$$\Delta_1 a_1(z) = 1 - z a_0(z), \qquad v = 0, \tag{3.50}$$

$$\Delta_{v+1} a_{v+1}(z) = a_{v-1}(z) - z a_v(z), \qquad v \geq 1. \tag{3.51}$$

$a_0(z) = (A(z), A)/(A, A) = \langle A(z)A^* \rangle / \langle AA^* \rangle$ is the normalized Laplace transformed relaxation function of the dynamical variable *A*. The relaxation function appears here as an autocorrelation function. By choosing the density fluctuation $\rho_k = \sum_{i=1}^{N} exp(-ikr_i)$ as a dynamical variable, one can relate $a_0(z)$ to the density-response function such that

$$1 - z a_0(z) = \frac{\chi(k,z)}{\chi(k)}, \tag{3.52}$$

where $\chi(k) = \chi(k, 0)$. The frequency-dependent response function is obtained by setting $z = i\omega + 0^+$. Dividing equations (3.50) and (3.51) by $a_0(z)$ and manipulating a little we have a continued fraction expression for $a_0(z)$ as:

$$a_0(z) = \frac{1}{z + \Delta_1 b_1(z)}, \tag{3.53}$$

where

$$b_1(z) = \frac{1}{z + \Delta_2 c_2(z)}$$

$$c_2(z) = \frac{1}{z + \Delta_3 d_3(z)},$$

…

Since $b_1(z)$ contains all Δ's except Δ_1 in the same manner as $a_0(z)$, it can be understood that $b_1(z)$ is the relaxation function of the random force f_1. Similarly, we get the same structure of continued fraction for $c_2(z)$, $d_3(z)$, etc. starting from Δ_3, Δ_4, etc. respectively. Therefore one understands that they are simply relaxation functions of higher-order random forces f_2, f_3, and so on.

While studying a OCP the Δ's are given by the frequency moments:

$$\Delta_1 = \frac{\langle\omega^2\rangle}{\langle\omega^0\rangle}, \quad \Delta_2 = \frac{\langle\omega^4\rangle}{\langle\omega^2\rangle} - \frac{\langle\omega^2\rangle}{\langle\omega^0\rangle}, \quad \ldots$$

Here $\langle\omega^{2n}\rangle = \langle\rho_k^{(n)}\left(\rho_k^{(n)}\right)^*\rangle$ stands for the second frequency moment.

In the case of investigation of DSF the frequency moments are $\langle\omega^{2n}\rangle = \int_{-\infty}^{\infty} d\omega\omega^{2n}\, S(k,\omega)$, that have the same meaning as in (2.23).

CONCLUSIONS

It has been shown in Section 1 how the unsystematic behavior of the fourth moment is corrected by the present approach to obtain a very satisfactory agreement with the simulation data. Finally, we mention that the short-time asymptotic behavior of the dynamic structure factor is qualitatively quite similar to that obtained in [9] where the recurrent relation method was used. Certainly, the ω^{-6} asymptotic behavior of the DSF observed in [9] follows directly from (1.52) as long as the imaginary part of the Nevanlinna parameter function $\zeta(k,\omega)$ is a positive constant.

We can conclude that the algorithm proposed within the method of moments with local constraints gives a quantitative agreement between the simulation data on the plasma dynamic characteristics and their non-rational counterparts reconstructed by a few integral characteristics, i.e., the power moments and the local constraints.

The agreement between our results on the dynamic structure factors of two-component plasmas and the corresponding MD results of Ref. [40] described in Section2 is qualitatively good. The introduction of the non-constant Nevanlinna parameter function (2.17), accounting for the exact high-frequency asymptotic expansion of the system dielectric function, permits to obtain a better agreement with respect to the position of the plasmon peaks, and also leads to an adequate broadening (damping) of the plasmon mode.

It has been shown in Section 3 that, at least, under the thermodynamic conditions considered above, the Drude-Lorentz model for the dynamic conductivity is qualitatively applicable. These results are in agreement with existing experimental and simulation data. Nevertheless, departures from the Drude-Lorentz model have also been studied and the results have been compared to recent simulation data with a semi-quantitative agreement being achieved.

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