What to do if there are no reliable small parameters in a physical system like a moderately or strongly coupled plasma and we have to describe its modes and other dynamic properties? Apply the method of moments! It is a mathematical approach dating back to the works by T.J. Stieltjes and M.G. Krein. We show how it works and describe its new fruitful modification, the method of moments with local constraints. Results of the moment approach application are provided. Destined to Ph.D. students in Statistical and Plasma Physics.

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978-3-659-23422-4

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Impressum / Imprint
Bibliografische Information der Deutschen Nationalbibliothek: Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über http://dnb.d-nb.de abrufbar.

Bibliographic information published by the Deutsche Nationalbibliothek: The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

Coverbild / Cover image: www.ingimage.com

Verlag / Publisher:
LAP LAMBERT Academic Publishing
ist ein Imprint der / is a trademark of
AV Akademikerverlag GmbH & Co. KG
Heinrich-Böcking-Str. 6-8, 66121 Saarbrücken, Deutschland / Germany
Email: info@lap-publishing.com

Herstellung: siehe letzte Seite /
Printed at: see last page
ISBN: 978-3-659-23422-4

THE METHOD OF MOMENTS AND ITS APPLICATIONS IN PLASMA PHYSICS

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Contents

Preface

This book 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 method of moments and its applications.

The book is basically destined to Plasma Physics Ph.D. students; their individual work with the above developments is presumed.

Solutions of most characteristic exercises and problems are provided in Part III. The theoretical part of Sect. 5 can be considered an Exercise as well.

Collaboration with a number of colleagues, in collaboration with a number of colleagues, V.M. Adamyan, D. Ballester, A.E. Davletov, G.M. Meirkanova, and others, is gratefully acknowledged.

I.M.T is grateful to the UPV for the sabbatical leave he was granted.

Finally, the financial support of the al-Farabi Kazakh National University and of the Spanish Ministerio de Educación y Ciencia (Projects ENE2007-67406-C02-02 and ENE2010-21116-C02-02) is acknowledged.

Part I

The mathematical introduction

Chapter 1

Asymptotic expansions [1]

Definition 1 *The series*

$$\sum_{n=0}^{\infty} \frac{c_n}{z^n},$$

possibly divergent, is called asymptotic expansion of a function f *on an infinite set* $\mathcal{M}$:

$$f(z) \sim \sum_{n=0}^{\infty} \frac{c_n}{z^n}, \tag{1.1}$$

if for any entire number $n \geq 0$ *it holds that for* $z \in \mathcal{M}$

$$\lim_{z \to \infty} z^n \left(f(z) - \sum_{k=0}^{n} \frac{c_k}{z^k} \right) = 0. \tag{1.2}$$

Proposition 2 *On a given set* $\mathcal{M}$ *the asymptotic expansion, if it exists, is unique.*

Proof. Indeed, it follows from (1.2) that for $n = 0$, $c_0 = \lim_{z \to \infty} f(z)$, for $n = 1$, $c_1 = \lim_{z \to \infty} z(f(z) - c_0)$, and in general,

$$c_n = \lim_{z \to \infty} z^n \left(f(z) - \sum_{k=0}^{n-1} \frac{c_k}{z^k} \right), \quad n = 0, 1, 2, \ldots, \text{ if it exists.}$$

■

Claim 3 *On the other hand, the same series (1.1) can serve as the asymptotic expansion for different functions. For example, the series which is identically equal to zero is the asymptotic expansion for the function identically equal to zero and of the function* $\exp(-x)$ *on the ray* $x > 0$ *and even in any sector* $|\arg z| < \frac{\pi}{2} - \alpha$, $\alpha > 0$*; indeed,* $\lim\limits_{z\to+\infty} x^n \exp(-x)$ *for any natural* n.

Claim 4 *Asymptotic series can be added, multiplied and even integrated term by term, but not always differentiated term by term. Indeed,* $\exp(-x)\sin\exp x \sim 0$ *on the ray* $x > 0$*, but* $(\exp(-x)\sin\exp x)' = \cos(\exp(x)) - (\sin(\exp x))\exp(-x)$ *has no asymptotic expansion at all, since on the ray* $x > 0$ *the limit, at* $x \to +\infty$*, does not exist.*

Example 5 *Prove that the integral exponential function*

$$E_1(x) = -\operatorname{Ei}(-x) = \int_x^\infty \exp(-t)\,\frac{dt}{t}$$

possesses on the ray $x > 0$ *the asymptotic expansion*

$$E_1(x) \sim \frac{\exp(-x)}{x}\left(1 - \frac{1}{x} + \frac{2!}{x^2} - \cdots + (-1)^n\frac{n!}{x^n} + \cdots\right). \tag{1.3}$$

Hint: a) Integrate repeatedly by parts to show that

$$\int_x^\infty \exp(x-t)\,\frac{dt}{t} = \frac{1}{x} - \frac{1}{x^2} + \frac{2!}{x^3} - \cdots + (-1)^{n-1}\frac{(n-)!}{x^n} + \cdots +$$

$$+ (-1)^n n! \int_x^\infty \exp(x-t)\,\frac{dt}{t^{n+1}}\ , \tag{1.4}$$

b) integrating by parts once more, find an estimate for (1.4) and prove that the condition (1.2) holds for the expansion (1.3).

Example 6 *Prove that on the ray* $x > 0$ *the error function*

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp\left(-t^2\right) dt$$

possesses the following asymptotic expansion

$$\operatorname{erf}(x) \sim 1 - \frac{2}{\sqrt{\pi}}\exp\left(-x^2\right)\left(\frac{1}{2x} - \frac{1}{2^2x^3} + \frac{1\cdot 3}{2^3x^5} - \frac{1\cdot 3\cdot 5}{2^4x^7} + \cdots\right).$$

Hint: Integrate repeatedly by parts to find the asymptotic expansion for the integral

$$\int_x^\infty \exp\left(x^2 - t^2\right) dt = -\frac{1}{2}\int_x^\infty \frac{1}{t} d\left(\exp\left(x^2 - t^2\right)\right)$$

and take into account that

$$\int_0^\infty \exp\left(-t^2\right) dt = \frac{\sqrt{\pi}}{2}.$$

Chapter 2

The method of moments

Dispersion relations

Claim 7 *If a continuous and complex-valued function $f(w)$ is defined on the real axis, and satisfies the Lipshitz condition*

$$|f(w) - f(w_0)| \leq C\,|w - w_0|^{\alpha}, \quad 0 < \alpha \leq 1, \quad C > 0,$$

and $f(w) \in L^2$, i.e.,

$$\int_{-\infty}^{\infty} |f(w)|^2\, dw < \infty,$$

then at $\forall w_0 \in \mathbb{R}$ there holds the formula of Sokhotsky-Plemelj:

$$\lim_{\varepsilon \downarrow 0} \int\limits_{-\infty}^{\infty} \frac{f(w')\, dw'}{w' - w_0 \mp \varepsilon} = P.V. \int\limits_{-\infty}^{\infty} \frac{f(w')\, dw'}{w' - w_0} \pm \pi i f(w_0), \tag{2.1}$$

P.V. standing for the Principal Value integral.

Example 8 *Find the boundary values for the real and imaginary parts of the dispersion function of classical plasmas:*

$$Z(\zeta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-t^2\right) \frac{dt}{t - \zeta}, \quad \operatorname{Im} \zeta > 0 \tag{2.2}$$

on the real axis.

Hint: a) The boundary value of the function $Z(\zeta)$ on the real axis is determined as

$$Z(x) = \lim_{\delta \downarrow 0} Z(x + i\delta);$$

apply (2.1) to $Z(x + i\delta)$ to prove that [1]

$$Z(0) = i\sqrt{\pi}; \tag{2.3}$$

b) differentiating (2.2) and integrating the expression obtained for $Z'(\zeta)$, demonstrate that $Z(\zeta)$ satisfies the differential equation

$$Z'(\zeta) + 2\zeta Z(\zeta) + 2 = 0;$$

c) solve this equation using the boundary condition (2.3).

Theorem 9 *Given a function $f(z)$ which is regular and bounded in the upper half-plane, if its boundary value on the real axis*

$$f(w) = \lim_{\delta \downarrow 0} f(w + i\delta)$$

is bounded and $f(w) \in \mathrm{L}^2$, then the real and imaginary parts of $f(w)$ are mutual Hilbert transforms:

$$\begin{aligned} \operatorname{Re} f(w) &= \tfrac{1}{\pi} V.P. \int_{-\infty}^{\infty} \tfrac{\operatorname{Im} f(w') dw'}{w' - w} , \\ \operatorname{Im} f(w) &= \tfrac{-1}{\pi} V.P. \int_{-\infty}^{\infty} \tfrac{\operatorname{Re} f(w') dw'}{w' - w} \end{aligned} \tag{2.4}$$

Hint: Apply the Sokhotsky-Plemelj formula (2.1) to the expression

$$f(w + i\delta) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f(w')\, dw'}{w' - w - i\delta} , \quad \delta \downarrow 0,$$

which stems directly from the Cauchy integral formula and separate the real and imaginary parts of the result.

Definition 10 *The relations (2.4) are called the Kramers-Kronig dispersion relations, and for the response functions or susceptibilities in physics or the Nevanlinna functions in mathematics, e.g. the plasma inverse dielectric function, they reflect the causality principle.*

Exercise 11 *Reconstruct the real part of the refraction index $n'(\omega)$, whose imaginary part is*

$$n''(\omega) = \frac{\Gamma}{(\omega - u)^2 + \Gamma^2} , \quad \operatorname{Re}\Gamma > 0 , \quad u > 0.$$

Hint: Apply the Kramers-Kronig relations (2.4).

[1] The integral $\int_{-\infty}^{\infty} \exp(-t^2) \frac{dt}{t} = 0$ due to the parity of the integrand.

Nevanlinna (response) functions and their mathematical properties [2]

Definition 12 *(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 13 *Let $x \in \mathbb{R}$ be a random variable with a distribution function $\sigma(x)$. If*

$$\sigma(x) = \int_{-\infty}^{x} f(s)\, ds \tag{2.5}$$

the function $f(x)$ is called the probability density function, p.d.f..

Claim 14 *The Nevanlinna functions are determined by the Riesz - Herglotz transform:*

$$F(z) = az + b + \int_{-\infty}^{\infty} \left(\frac{1}{x-z} - \frac{x}{1+x^2} \right) dg(x) \quad , \tag{2.6}$$

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

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

Claim 15 *Notice that we can always choose the function $g(x)$ so that b were equal to*

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

Claim 16 *Observe also that for $\forall r \in (-1,1)$, $\forall s \in \mathbb{R}$ and $\operatorname{Im} z > 0$ (see Section IV)*

$$W_{r+is}(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{|x|^{r+is}\, dx}{x-z} = \frac{i z^{r+is}}{\exp\left(\frac{\pi i(r+is)}{2}\right) \cos\left(\frac{\pi(r+is)}{2}\right)} \quad , \tag{2.7}$$

particularly,

$$\frac{h}{\pi} \lim_{r,s \to 0} \int_{-\infty}^{\infty} \frac{|x|^{r+is}\, dx}{x-z} = ih \ , h \in \mathbb{R},$$

and that the integral

$$\int_{-\infty}^{\infty} \frac{|x|^{r+is}\,dx}{1+x^2} = 2\int_{0}^{\infty} \frac{x^r \exp\left(is\ln u\right)dx}{1+x^2}$$

converges [2]*; it is also easy to see that*

$$a = \lim_{y\to+\infty} \frac{\operatorname{Im} F\left(iy\right)}{y}.$$

Definition 17 *(The class of functions $\mathfrak{R}_0$): A function $G\left(z\right) \in \mathfrak{R}_0$ if $G\left(z\right) \in \mathfrak{R}$ and*

$$\lim_{z\to\infty} \frac{G\left(z\right)}{z} = 0, \quad \operatorname{Im} z > 0, \tag{2.8}$$

so that for such functions from (2.6) we have:

$$G(z) = \int_{-\infty}^{\infty} \frac{dg\left(x\right)}{x-z} + ih\ , h > 0 \tag{2.9}$$

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]For $r < 0$ pass to a new variable $u = x^{1+r}$.

The classical (untruncated) Hamburger problem of moments

Definition 18 *The real numbers*

$$\mu_m \equiv \langle x^m \rangle = \int_{-\infty}^{\infty} x^m d\sigma(x) \quad , \quad m = 0, 1, 2, \ldots \tag{2.10}$$

are the (power) moments of the distribution $\sigma(x)$. *If the distribution* $\sigma(x)$ *is differentiable and* $f(x) = \sigma'(x)$ *is symmetric, all odd-order moments (2.10) vanish.*

Let us summarize some notions and results of the classical theory of moments [2, 3], [4].

The Hamburger problem is formulated in the following way.

Problem 19 *Given a set of real numbers* $\{\mu_0, \mu_1, \mu_2, \ldots\}$, *find all distributions* $\sigma(x)$ *such that*

$$\int_{-\infty}^{\infty} x^m d\sigma(x) = \mu_m \ , \ m = 0, 1, 2, \ldots . \tag{2.11}$$

The Hamburger moment problem is solvable, i.e., there exists at least one distribution (p.d.f.) which satisfies (2.11), if and only if the given set of numbers $\{\mu_m\}_{m=0}^{\infty}$ *is non-negative, i.e., if the Hankel matrix* $\Gamma = \left(\mu_{m+n}\right)_{m,n=0}^{\infty} \geq 0$. *If the problem is solvable, it can have a unique solution (a determinate problem) or an infinite number of solutions (an indeterminate problem).*

Definition 20 *Notice that if* $\sigma(x < 0) \equiv const$ *(i.e., if* $f(x < 0) \equiv 0$*), we have the Stieltjes moment problem, and if* $\sigma(x) \equiv const$ $(f(x) \equiv 0)$ *for* $x < a$, $x > b$, $a, b \in \mathbb{R}$, *we deal with the Hausdorff problem finite interval moment problem.*

Theorem 21 *[5] In order that a Hamburger moment problem (2.11) shall have a solution it is necessary that*

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

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

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

The problem (2.11) is determinate if and only if

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

Claim 22 *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 [2]; this correspondence is described by the Nevanlinna formula, see below.*

Claim 23 *Given a set of real numbers* $\{s_0, s_1, s_2, \ldots\}$*, the solvability conditions of the Stieltjes moment problem*

$$\int_0^{\infty} x^m d\sigma(x) = s_m \ , \quad m = 0, 1, 2, \ldots$$

is the non-negativity of two Hankel matrices, $(s_{m+n})_{m,n=0}^{\infty}$ *and* $(s_{m+n+1})_{m,n=0}^{\infty}$*, for further details, see [5, 2].*

Theorem 24 *[5] Given a set of real numbers* $\{c_0, c_1, c_2, \ldots\}$*, a necessary and sufficient condition that the one-dimensional Hausdorff moment problem*

$$\int_0^{1} x^m d\sigma(x) = c_m \ , \quad m = 0, 1, 2, \ldots \tag{2.12}$$

shall have a solution is that all differences

$$\Delta^k c_m \equiv c_m - \binom{k}{1} c_{m+1} + \binom{k}{2} c_{m+2} + \cdots + (-1)^k \binom{k}{1} c_{m+k} \geq 0 \ , \quad m, k = 0, 1, 2, \ldots .$$

Claim 25 *A solvable Hausdorff one-dimensional problem is always determinate.*

Claim 26 *A truncated Hamburger moment problem [2], i.e., a moment problem with a finite set of given numbers, i.e.,* $\{\mu_m\}_{m=0}^{2\nu}$*,* $\nu = 0, 1, 2, \ldots$ *is solvable if the Hankel matrix* $\Gamma_\nu = \left(\mu_{m+n}\right)_{m,n=0}^{\nu} > 0$*, [6], see also [7] and [8]. In the degenerate case of a singular Hankel matrix* Γ_ν *the problem of moments (under some special conditions established in [8] and [6], [7]) has a unique solution described in [6], [7].*

Theorem 27 *[9, 5, 2] A sufficient condition that the Hamburger moment problem (2.10) be determinate is that (Carleman's criterion)*

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

Corollary 28 *[10, 5, 3] If the Hamburger moment problem (2.10) has a solution (2.5), where* $f(x) \geq 0$ *and*

$$\int_{-\infty}^{\infty} e^{\delta|x|} \left[f(x)\right]^q dx < \infty,$$

for some $q \geq 1$ *and* $\delta > 0$*, then the problem is determinate, i.e., it has only one solution.*

Theorem 29 *[2, 3] If*

$$\int_{-\infty}^{\infty} \frac{\ln f(x)}{1+x^2} dx > -\infty,$$

the Hamburger moment problem (2.10) has an infinite number of solutions.

Example 30 *The p.d.f.*

$$f_\alpha(x;\gamma) = \frac{\alpha\gamma^{1/\alpha}}{2\Gamma\left(\frac{1}{\alpha}\right)} \exp\left(-\gamma\left|x\right|^\alpha\right), \quad \alpha,\gamma > 0, \tag{2.13}$$

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

$$\begin{aligned} \mu_{2m}\left(\alpha;\gamma\right) &= \int_{-\infty}^{\infty} x^{2m} f_\alpha(x) dx = \frac{\Gamma\left(\frac{2m+1}{\alpha}\right)}{\gamma^{2m/\alpha}\Gamma\left(\frac{1}{\alpha}\right)}, \qquad (2.14) \\ \mu_{2m+1}\left(\alpha;\gamma\right) &= 0\ , \quad m = 0,1,2,\ldots \end{aligned}$$

but the Hamburger moment problem for the set of numbers

$$\left\{1,0,\frac{\Gamma\left(\frac{3}{\alpha}\right)}{\gamma^{2/\alpha}\Gamma\left(\frac{1}{\alpha}\right)},0,\frac{\Gamma\left(\frac{5}{\alpha}\right)}{\gamma^{4/\alpha}\Gamma\left(\frac{1}{\alpha}\right)},0,\ldots\right\} \tag{2.15}$$

has, as it stems from the Carleman criterion, a unique solution, which is the p.d.f. (2.13), if $\alpha > 1$, in particular the Gaussian density $f_2(x;\frac{1}{2a^2})$, $a > 0$, and an infinite number of solutions if $\alpha \leq 1$. In this latter case, all solutions of the moment problem are described by the Nevanlinna formula ([2]), see below.

Other examples of sets $\{\mu_m\}_{m=0}^{\infty}$ which generate indeterminate moment problems are provided in [3].

In (solvable) problems where we already have at least one p.d.f. with an infinite 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, $\{\mu_m\}_{m=0}^{\infty}$.

Claim 31 *If in the vicinity of the point $s = 0$ there exists the moment generating function (m.g.f.)*

$$M_x(s) \equiv \int_{-\infty}^{\infty} e^{sx} f(x) dx = \sum_{m=0}^{\infty} \mu_m \frac{s^m}{m!}, \tag{2.16}$$

then the p.d.f., $f(x)$ and its moments can be expressed through the m.g.f., $M_x(s)$ in the unique way:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-isx} M_x(is)ds,$$
$$\mu_m = \frac{d^m}{ds^m} M_x(s)\Big|_{s=0}.$$

Claim 32 *Notice that, e.g., for the density $f_\alpha(x;\gamma)$ with $\alpha \le 1$ the m.g.f. exists only at the point $s = 0$ (the zero moment) and cannot be prolongated analytically to a vicinity of this point. For $\alpha > 1$*

$$M_x(s) = \frac{\alpha\gamma^{1/\alpha}}{\Gamma\left(\frac{1}{\alpha}\right)} \int_0^{\infty} \exp\left(-\gamma x^\alpha\right)\cosh(sx)dx, \quad s \in \mathbb{R}, \tag{2.17}$$

which is also the sum of the series

$$\sum_{m=0}^{\infty} \mu_{2m}(\alpha;\gamma)\frac{s^{2m}}{(2m)!} \tag{2.18}$$

for any real s. For $\alpha \le 1$ the series (2.18) and the integral (2.17) converge only along the imaginary axis $s = iy$ $y \in \mathbb{R}$, but diverges in any band along this axis, i.e., for any $s = x + iy$, $x \ne 0$: the problem is indeterminate.

Claim 33 *The above relations of uniqueness of the solution hold for the probability distributions of practical interest. For example, moments and moment generating functions of normal, uniform and parabolic p.d.f.'s are shown in Table 1. The latter two distributions correspond to the determinate Hausdorff problems, like any other so called bounded p.d.f.'s with a given infinite set of moments, and they are uniquely determined by the latter. Due to the Carleman criterion the normal p.d.f. is defined by its moments in the unique way as well.*

Table 1. Moments and moment generating functions of normal, uniform and parabolic distributions.

	$f(x)$	μ_{2m}	$M_x(s)$
normal $x \in \mathbb{R}$	$\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{x^2}{2\sigma^2}\right)$	$(2m-1)!!a^{2m}$	$\exp\left(\frac{(\sigma s)^2}{2}\right)$
uniform $x \in [-a, a]$	$\frac{1}{2a}$	$\frac{a^{2m}}{2m+1}$	$\frac{\sinh as}{as}$
parabolic $x \in [-a, a]$	$\frac{3(a^2-x^2)}{4a^3}$	$\frac{3a^{2m}}{(2m+1)(2m+3)}$	$3\left(\frac{\cosh as}{(as)^2} - \frac{\sinh as}{(as)^3}\right)$

Orthogonal polynomials and the Nevanlinna formula

Theorem 34 *(Nevanlinna) There is a one-to-one correspondence between all solutions of the Hamburger problem (19), or all complex Nevanlinna functions*

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{d\sigma(x)}{x-z}, \tag{2.19}$$

and all Nevanlinna functions $q(z) \in \mathfrak{R}_0$ *such that*

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{d\sigma(x)}{z-x} = \frac{E_{n+1}(z) + q(z) E_n(z)}{D_{n+1}(z) + q(z) D_n(z)}. \tag{2.20}$$

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

Definition 35 *Here* $D_k(z)$ *are orthonormalized polynomials with respect to the measure* $d\sigma$ *[3]:*

$$\int_{-\infty}^{\infty} D_n(x) D_m(x) d\sigma(x) = \delta_{nm}, \quad n, m = 0, 1, \ldots, \tag{2.21}$$

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

$$E_n(z) = \int_{-\infty}^{\infty} \frac{D_n(z) - D_n(t)}{z-t} d\sigma(t). \tag{2.22}$$

Precisely,

$$D_0 = \frac{1}{\sqrt{\mu_0}}, \ \ \Delta_{-1} = 1, \ \ \Delta_0 = \mu_0,$$

$$D_k(t) = \frac{1}{\sqrt{\Delta_k \Delta_{k-1}}} \det \begin{bmatrix} \mu_0 & \cdots & \mu_{k-1} & 1 \\ \mu_1 & \cdots & \mu_k & t \\ \vdots & \vdots & \vdots & \vdots \\ \mu_k & \cdots & \mu_{2k-1} & t^k \end{bmatrix}, \tag{2.23}$$

$$\Delta_k = \det \begin{bmatrix} \mu_0 & \cdots & \mu_k \\ \vdots & \vdots & \vdots \\ \mu_k & \cdots & \mu_{2k} \end{bmatrix}, \ k = 1, 2, \ldots. \tag{2.24}$$

Let us point out the properties of these orthonormalized polynomials:

Claim 36 *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:*

$$\begin{aligned} D_0(z) &= \frac{1}{\sqrt{\mu_0}}\ ,\ D_1(z) = \frac{1}{\sqrt{\mu_0}} \frac{z - a_0}{b_0}\ , \\ D_2(z) &= \frac{\left(\mu_0\mu_2 - \mu_1^2\right) z^2 + z\left(\mu_1\mu_2 - \mu_0\mu_3\right) + \left(\mu_3\mu_1 - \mu_2^2\right)}{\sqrt{\left(\mu_0\mu_2 - \mu_1^2\right)\Delta_2}}, \\ E_0(z) &= 0\ ,\ E_1(z) = \frac{\sqrt{\mu_0}}{b_0}\ , \\ E_2(z) &= \frac{\mu_0\left(\mu_0\mu_2 - \mu_1^2\right) z + \left(\mu_0\mu_2 - \mu_1^2\right)\mu_1 + \mu_0\left(\mu_1\mu_2 - \mu_0\mu_3\right)}{\sqrt{\left(\mu_0\mu_2 - \mu_1^2\right)\Delta_2}}, \ldots. \end{aligned} \tag{2.25}$$

Besides:

1. The zeros of the polynomials $D_k(t)$ and $E_k(t)$, $k \in \mathbb{N}$, are all real;

2. The zeros of the polynomials $D_k(t)$ and $D_{k-1}(t)$, $k \in \mathbb{N}$, are all real and alternate. The zeros of the polynomials $D_k(t)$ and $E_k(t)$, $k \in \mathbb{N}$, alternate;

3. The polynomials $D_k(t)$ and $E_k(t)$, $k \in \mathbb{N}$, can be expressed in terms of each other:

$$zD_k(z) = b_{k-1}D_{k-1}(z) + a_kD_k(z) + b_kD_{k+1}(z)\ ,\ k = 1, 2, \ldots \tag{2.26}$$

or

$$zE_k(z) = b_{k-1}E_{k-1}(z) + a_kE_k(z) + b_kE_{k+1}(z)\ ,\ k = 1, 2, \ldots, \tag{2.27}$$

where

$$\begin{aligned} a_k &= a_{k,k} = \int_{-\infty}^{\infty} tD_k(t)D_k(t)d\sigma(t)\ , \\ b_k &= a_{k,k+1} = \int_{-\infty}^{\infty} tD_k(t)D_{k+1}(t)d\sigma(t) = \frac{\sqrt{\Delta_{k-1}\Delta_{k+1}}}{\Delta_k},\ k = 0, 1, 2, \ldots; \end{aligned}$$

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

$$D_{n-1}(z)E_n(z) - D_n(z)E_{n-1}(z) = \frac{1}{b_{n-1}} = \frac{\Delta_{n-1}}{\sqrt{\Delta_{n-2}\Delta_n}}\ ,\ n = 2, 3, \ldots. \tag{2.28}$$

Claim 37 *The latter relation permits to define these polynomials in the recurrent way. Indeed, since*

$$\begin{aligned} D_0(z) &= \frac{1}{\sqrt{\mu_0}}\ ,\ D_1(z) = \frac{1}{\sqrt{\mu_0}}\frac{z-a_0}{b_0}\ , \\ E_0(z) &= 0\ ,\ E_1(z) = \frac{\sqrt{\mu_0}}{b_0}\ , \end{aligned}$$

we have that

$$\begin{aligned} D_2(z) &= \frac{(z-a_1)\,D_1(z) - b_0 D_0(z)}{b_1} = \\ &= \frac{(\mu_0\mu_2 - \mu_1^2)\,z^2 + z\,(\mu_1\mu_2 - \mu_0\mu_3) + (\mu_3\mu_1 - \mu_2^2)}{\sqrt{(\mu_0\mu_2 - \mu_1^2)\,\Delta_2}}, \end{aligned}$$

$$\begin{aligned} E_2(z) &= \frac{(z-a_1)\,E_1(z) - b_0 E_0(z)}{b_1} = \\ &= \frac{\mu_0\,(\mu_0\mu_2 - \mu_1^2)\,z + (\mu_0\mu_2 - \mu_1^2)\,\mu_1 + \mu_0\,(\mu_1\mu_2 - \mu_0\mu_3)}{\sqrt{(\mu_0\mu_2 - \mu_1^2)\,\Delta_2}}. \end{aligned}$$

and so on. This procedure can be easily programmed.

Exercise 38 *Check that the polynomials $D_j(z)$, $j = 0, 1, 2$ are normalized to unity and mutually orthogonal.*

Exercise 39 *Initiate the construction of the set of orthogonal (but not normalized) polynomials $\{\mathrm{D}_k(t)\}_{k=0}^{\infty}$ from the canonical basis of the Hilbert vector space of polynomials,*

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

but with the scalar product and the norm defined as

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

by means of the standard Gram-Schmidt procedure.

Canonical and degenerate solutions of a solvable truncated Hamburger moment problem

Claim 40 *It is clear that, at least, due to numerical and measurement problems, we never possess 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

$$\mu_m = \int_{-\infty}^{\infty} x^m d\sigma(x) = \int_{-\infty}^{\infty} x^m f(x)dx, \quad m = 0, 1, 2, \ldots, 2\nu, \quad \nu = 0, 1, 2, \ldots, \tag{2.29}$$

one could first consider a step-like distribution

$$d\sigma(x) = \sum_{j=0}^{2\nu} m_j \delta(x - x_j)\, dx \tag{2.30}$$

with the density which actually consists of $2\nu + 1$ point masses located at some distinct points of the real axis $\{x_j\}_{j=0}^{2\nu}$. This is a so called *canonical solution* of the problem. Then the assumption (2.30) can be substituted to the conditions (2.29) 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 $\{x_j\}_{j=0}^{2\nu}$:

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_{2\nu} \\ \vdots & \vdots & \ddots & \vdots \\ x_0^{2\nu} & x_1^{2\nu} & \cdots & x_{2\nu}^{2\nu} \end{bmatrix} \begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_{2\nu} \end{bmatrix} = \begin{bmatrix} \mu_0 \\ \mu_1 \\ \vdots \\ \mu_{2\nu} \end{bmatrix}. \tag{2.31}$$

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

Example 41 ***Gaussian distribution*** $\exp(-x^2)$. *Consider a truncated problem generated by the moments*

$$\begin{aligned} \mu_m &= \int_{-\infty}^{\infty} x^m \exp\left(-x^2\right) dx, \quad m = 0, 1, 2 : \\ \mu_0 &= \sqrt{\pi}, \mu_1 = 0, \mu_2 = \frac{\sqrt{\pi}}{2}. \end{aligned}$$

Then the system (2.31) becomes:

$$\begin{bmatrix} 1 & 1 & 1 \\ x_0 & x_1 & x_2 \\ x_0^2 & x_1^2 & x_2^2 \end{bmatrix} \begin{bmatrix} m_0 \\ m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} \sqrt{\pi} \\ 0 \\ \frac{\sqrt{\pi}}{2} \end{bmatrix}.$$

Its solution is just:

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

Exercise 42 ***Nevertheless,*** *for the moment set* $\{\mu_0, 0, \mu_2\}$, *there exists the following canonical solution of the moment problem*

$$\int_{-\infty}^{\infty} x^m f(x)\, dx = \mu_m, \quad m = 0, 1, 2:$$

$$f(x) = \frac{\mu_0}{2} [\delta(x - \xi) + \delta(x + \xi)],$$

where

$$\xi^2 = \frac{\mu_2}{\mu_0}.$$

Exercise 43 ***While,*** *for the moment set* $\{\mu_0, 0, \mu_2, 0, \mu_4\}$, *there exists the following canonical solution of the moment problem*

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

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

where

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

This solution will be interpreted later, e.g., in Chapter 4 dedicated to the investigation of one-component plasmas. The positivity of the central feature intensity, $\left(1 - (\xi_1/\xi_2)^2\right)$ *follows from the Cauchy-Schwarz inequality, see Section IV.*

Example 44 ***Degenerate case.*** *Consider now a degenerate truncated problem generated by the moments*

$$\mu_0 = 1, \mu_1 = \sqrt{2}, \mu_2 = 2, \tag{2.32}$$

whose Hankel matrix

$$\Gamma_1 = \begin{bmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 2 \end{bmatrix}$$

is obviously singular ($\Delta_1 = \det \Gamma_1 = 0$). 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 Γ_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 $\{x_i\}_{i=1}^{\nu}$ of the masses in the degenerate solution

$$d\sigma(x) = \sum_{i=1}^{\nu} m_i \delta\left(x - x_i\right) dx,$$

and determine the corresponding masses from the moment conditions (2.29). Particularly, for the moments (2.32) we have

$$d\sigma(x) = \delta\left(x - \sqrt{2}\right) dx,$$

which automatically satisfies the conditions

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

Claim 45 *Certainly, in physical problems we are basically interested in non-canonical, 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.*

But let us start with

An example: the Drude – Lorentz model

The Drude - Lorentz formula

Consider the simplest case of the Nevanlinna formula (2.20) with $n = 0$. Choose the p.d.f.

$$f(\omega) = \operatorname{Re}\sigma^{int}(\omega),$$

which is an even function of frequency, and assume that the (internal) static conductivity

$$\sigma_0 = \lim_{\eta\downarrow 0}\sigma^{int}(i\eta) = \frac{\omega_p^2\tau}{4\pi}$$

exists and the power moment

$$c_0 = \int_{-\infty}^{\infty}\operatorname{Re}\sigma^{int}(\omega)\,d\omega = \omega_p^2/4$$

converges due to the the f-sum rule [11] [3], while

$$c_1 = \int_{-\infty}^{\infty}\omega\operatorname{Re}\sigma^{int}(\omega)\,d\omega = 0.$$

Here $\omega_p = \sqrt{4\pi n_e e^2/m_e}$ is the (electronic) plasma frequency and τ is the relaxation time defined, e.g., by the Spitzer formula; n_e and m_e, as usually, are the number density and mass of plasma electrons. Remember that in the absence of the spatial dispersion, the plasma dielectric function

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma^{int}(\omega)$$

is a response or Nevanlinna function [12]. Introduce the Hilbert transform

$$\sigma^{int}(z) = \frac{1}{\pi i}\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma^{int}(\omega)}{\omega - z}d\omega.$$

Observe that due to the Kramers - Kronig relations,

$$\begin{aligned}\sigma^{int}(\omega) &= \frac{1}{\pi i}\lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma^{int}(\omega')}{\omega' - \omega - i\eta}d\omega' = \frac{1}{\pi i}P.V.\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma^{int}(\omega')}{\omega' - \omega}d\omega' + \operatorname{Re}\sigma(\omega) = \\ &= \operatorname{Re}\sigma^{int}(\omega) + i\operatorname{Im}\sigma^{int}(\omega),\end{aligned}$$

and that $\operatorname{Im}\sigma^{int}(\omega = 0) = 0$.

[3] We will later justify this result independently.

Consider the asymptotic expansion of $\sigma^{int}(z)$ in the upper half-plane:

$$\begin{aligned}\sigma^{int}(z) &= \frac{1}{\pi i}\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma^{int}(\omega)}{\omega - z}d\omega = \frac{i}{\pi z}\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma^{int}(\omega)}{1-\frac{\omega}{z}}d\omega \\ &\underset{z\to\infty}{\simeq} \frac{i}{\pi z}\int_{-\infty}^{\infty}\operatorname{Re}\sigma^{int}(\omega)\left(1+\frac{\omega}{z}\right)d\omega \\ &\underset{z\to\infty}{\simeq} \frac{ic_0}{\pi z} + \mathrm{o}\left(\frac{1}{z}\right).\end{aligned}$$

Hence,

$$\epsilon(z\to\infty) = 1 + \frac{4\pi i}{z}\sigma^{int}(z\to\infty) \simeq 1 - \frac{\omega_p^2}{z^2},\ \ \operatorname{Im} z > 0.$$

According to the above definitions,

$$D_0 = c_0^{-1/2}, E_0 = 0,$$

$$D_1(z) = c_0 z/\sqrt{\Delta_{-1}\Delta_1}, E_1(z) = c_0^2/\sqrt{\Delta_{-1}\Delta_1} \Longrightarrow$$

$$\sigma^{int}(z) = \frac{1}{\pi i}\int_{-\infty}^{\infty}\frac{\operatorname{Re}\sigma(\omega)}{\omega - z}d\omega = \frac{i}{\pi}\frac{E_1(z) + Q_0(z)E_0(z)}{D_1(z) + Q_0(z)D_0(z)} =$$

$$= \frac{i}{\pi}\frac{c_0^2/\sqrt{\Delta_{-1}\Delta_1}}{c_0 z/\sqrt{\Delta_{-1}\Delta_1} + c_0^{-1/2}q_0(z)} = \frac{i}{\pi}\frac{c_0}{z + q_0(z)} =$$

$$= \frac{i\omega_p^2}{4\pi}\frac{1}{z+q_0(z)} = \frac{\sigma_0}{1 - iz\tau},\quad q_0(z) = ih_0 = \frac{i}{\tau}.$$

A generalization of the Drude-Lorentz model

Consider now the simplified case with $n = 1$:

$$c_0 = \int_{-\infty}^{\infty} \mathrm{Re}\,\sigma^{int}(\omega)\,d\omega = \omega_p^2/4 \quad , \quad c_1 = 0 \quad ,$$

$$c_2 = \int_{-\infty}^{\infty} \omega^2\,\mathrm{Re}\,\sigma^{int}(\omega)\,d\omega := \omega_p^2\Omega^2/4, \implies$$

$$\sigma^{int}(z) = \frac{i}{\pi}\frac{E_2(z) + Q_1(z)\,E_1(z)}{D_2(z) + Q_1(z)\,D_1(z)} = \frac{i}{4\pi}\frac{\omega_p^2\,(z + q_1(z))}{z^2 - \Omega^2 + zq_1(z)}. \tag{2.33}$$

With the choice

$$q_1(z) = q_1(z = 0) = ih_1 = i\tau\Omega^2, \tag{2.34}$$

$$\sigma^{int}(z) = \frac{i\omega_p^2}{4\pi}\frac{z + i\tau\Omega^2}{z^2 - \Omega^2\,(1 - iz\tau)} \underset{z\to\infty}{\simeq} \frac{i\omega_p^2}{4\pi z} + \frac{i\omega_p^2\Omega^2}{4\pi z^3} + \mathrm{o}\left(\frac{1}{z^3}\right), \quad \mathrm{Im}\,z > 0. \tag{2.35}$$

If $\tau\Omega \leq \sqrt{2}$, the real part of (2.35) on the real axis,

$$\mathrm{Re}\sigma^{int}(\omega) = \frac{\sigma_0\Omega^4}{(\omega^2 - \Omega^2)^2 + \omega^2\tau^2\Omega^4} \tag{2.36}$$

possesses two symmetric maxima shifted to

$$\omega_{\max} = \pm\Omega\sqrt{1 - \frac{\tau^2\Omega^2}{2}}. \tag{2.37}$$

Otherwise, its behavior is qualitatively similar to that of the Drude-Lorentz conductivity.

Exercise 46 *Prove the expansion (2.35).*

Dynamic conductivity of aluminum plasmas

These results were used in [13] to analyze recent **data on aluminum plasmas** obtained by means of Quantum Molecular Dynamics simulations (QMD) [14]. This simulation technique uses the Density Functional Theory (to treat the electronic subsystem through the package VASP) and the Kubo-Greenwood formula.

Then, for the reconstruction of the dynamic conductivity, the values of the moments c_0 and c_2 were calculated from the computed spectra kindly provided to us by the authors of [14]. We understand that the plasma frequency computed from the simulations is an effective one, accounting for the total electronic density.

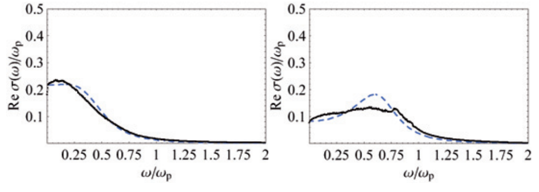

Fig. 1. Here we show the dynamic conductivity real part of (2.36), which gives the best approximation to the simulation data of [14]. We can clearly identify the maxima shown by this model at the values given by (2.37), which appear for $\tau\Omega \leq \sqrt{2}$. Temperature is 25 kK and the density varies from 1.0 $g \cdot cm^{-3}$ to 0.5 $g \cdot cm^{-3}$.

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

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

$$\left\{\mu_0, \mu_1, \mu_2, \ldots, \mu_{2\nu-1}, \mu_{2\nu}\right\}, \quad \nu = 0, 1, 2, \ldots,$$

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. $f(x)$ such that

$$\mu_l = \int_{-\infty}^{\infty} x^l f(x)\, dx, \quad l = 0, 1, 2, \ldots, 2\nu, \quad \nu = 0, 1, 2, \ldots. \tag{2.38}$$

The Nevanlinna formula in this case takes the following form:

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{f(x)\, dx}{x - z} = -\frac{E_{\nu+1}(z) + Q_\nu(z) E_\nu(z)}{D_{\nu+1}(z) + Q_\nu(z) D_\nu(z)}. \tag{2.39}$$

Claim 47 *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 (2.38) independently of our choice of this parameter function.*

Indeed, along any ray within the upper half-plane $\operatorname{Im} z > 0$,

$$\varphi(z \to \infty) = -\frac{1}{z} \int_{-\infty}^{\infty} \frac{f(x)\, dx}{1 - \frac{x}{z}} \simeq$$

$$\underset{z\to\infty}{\simeq} -\frac{1}{z} \int_{-\infty}^{\infty} f(x) \left(\sum_{l=0}^{2\nu} \left(\frac{x}{z}\right)^l + \mathrm{O}\left(\frac{1}{z}\right)^{2\nu+1} \right) dx =$$

$$= -\sum_{l=0}^{2\nu} \frac{1}{z^{l+1}} \int_{-\infty}^{\infty} x^l f(x)\, dx + \mathrm{O}\left(\frac{1}{z}\right)^{2\nu+2} =$$

$$= -\sum_{l=0}^{2\nu} \frac{\mu_l}{z^{l+1}} + \mathrm{O}\left(\frac{1}{z}\right)^{2\nu+2}. \tag{2.40}$$

In other words, the contribution related to the Nevanlinna parameter function $Q_\nu(z)$, due to the additional property (2.8), will appear in the asymptotic expansion (2.40) only in the correction of excessive order $2\nu+2$. We will see, how this happens in specific examples.

By definition, on the real axis $\operatorname{Im} z = 0$,

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

Let

$$Q(x) = \operatorname{Re}Q(x) + i\operatorname{Im}Q(x)\,,\quad \overline{Q(x)} = \operatorname{Re}Q(x) - i\operatorname{Im}Q(x)$$

and observe that, also by definitions (2.23) and (2.24), we have:

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

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

$$\Delta_\nu = \det\begin{bmatrix}\mu_0 & \cdots & \mu_{\nu-1} & \mu_\nu\\ \mu_1 & \cdots & \mu_\nu & \mu_{\nu+1}\\ \vdots & \cdots & \vdots & \vdots\\ \mu_{\nu-1} & \cdots & \mu_{2\nu-1} & \mu_{2\nu}\end{bmatrix}. \tag{2.41}$$

Hence,

$$D_{\nu+1}(t) = \sqrt{\frac{\Delta_\nu}{\Delta_{\nu+1}}}\mathrm{D}_{v+1}(t)\,,\quad D_\nu(t) = \sqrt{\frac{\Delta_{\nu-1}}{\Delta_\nu}}\mathrm{D}_v(t)\,, \tag{2.42}$$

where $\{\mathrm{D}_l(t)\}_{l=0}^{\nu+1}$ are orthogonal monic polynomials with respect to the measure density $f(x)$, i.e., the polynomials with the coefficient of the term of highest degree equal to one. We show how these polynomials can be constructed by the Gram-Schmidt procedure applied to the canonical, non-orthogonal basis

$$\{1, t, t^2, \ldots\}$$

in Exercise 39. Thus [4], due to the Liouville-Ostrogradsky equality (2.28),

$$\begin{aligned} f(x) &= -\frac{1}{\pi}\operatorname{Im}\frac{E_{\nu+1}(x)+Q_\nu(x)E_\nu(x)}{D_{\nu+1}(x)+Q_\nu(x)D_\nu(t)} = \\ &= \frac{1}{2\pi i}\left(\frac{E_{\nu+1}(x)+\overline{Q_\nu(x)}E_\nu(x)}{D_{\nu+1}(x)+\overline{Q_\nu(x)}D_\nu(x)} - \frac{E_{\nu+1}(x)+Q_\nu(x)E_\nu(x)}{D_{\nu+1}(x)+Q_\nu(x)D_\nu(x)}\right) = \\ &= \frac{Q_\nu(x)-\overline{Q_\nu(x)}}{2\pi i}\frac{D_\nu(x)E_{\nu+1}(x)-E_\nu(x)D_{\nu+1}(x)}{\left|D_{\nu+1}(x)+Q_\nu(x)D_\nu(x)\right|^2} = \\ &= \frac{\Delta_\nu}{\pi\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}}\frac{\operatorname{Im}Q_\nu(x)}{\left|D_{\nu+1}(x)+Q_\nu(x)D_\nu(x)\right|^2}. \end{aligned}$$

The "problem" is that the determinant $\Delta_{\nu+1}$ (see (2.41)) 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 $\{D_l(t)\}_{l=0}^{\nu+1}$: use instead the monic polynomials $\{\mathrm{D}_l(t)\}_{l=0}^{2\nu}$:

$$\begin{aligned} f(x) &= \frac{\Delta_\nu}{\pi\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}}\frac{\operatorname{Im}Q_\nu(x)}{\left|D_{\nu+1}(x)+Q_\nu(x)D_\nu(x)\right|^2} = \\ &= \frac{\Delta_\nu}{\pi\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}}\frac{\operatorname{Im}Q_\nu(x)}{\left|\sqrt{\frac{\Delta_\nu}{\Delta_{\nu+1}}}\mathrm{D}_{v+1}(x)+Q_\nu(x)\sqrt{\frac{\Delta_{\nu-1}}{\Delta_\nu}}\mathrm{D}_v(x)\right|^2} = \\ &= \frac{\Delta_\nu}{\pi\Delta_{\nu-1}}\frac{\operatorname{Im}q_\nu(x)}{\left|\mathrm{D}_{v+1}(x)+q_\nu(x)\mathrm{D}_v(x)\right|^2} > 0, \end{aligned} \tag{2.43}$$

where

$$q_\nu(x) = Q_\nu(x)\sqrt{\frac{\Delta_{\nu+1}\Delta_{\nu-1}}{\Delta_\nu^2}}.$$

Notice that due to the positivity of the moment sequence (2.38), 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 $f(z)$, $\operatorname{Im} z < 0$ are the roots of the "polynomial" equation

$$\mathrm{D}_{v+1}(z) + q_v(z)\,\mathrm{D}_v(z) = 0, \tag{2.44}$$

[4]Remember that for any $z \in \mathbb{C}$,

$$\operatorname{Im} z = \operatorname{Im}(x+iy) = \frac{1}{2i}(z-\bar{z}) = ((x+iy)-(x-iy)).$$

which "starts" from z^{v+1}, i.e., if we approximate

$$q_v\left(z\right) = q_v\left(z = 0\right) = ih,$$

equation (2.44) acquires the form of the genuine polynomial equation of the order $v + 1$.

The method of moments with local constraints

The problem set-up

Consider the mixed Löwner-Nevanlinna problem [15, 2, 3, 6, 16], see also [17] for the matrix version of the problem.

Problem 48 *Given a set of real numbers $(\mu_0, \mu_1, ..., \mu_{2\nu})$, a finite set of points $(t_1, ..., t_p)$ on the real axis, and a set of complex numbers $(w_1, ..., w_p)$ with non-negative imaginary parts, find a function of the Nevanlinna class, $\varphi \in \mathfrak{R}_0$ such that asymptotically, for $z \to \infty$ inside any angle $\delta < \arg z < \pi - \delta$, $\delta > 0$,*

$$\varphi(z) = -\sum_{r=1}^{2\nu+1} \frac{\mu_{r-1}}{z^r} + \mathrm{o}\left(|z|^{-2\nu-1}\right) , \tag{2.45}$$

possesses continuous boundary values in some vicinities of the points $(t_1, ..., t_p)$ and

$$\varphi(t_s + i0) = w_s,\ s = 1, .., p. \tag{2.46}$$

Notice [3] that the condition (2.45) is equivalent to the moment conditions

$$\int_{-\infty}^{\infty} t^k f\,(t)\,dt = \mu_l,\ l = 0, 1, ..., 2\nu. \tag{2.47}$$

for the generating distribution density $f(t)$, such that

$$\varphi(z) = \int\limits_{-\infty}^{\infty} \frac{f\,(t)\,dt}{t - z},\ \mathrm{Im}\, z > 0. \tag{2.48}$$

The suggested Problem 48 is a mixture of the truncated Hamburger moment problem [16] with the Löwner-type interpolation problem in the class of Nevanlinna functions [15].

We describe and test numerically (see below) an algorithm for finding of non-rational solutions of this problem. We are interested in the possibility to solve the problem when only a very small number of moments and constraints (data at the interpolation nodes) is known. The behavior of the problem solution when the number of interpolation nodes grows is treated in [18].

The mixed problem solution

Solvability and contractive functions

Assume that the truncated Hamburger moments problem is solvable and that there exists an infinite set of non-negative measures densities $f(t)$ on the real axis satisfying (2.47).

As we know, these solutions of the truncated Hamburger moment problem are parametrized by the Nevanlinna parameter functions $\zeta_\nu(z) \in \mathfrak{R}_0$ by the Nevanlinna formula (2.20),

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{f(t)\,dt}{t-z} = -\frac{E_{\nu+1}(z) + \zeta_\nu(z) E_\nu(z)}{D_{\nu+1}(z) + \zeta_\nu(z) D_\nu(z)}, \quad \operatorname{Im} z > 0, \quad \nu = 0, 1, 2, \ldots, \tag{2.49}$$

which, according to the Nevanlinna theorem [2], establishes a one-to-one correspondence between the set of all Nevanlinna functions $\varphi(z)$ satisfying (2.45) and the elements $\zeta(z)$ of the subclass $\mathfrak{R}_0$.

Notice that since the zeros of each orthogonal polynomial $D_\nu(z)$ are real and by virtue of the Liouville-Ostrogradsky identity (2.28), the zeros of $D_\nu(z)$ alternate with the zeros of $D_{\nu+1}(z)$ as well as with the zeros of $E_\nu(z)$. Therefore *any function $\varphi(z)$ given by the expression on the right hand side of (2.49) has a continuous boundary value on the real axis if and only if the corresponding Nevanlinna function $\zeta_\nu(z) \in \mathfrak{R}_0$ is continuous in the closed upper half-plane and such that $\zeta_\nu(z)D_\nu(z)$ has no joint zeros with $D_{\nu+1}(z)$.*

To meet the constraints (2.46) it is enough to substitute into the r.h.s. of (2.49) any function $\zeta_\nu(z) \in \mathfrak{R}_0$ which is continuous in the closed upper half-plane and satisfies the following conditions:

$$\xi_s^{(\nu)} = \zeta_\nu(t_s) = -\frac{w_s D_{\nu+1}(t_s) + E_{\nu+1}(t_s)}{w_s D_\nu(t_s) + E_\nu(t_s)}, \; s = 1, .., p. \tag{2.50}$$

Note that by (2.28),

$$\operatorname{Im} \xi_s^{(\nu)} = \frac{\Delta_\nu}{\sqrt{\Delta_{\nu-1}\Delta_{\nu+1}}} \frac{\operatorname{Im} w_s}{|w_s D_\nu(t_s) + E_\nu(t_s)|^2} > 0, \; s = 1, ..., p.$$

Thus Problem 5 reduces to

Problem 49 *Given a finite number of distinct points $t_1, ..., t_p$ of the real axis and a set of complex numbers $w_1, ..., w_p$ with positive imaginary parts, find the set of functions $\zeta_\nu(z) \in \mathfrak{R}_0$ continuous in the closed upper half-plane which satisfy conditions (2.50).*

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

$$\zeta_\nu(z) = i\frac{1 + \theta^{(\nu)}(z)}{1 - \theta^{(\nu)}(z)}, \tag{2.51}$$

where

$$\theta^{(\nu)}(z) = \frac{\zeta_\nu(z) - i}{\zeta_\nu(z) + i} \tag{2.52}$$

is a holomorphic function on the upper half-plane with *contractive* values, i.e. $\left|\theta^{(\nu)}(z)\right| \leq 1, \ \mathrm{Im}\, z > 0$. The function $\theta^{(\nu)}(z)$ connected with the Nevanlinna function $\zeta_\nu(z)$ by the linear fractional transformation (2.52) is continuous in the closed upper half-plane if $\zeta_\nu(z)$ satisfies this condition. On the other hand, the Nevanlinna function $\zeta_\nu(z)$ given as the linear fractional transformation (2.51) of a function $\theta^{(\nu)}(z)$ which is holomorphic on the upper half-plane, continuous in its closure, and has contractive values, is continuous at the points of the closed upper half-plane where $\theta^{(\nu)}(z) \neq 1$. Therefore Problem 49 is equivalent to the following problem for contractive functions.

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

Problem 50 *Given a finite number of distinct points $t_1, ..., t_p$ of the real axis and a set of points $\lambda_1^{(\nu)}, ..., \lambda_p^{(\nu)}$,*

$$\lambda_s^{(\nu)} = \frac{\xi_s^{(\nu)} - i}{\xi_s^{(\nu)} + i}, \ \left|\lambda_s^{(\nu)}\right| \leq 1, \ s = 1, ..., p. \tag{2.53}$$

find a set of functions $\theta^{(\nu)} \in \mathfrak{B}$ such that

$$\theta^{(\nu)}(t_s) = \lambda_s^{(\nu)}, \ s = 1, ..., p. \tag{2.54}$$

Problem 50 is a limiting case of the Nevanlinna-Pick problem [3, 2] with interpolation nodes on the real axis. Its solvability for any interpolation data $\lambda_1^{(\nu)}, ..., \lambda_p^{(\nu)}$ inside the unit circle was actually proven in [19]. The point is that the associated Pick matrix is automatically positive definite for given contractive interpolation values once the interpolation nodes are close enough to the axis; this guarantees that the approximate Nevanlinna-Pick problem is solvable once the interpolation nodes are close enough to the real line. Then one applies the Vitali-Montel theorem to take the limit as the interpolation nodes go to the real line. This implies also that the Nevanlinna-Pick problem is solvable even if some or all $\left|\lambda_s^{(\nu)}\right| = 1$.

We describe below an algorithm of solution of Problem 50 when all $\left|\lambda_s^{(\nu)}\right| < 1$, 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 $\left|\lambda_s^{(\nu)}\right| = 1$ [16].

Schur algorithm

Note that a function $\theta^{(\nu)} \in \mathfrak{B}$ satisfies the condition

$$\theta^{(\nu)}(t_1) = \lambda_1^{(\nu)}, \ \left|\lambda_1^{(\nu)}\right| < 1,$$

if and only if it admits the representation

$$\theta^{(\nu)}(z) = \frac{\phi_\nu(z) + \lambda_1^{(\nu)}}{\overline{\lambda_1^{(\nu)}}\phi_\nu(z) + 1}\ , \tag{2.55}$$

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

$$\phi_\nu(z) = \frac{z - t_1}{z - \overline{t_1}}\chi_\nu(z)\ ,$$

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

Here we carry out the reconstruction procedure using the non-rational functions, in particular, using the function [16]

$$\phi_\nu(z) = \theta_1^{(\nu)}(z) \exp\left\{\frac{\alpha}{\pi i}\int\limits_{t_1-1}^{t_1+1} \frac{1+tz}{t-z} \ln|t-t_1| \frac{dt}{t^2+1}\right\} := \theta_1^{(\nu)}(z)\, u_1^{(\nu)}(z)\,, \tag{2.56}$$

with a unique free parameter $\alpha \in (0,1)$ [5] Here $\theta_1^{(\nu)}$ is any function from $\mathfrak{B}$ such that

$$\theta_1^{(\nu)}(t_s) = \left(\lambda_s^{(\nu)}\right)' = \frac{1}{u_1^{(\nu)}(t_s)} \frac{\lambda_s^{(\nu)} - \lambda_1^{(\nu)}}{1 - \overline{\lambda_1^{(\nu)}}\lambda_s^{(\nu)}},\ s = 2, ..., p. \tag{2.57}$$

Such a choice of $\theta_1^{(\nu)}(z)$ guarantees the verification of all of the conditions (2.54). Hence Problem 50 with p nodes of interpolation on the real axis and strictly contractive values of the functions to find at these nodes, reduces to the same problem but with $p-1$ nodes of interpolation and modified values at these nodes given by (2.57). 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 $t_{s+1}, ..., t_p$ according to (2.57), permits to obtain some solution of Problem 50. Observe that contrary to the Nevanlinna-Pick

[5] This parameter can be found by the Shannon entropy maximization procedure [20].

problem with nodes in the open upper half-plane, our Problem 50 is always solvable if the values of the function to reconstruct are contractive at the nodes of interpolation.

Let $\theta_{s-1}^{(\nu)} \in \mathfrak{B}$ be a contractive function emerging after the $s-1$ step in the course of the Problem 50 solution by the above method, and let $\left(\lambda_s^{(\nu)}\right)^{(s-1)} = \theta_{s-1}^{(\nu)}(t_s)$, $\left(\lambda_1^{(\nu)}\right)^{(0)} = \lambda_1^{(\nu)}$. It follows from the above arguments that should the initial parameters $\lambda_1^{(\nu)}, ..., \lambda_p^{(\nu)}$ be strictly contractive, there exists a set of solutions of Problem 50 described by the formula

$$\theta^{(\nu)}(z) = \frac{a^{(\nu)}(z)\mu^{(\nu)}(z) + b^{(\nu)}(z)}{c^{(\nu)}(z)\mu^{(\nu)}(z) + d^{(\nu)}(z)}, \tag{2.58}$$

where the elements of the matrix of the linear fractional transformation (2.58) are non-rational functions constructed as above and $\mu^{(\nu)}(z)$ runs the subset of all functions from $\mathfrak{B}$ satisfying the condition $\mu^{(\nu)}(t_p) = \left(\lambda_p^{(\nu)}\right)^{(p-1)}$. This matrix can be calculated as

$$\begin{pmatrix} a^{(\nu)}(z) & b^{(\nu)}(z) \\ c^{(\nu)}(z) & d^{(\nu)}(z) \end{pmatrix} = \overset{\curvearrowright}{\prod_{s=1}^{p-1}} \begin{pmatrix} \dfrac{u_s^{(\nu)}(z)}{\left(\lambda_s^{(\nu)}\right)^{(s-1)}} u_s^{(\nu)}(z) & \left(\lambda_s^{(\nu)}\right)^{(s-1)} \\ & 1 \end{pmatrix}, \tag{2.59}$$

where numbers s in matrix factors on the right hand side increase from left to right.

Observe that the simplest choice for the function $\mu(z)$ in (2.58) is just $\mu^{(\nu)}(z) \equiv \left(\lambda_p^{(\nu)}\right)^{(p-1)}$. Hence, if initial parameters $\lambda_1^{(\nu)}, ..., \lambda_p^{(\nu)}$ in Problem 50 are strictly contractive, then among the solutions of this problem there are non-rational functions of the type we consider.

A numerical testing of this representation is given in the next Section.

An example

Consider a physically interesting case of $\nu = 2$ and $p = 1$.

Precisely, let

$$\varphi(z) = \int_{-\infty}^{\infty} \frac{f(\omega)\, d\omega}{\omega - z}, \ \operatorname{Im} z > 0. \tag{2.60}$$

with

$$f(\omega) = -\frac{\operatorname{Im} \epsilon^{-1}(\omega)}{\pi\omega}, \tag{2.61}$$

$$\epsilon^{-1}(\omega) = 1 - \frac{4\pi i}{\omega}\sigma^{ext}(\omega)$$

being the inverse dielectric function, compare to Section 2. Notice also that

$$f(\omega) = 4\,\mathrm{Re}\,\sigma^{ext}(\omega)/\omega^2, \tag{2.62}$$

where $\sigma^{ext}(\omega)$ is the system external conductivity,

$$\sigma^{ext}(\omega) = \frac{\sigma^{int}(\omega)}{1+\frac{4\pi i}{\omega}\sigma^{int}(\omega))}$$

and $\sigma^{int}(\omega)$ is the system internal conductivity such that $\sigma_0 = \sigma^{int}(\omega=0) < \infty$ is the static conductivity. Then we have the following sum rules [21]:

$$C_0 = \int_{-\infty}^{\infty} f(t)dt = 1, \quad C_1 = C_3 = 0, \tag{2.63}$$

$$C_2 = \int_{-\infty}^{\infty} t^2 f(t)dt = \omega_p^2 \quad , \tag{2.64}$$

(ω_p, as before, is the plasma frequency), and

$$C_4 = \int_{-\infty}^{\infty} t^4 f(t)dt := \omega_p^2\left(\omega_p^2+\Omega^2\right), \tag{2.65}$$

since, due to the Cauchy-Schwarz inequality (see Section IV), $C_0C_4 - C_2^2 > 0$.

Hence, by virtue of the Nevanlinna theorem,

$$\varphi_2(z) = -\frac{\mathrm{E}_3(z)+q_2(z)\mathrm{E}_2(z)}{\mathrm{D}_3(z)+q_2(z)\mathrm{D}_2(z)}, \quad \mathrm{Im}\,z>0, \tag{2.66}$$

where we can put

$$\begin{aligned} &\mathrm{D}_0(z)=1, \quad \mathrm{D}_1(z)=z, \quad \mathrm{D}_2(z)=z^2-\omega_p^2,\\ &\mathrm{D}_3(z)=z^3-z\left(\omega_p^2+\Omega^2\right), \quad \mathrm{E}_0(z)\equiv 0, \quad \mathrm{E}_1(z)=C_0,\\ &\mathrm{E}_2(z)=C_0 z, \quad \mathrm{E}_3(z)=C_0\left(z^2-\Omega^2\right), \end{aligned} \tag{2.67}$$

and

$$\omega_1^2 = \frac{C_2}{C_0} = \omega_p^2\,, \quad \omega_2^2 = \frac{C_4}{C_2} = \omega_p^2+\Omega^2\ . \tag{2.68}$$

Thus, at $z=\omega_0\in\mathbb{R}$ let

$$\Phi = \varphi_2(\omega_0) = -P.V.\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,\epsilon^{-1}(\omega)\,d\omega}{\pi\omega(\omega-\omega_0)} + \frac{\mathrm{Im}\,\epsilon^{-1}(\omega_0)}{i\omega_0}\in\mathbb{C},$$

and

$$\begin{aligned}\psi &= \Phi\omega_0+1 = \omega_0\varphi(\omega_0)+1 = \\ &= 1-\omega_0 P.V.\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,\epsilon^{-1}(\omega)\,d\omega}{\pi\omega(\omega-\omega_0)} - i\,\mathrm{Im}\,\epsilon^{-1}(\omega_0)\\ &= 1+\epsilon^{-1}(\omega=0)-\epsilon^{-1}(\omega=\omega_0) = 1-\epsilon^{-1}(\omega_0)\,.\end{aligned} \tag{2.69}$$

Observe that the latter expression was obtained using the Kramers-Kronig relations,

$$\epsilon^{-1}(\omega) = 1 + P.V. \int_{-\infty}^{\infty} \frac{\operatorname{Im} \epsilon^{-1}(s)\, ds}{\pi (s-\omega)} + i \operatorname{Im} \epsilon^{-1}(\omega)$$

and that with $\sigma_0 < \infty$,

$$\epsilon^{-1}(0) = \lim_{\omega \to 0} \left(1 + \frac{4\pi i}{\omega} \sigma^{int}(\omega) \right)^{-1} = 0$$

so that with $\omega_0 = 0$ in (2.69), $\psi = 1$, while, due to the parity of (2.61),

$$\Phi_0 = \varphi_2(0) = \lim_{\omega \to 0} \frac{\operatorname{Im} \epsilon^{-1}(\omega)}{i\omega}$$

with $\operatorname{Im} \Phi_0 > 0$. It is important that the latter parameter has a clear physical meaning. Indeed, since

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega} \sigma^{int}(\omega)$$

with

$$\operatorname{Re} \sigma^{int}(\omega = 0) = \sigma_0 = \frac{\omega_p^2 \tau}{4\pi}, \quad \operatorname{Im} \sigma^{int}(\omega = 0) = 0, \;\; \Phi_0 = \frac{i}{\tau \omega_p^2}. \tag{2.70}$$

Then

$$\gamma = \frac{Q_2(\omega_0)}{\omega_p} = -\frac{1}{\omega_p} \frac{\Phi_0 \mathrm{D}_3(\omega_0) + \mathrm{E}_3(\omega_0)}{\Phi_0 \mathrm{D}_2(\omega_0) + \mathrm{E}_2(\omega_0)} = -\frac{\omega_0}{\omega_p} + \frac{\psi \Omega^2}{\left(\psi \omega_0 - \Phi_0 \omega_p^2\right) \omega_p} \in \mathbb{C} \tag{2.71}$$

with

$$\gamma_0 = \frac{Q_2(0)}{\omega_p} = -\frac{\Omega^2}{\Phi_0 \omega_p^3} = i \frac{\tau \Omega^2}{\omega_p} := ih.$$

To mention that if we possess numerical data on the loss function (2.61) or the measure (2.62), we can use the latter of the relations (2.70) to find the transport relaxation time τ and the static conductivity.

We want to reconstruct the Nevanlinna function $q_2(z) \in \mathfrak{R}_0$ such that (2.71) would hold. Our Shur-like algorithm reduces the search for the function $q_2(z)$ to the construction of a contractive function $r(z)$

$$r(z) = \frac{q_2(z) - i\omega_p}{q_2(z) + i\omega_p} \tag{2.72}$$

such that

$$v = r(z = \omega_0) = \frac{\gamma - i}{\gamma + i}, \; |v| < 1. \tag{2.73}$$

By virtue of (2.59),

$$r(z) = \frac{u(z)+1}{\overline{v}u(z)+v^{-1}}, \tag{2.74}$$

with

$$u(z) = \exp\left\{\frac{\alpha}{\pi i}\int_{\omega_0-1}^{\omega_0+1}\frac{1+sz}{s-z}\ln|s-\omega_0|\frac{ds}{s^2+1}\right\},\ \alpha\in(0,1)\,, \tag{2.75}$$

which vanishes at $z=\omega_0$ [6]. Thus,

$$q_2(z) = i\omega_p\frac{1+r(z)}{1-r(z)} = i\omega_p\frac{(\overline{v}+1)\,u(z)+v^{-1}+1}{(\overline{v}-1)\,u(z)+v^{-1}-1} \tag{2.76}$$

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

$$q_2(0) = i\tau\Omega^2\ . \tag{2.77}$$

The corresponding model expression for the internal conductivity,

$$\sigma^{int}\,(z) = \frac{i\omega_p^2}{4\pi}\frac{z+i\tau\Omega^2}{z^2-\Omega^2\,(1-iz\tau)} \tag{2.78}$$

automatically satisfies the sum rules (2.63), (2.64) and (2.65) and interpolates between the static conductivity $\sigma_0=\omega_p^2\tau/4\pi$ and the asymptotic expansion

$$\sigma^{int}\,(z\to\infty) \simeq \frac{i\omega_p^2}{4\pi z}+\frac{i\omega_p^2\Omega^2}{4\pi z^3}+\cdots\,,\quad \operatorname{Im} z>0. \tag{2.79}$$

We can obtain a rational model for the Nevanlinna parameter function if we put, e.g., $u\,(z)=z/\,(z+is)$ with some positive parameter s. Then

$$q_2\,(z) = ih^2\omega_p\frac{z+i\delta}{z+ih\delta}, \tag{2.80}$$

where

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

Alternatively, a non-rational model for the function $q_2\,(z)$ follows from (2.76), (2.73), and (2.71).

Exercise 51 *Obtain the asymptotic expansion (2.79).*

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[6] Notice that $\operatorname{Im}\left(\frac{1}{\pi}\int_{t-1}^{t+1}\frac{1+sz}{s-z}\ln|s-t|\,\frac{ds}{s^2+1}\right)\underset{z\downarrow t}{\to}-\infty.$

Part II

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 (see Sections 4 and 5), and provide an example of application of the method of moments with local constraints, Section 4. We start with the

Chapter 3

Calculation of power moments on the basis of the Kubo linear theory

Introduction and the zero moment

In Chapter 2 we have seen that the method of moments expresses the dynamic (i.e., frequency-dependent) characteristics of the system in terms of the static (frequency-independent) ones. 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 system inverse (longitudinal) dielectric function, $\epsilon^{-1}(k,\omega)$ (IDF), the sum rules are effectively the power frequency moments of the (positive) loss function $\mathcal{L}(k,\omega) = -\operatorname{Im}\epsilon^{-1}(k,\omega)/\omega$:

$$C_\nu(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^\nu \mathcal{L}(k,\omega)\, d\omega, \quad \nu = 0, 2, 4. \tag{3.1}$$

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

$$\omega_1^2(k) = \frac{C_2}{C_0(k)}, \quad \omega_2^2(k) = \frac{C_4(k)}{C_2}. \tag{3.2}$$

The procedure we will describe here is applicable to the calculation of higher order convergent moments as well.

Since the IDF is a genuine response function [11] and thus satisfies, by virtue of the causality principle, the Kramers-Kronig relations (2.4), some general properties of the static dielectric function $\epsilon(k,0)$ can be obtained, Besides, we know that the moments (3.1) determine the asymptotic expansion of the IDF [3], see Section 2. Indeed, due to the the Kramers-Kronig relations (see also (5.24)),

$$\epsilon^{-1}(k,z) = 1 + \frac{1}{\pi}\int\limits_{-\infty}^{\infty} \frac{\operatorname{Im}\epsilon^{-1}(k,\omega)}{\omega - z} d\omega \,,\operatorname{Im} z > 0, \tag{3.3}$$

with the limiting value at $\operatorname{Im} z = 0$ understood as

$$\begin{aligned}\epsilon^{-1}(k,\omega) &= 1 + \frac{1}{\pi}\lim_{\eta\downarrow 0}\int\limits_{-\infty}^{\infty} \frac{\operatorname{Im}\epsilon^{-1}(k,\omega')}{\omega' - \omega - i\eta} d\omega' = \\ &= 1 + \frac{1}{\pi} P.V. \int\limits_{-\infty}^{\infty} \frac{\operatorname{Im}\epsilon^{-1}(k,\omega')}{\omega' - \omega} d\omega' + i \operatorname{Im}\epsilon^{-1}(k,\omega) \end{aligned} \tag{3.4}$$

Particularly, since the imaginary part is an odd function of frequency and thus vanishes at $\omega = 0$,

$$\epsilon^{-1}(k,0) = 1 + \frac{1}{\pi} P.V. \int\limits_{-\infty}^{\infty} \frac{\operatorname{Im}\epsilon^{-1}(k,\omega)}{\omega} d\omega.$$

We assume here that the static dielectric function $\epsilon(k,0)$ exists. We will see that the integrand in this principal value integral has a removable singularity, which means that it converges as a usual Riemann integral. The latter is actually the zero power moment of the loss function:

$$C_0(k) = -\int_{-\infty}^{\infty} \frac{\operatorname{Im}\epsilon^{-1}(k,\omega)}{\pi\omega} d\omega = 1 - \epsilon^{-1}(k,0)\,. \tag{3.5}$$

The relation of the zero moment to the system static structure factor charge-charge is discussed below in Sect. 5.

The power moments C_2 and C_4 are found in Appendix IV; particularly, it matters that even if the interparticle interaction might be different from the bare Coulomb one and is described by an effective potential, the second power moment of the loss function, due to the f-sum rule [11], remains unchanged and equal to the square of the dust plasma frequency (for simplicity we deal here with a hydrogen-like completely ionized plasma in thermal equilibrium with the species $a = 0, 1, \dots s$ whose charge numbers and masses are Z_a and m_a):

$$C_2 = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^2 \mathcal{L}(k,\omega)\, d\omega \equiv \omega_p^2 = \sum_{a=0}^{s} \frac{4\pi Z_a^2 e^2 n_a}{m_a}, \tag{3.6}$$

Like in (2.40) one can study the asymptotic expansion of the IDF along any ray in the upper half-plane:

$$\epsilon^{-1}(k,z) = \epsilon^{-1}(k,0) + \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\mathcal{L}(k,\omega)\,d\omega}{1-\frac{\omega}{z}}$$

$$\underset{z\to\infty}{\simeq} \epsilon^{-1}(k,0) + \frac{1}{\pi}\int_{-\infty}^{\infty}\left(1+\frac{\omega}{z}+\left(\frac{\omega}{z}\right)^2+\left(\frac{\omega}{z}\right)^3+\left(\frac{\omega}{z}\right)^4+\cdots\right)\mathcal{L}(k,\omega)\,d\omega =$$

$$= \epsilon^{-1}(k,0) + C_0(k) + \frac{C_2}{z^2} + \frac{C_4(k)}{z^4} + \cdots =$$

$$= 1 + \frac{\omega_{pd}^2}{z^2} + \frac{\omega_{pd}^2\omega_2^2(k)}{z^4} + \cdots .$$

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

$$\epsilon(k,z) \underset{z\to\infty}{\simeq} 1 - \frac{\omega_p^2}{z^2} - \frac{\omega_p^2}{z^4}\left(\omega_2^2(k) - \omega_{pd}^2\right) + \cdots . \tag{3.7}$$

The loss function second and fourth power moments

Definitions

For the higher order power frequency moments (3.1),

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

directly, from the Kubo linear reaction theory formula applied to our model system, we get:

$$\begin{aligned}\mathcal{L}(k,\omega) &= \frac{2\pi^2}{\hbar\omega k^2}\int_{-\infty}^{\infty} \Phi(\mathbf{k},t)\, e^{i\omega t} dt,\\ \omega^\nu \mathcal{L}(k,\omega) &= \frac{2\pi^2}{\hbar k^2} i \int_{-\infty}^{\infty} \frac{\partial^{\nu-1}\Phi(\mathbf{k},t)}{\partial t^{\nu-1}} e^{i\omega t} dt.\end{aligned} \tag{3.8}$$

To obtain expression (3.8) we have used the limiting property

$$\lim_{t\to\pm\infty} \Phi(\mathbf{k},t) = 0$$

of the correlation function

$$\Phi(\mathbf{k},t) = \langle [n_{\mathbf{k}}(t),\ n_{-\mathbf{k}}(0)] \rangle,$$

and have integrated by part $\nu - 1$ times.

These formulas are valid if $\Phi(\mathbf{k},t)$ is differentiable with respect to time and has integrable time derivatives. Then, by virtue of the time reversibility, we obtain:

$$C_\nu(k) = \frac{4\pi i}{\hbar k^2}\frac{\partial^{\nu-1}\Phi(\mathbf{k},0)}{i^{1-\nu}\partial t^{\nu-1}} = \frac{4\pi i}{\hbar k^2}\left\langle \left[\overset{(\nu-1)}{\rho_{\mathbf{k}}}(0),\ \rho_{-\mathbf{k}}(0) \right] \right\rangle. \tag{3.9}$$

The operator derivatives in (3.9) are determined by the formulas:

$$\dot{\rho}_{\mathbf{k}}(0) = \frac{1}{i\hbar}\left[\rho_{\mathbf{k}}(0),\ \hat{H}_0\right], \quad \ddot{\rho}_{\mathbf{k}}(0) = \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}}(0),\ \hat{H}_0\right], \ldots, \tag{3.10}$$

where $\hat{H}_0$ is the system Hamiltonian in the absence of the external field. Since for arbitrary Heisenberg operators $\hat{A}$ and $\hat{B}$ taken at simultaneous time instants, we have that

$$\left\langle \left[\dot{\hat{A}},\ \hat{B} \right] \right\rangle = -\left\langle \left[\hat{A},\ \dot{\hat{B}} \right] \right\rangle,$$

even order moments

$$C_{2l}(k) = \frac{4\pi i}{\hbar k^2}\left\langle\left[\overset{(l+1)}{\rho_{\mathbf{k}}}(0)\,,\ \overset{(l)}{\rho_{-\mathbf{k}}}(0)\right]\right\rangle, \quad l = 1, 2. \tag{3.11}$$

To calculate the moments explicitly, use now the representation of the charge density operator $\rho_{\mathbf{k}}(0) \equiv \rho_{\mathbf{k}}$ in terms of the operators of creation and annihilation of the species a particles possessing a quantal momentum $\hbar\mathbf{q}$ and being in a spin state τ, $a^{+}_{\mathbf{q}\tau}$, $a_{\mathbf{q},\tau}$, respectively,

$$\rho_{\mathbf{k}} = \frac{e}{\sqrt{V}}\sum_{a,\mathbf{q},\tau} Z_a a^{+}_{\mathbf{q}-\mathbf{k},\tau} a_{\mathbf{q},\tau}\ , \tag{3.12}$$

(V is the system volume) and the explicit representation of the external-field-free Hamiltonian,

$$\hat{H}_0 = \hat{K} + \hat{W} = \sum_{a,\mathbf{q},\tau}\frac{\hbar^2 q^2}{2m_a} a^{+}_{\mathbf{q},\tau} a_{\mathbf{q},\tau} + \frac{1}{2}\sum_{a,b}\sum_{\mathbf{q}}{}' W_{ab}(q)\left(n^a_{\mathbf{q}} n^b_{-\mathbf{q}} - \delta_{ab} n_a\right). \tag{3.13}$$

Here m_a is the species a mass; the prime at the sum over $\mathbf{q}$ means that the value $\mathbf{q} = \mathbf{0}$ must be omitted. In what follows we omit the spin indices, they cannot influence the results since the interaction (3.14) we consider is spin-independent; these results will be mainly independent of the statistics type.

We consider a quite general case with

$$W_{ab}(q) = \frac{4\pi e^2}{q^2}\zeta_{ab}(q)\,, \quad \zeta_{ab}(q) = \zeta_{ba}(q)\,, \tag{3.14}$$

being the effective interaction potential for the particles of species a and b (in a purely Coulomb system $\zeta_{ab} = Z_a Z_b$), while

$$n^a_{\mathbf{q}} = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a^{+}_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\ ;\ \langle n^a_{\mathbf{0}}\rangle = \frac{N_a}{\sqrt{V}} = n_a\sqrt{V}, \tag{3.15}$$

where N_a is the number of charged particles of the species a in the volume V occupied by the system we consider, $N_a = n_a V$. The averaging in (3.9) and further is carried out over the canonical ensemble defined by the Hamiltonian (3.13).

The f-sum rule

Thus with $\dot{\rho}_{\mathbf{k}} = \overset{(1)}{\rho_{\mathbf{k}}}$ and $\rho_{\mathbf{k}} = \overset{(0)}{\rho_{\mathbf{k}}}$, we obtain:

$$C_2(k) = \frac{4\pi i}{\hbar k^2}\left\langle\left[\dot{\rho}_{\mathbf{k}}, \rho_{-\mathbf{k}}\right]\right\rangle. \tag{3.16}$$

Since the f-sum rule is independent of the direct interaction contribution to the Hamiltonian, we observe that $\left[\rho_{\mathbf{k}}, \hat{W}\right] = 0$ and that the density operator time derivative can be calculated simply as

$$\dot{\rho}_{\mathbf{k}} = \frac{1}{i\hbar}\left[\rho_{\mathbf{k}}, \hat{K}\right] = \frac{e}{i\hbar\sqrt{V}} \sum_{a,b,\mathbf{q},\mathbf{p}}{}' Z_a \varepsilon_b(\mathbf{p}) \left[a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}}, b^+_{\mathbf{p}} b_{\mathbf{p}}\right]$$

with

$$\varepsilon_a(\mathbf{p}) = \frac{\hbar^2 |\mathbf{p}|^2}{2m_a} = \frac{\hbar^2 p^2}{2m_a}.$$

We presume that the charged particles are all fermions and we know that for fermions the anticommutators

$$\left\{a^+_{\mathbf{s}}, b^+_{\mathbf{r}}\right\} = a^+_{\mathbf{s}} b^+_{\mathbf{r}} + b^+_{\mathbf{r}} a^+_{\mathbf{s}} = 0, \tag{3.17}$$

$$\left\{a_{\mathbf{s}}, b_{\mathbf{r}}\right\} = a_{\mathbf{s}} b_{\mathbf{r}} + b_{\mathbf{r}} a_{\mathbf{s}} = 0, \tag{3.18}$$

but

$$\left\{a^+_{\mathbf{s}}, b_{\mathbf{r}}\right\} = a^+_{\mathbf{s}} b_{\mathbf{r}} + b_{\mathbf{r}} a^+_{\mathbf{s}} = \delta_{ab}\delta_{\mathbf{sr}} \tag{3.19}$$

and

$$\left\{b^+_{\mathbf{s}}, a_{\mathbf{r}}\right\} = b^+_{\mathbf{s}} a_{\mathbf{r}} + a_{\mathbf{r}} b^+_{\mathbf{s}} = \delta_{ab}\delta_{\mathbf{sr}} \ . \tag{3.20}$$

Exercise 52 *Prove that*

$$\left[a^+_{\mathbf{s}} a_{\mathbf{u}}, b^+_{\mathbf{r}} b_{\mathbf{t}}\right] = \delta_{ab}\left(\delta_{\mathbf{ur}} a^+_{\mathbf{s}} b_{\mathbf{t}} - \delta_{\mathbf{st}} b^+_{\mathbf{r}} a_{\mathbf{u}}\right), \tag{3.21}$$

where δ_{ab} and $\delta_{\mathbf{rs}}$ are, of course, the Kronecker symbols.

Exercise 53 *Prove that*

$$\left[a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}}, \ \left(n^c_{\mathbf{p}} n^b_{-\mathbf{p}} - \delta_{cb} n_a\right)\right] =$$

$$= \frac{\delta_{ab}}{\sqrt{V}}\left(n^c_{\mathbf{p}} a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}-\mathbf{p}} - n^c_{\mathbf{p}} a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}} a_{\mathbf{q}}\right) + \frac{\delta_{ac}}{\sqrt{V}}\left(a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}+\mathbf{p}} n^b_{-\mathbf{p}} - a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}} a_{\mathbf{q}} n^b_{-\mathbf{p}}\right). \tag{3.22}$$

Now, we are able to simplify the first derivative:

$$\begin{aligned}
\dot{\rho}_{\mathbf{k}} &= \frac{1}{i\hbar}\left[\rho_{\mathbf{k}}, \ \hat{H}_0\right] = \frac{e}{i\hbar\sqrt{V}} \sum_{a,b,\mathbf{q},\mathbf{p}}{}' Z_a \varepsilon_b(\mathbf{p})\, \delta_{ab} \left[a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}}, b^+_{\mathbf{p}} b_{\mathbf{p}}\right] = \\
&= \frac{e}{i\hbar\sqrt{V}} \sum_{a,\mathbf{q},\mathbf{p}} Z_a \varepsilon_a(\mathbf{p}) \left(\delta_{\mathbf{pq}} a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{p}} - \delta_{\mathbf{q}-\mathbf{k},\mathbf{p}} a^+_{\mathbf{p}} a_{\mathbf{q}}\right) = \\
&= \frac{e}{i\hbar\sqrt{V}} \sum_{a,\mathbf{q},\mathbf{p}} Z_a \left(\varepsilon_a(\mathbf{q})\, a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}} - \varepsilon_a(\mathbf{q}-\mathbf{k})\, a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}}\right) = \\
&= \frac{e\hbar}{2i\sqrt{V}} \sum_{a,\mathbf{q}} \frac{Z_a}{m_a} \left(q^2 - (\mathbf{q}-\mathbf{k})^2\right) a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}} = \\
&= \frac{e\hbar}{i\sqrt{V}} \sum_{a,\mathbf{q}} \frac{Z_a}{m_a} \left(\mathbf{q}\cdot\mathbf{k} - \frac{k^2}{2}\right) a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}}.
\end{aligned} \tag{3.23}$$

From (3.12) and (3.23) we have:

$$\begin{aligned}\left[\dot{\rho}_{\mathbf{k}},\ \rho_{-\mathbf{k}}\right] &= \left[\frac{e\hbar}{i\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-k^2/2\right)a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ \frac{e}{\sqrt{V}}\sum_{b,\mathbf{p}}Z_b b^+_{\mathbf{p}+\mathbf{k}}b_{\mathbf{p}}\right] = \\ &= \frac{e^2\hbar}{iV}\sum_{a,b,\mathbf{q},\mathbf{p}}{}' \frac{Z_aZ_b}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-k^2/2\right)\left[a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}}, b^+_{\mathbf{p}+\mathbf{k}}b_{\mathbf{p}}\right] =\end{aligned}$$

$$= \frac{e^2\hbar}{iV}\sum_{a,b,\mathbf{q},\mathbf{p}}{}' \frac{Z_aZ_b}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-k^2/2\right)\delta_{ab}\left(\delta_{\mathbf{p}+\mathbf{k},\mathbf{q}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{p}}-\delta_{\mathbf{q}-\mathbf{k},\mathbf{p}}a^+_{\mathbf{p}+\mathbf{k}}a_{\mathbf{q}}\right) =$$

$$\begin{aligned} &= \frac{e^2\hbar}{iV}\sum_{a,\mathbf{q}}\frac{Z_aZ_b}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-k^2/2\right)\left(a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}-\mathbf{k}}-a^+_{\mathbf{q}}a_{\mathbf{q}}\right) = \\ &= \frac{e^2\hbar}{iV}\sum_{a,\mathbf{q}}\frac{Z_a^2}{m_a}\left(\left((\mathbf{q}+\mathbf{k})\cdot\mathbf{k}-k^2/2\right)-\left(\mathbf{q}\cdot\mathbf{k}-k^2/2\right)\right)a^+_{\mathbf{q}}a_{\mathbf{q}} = \\ &= \frac{e^2\hbar}{iV}k^2\sum_{a,\mathbf{q}}\frac{Z_a^2}{m_a}a^+_{\mathbf{q}}a_{\mathbf{q}}\ ,\end{aligned}$$

wherefrom

$$\begin{aligned} C_2(k) &= \frac{4\pi i}{\hbar k^2}\left\langle\left[\dot{\rho}_{\mathbf{k}},\rho_{-\mathbf{k}}\right]\right\rangle = \frac{4\pi i}{\hbar k^2}\left\langle\frac{e^2\hbar}{iV}k^2\sum_{a,\mathbf{q}}\frac{Z_a^2}{m_a}a^+_{\mathbf{q}}a_{\mathbf{q}}\right\rangle = \\ &= 4\pi e^2\sum_a\frac{Z_a^2 n_a}{m_a}.\end{aligned}$$

Here, as before,

$$n_a = \frac{1}{V}\sum_{\mathbf{q}}\left\langle a^+_{\mathbf{q}}a_{\mathbf{q}}\right\rangle = \frac{N_a}{V}.$$

is the species a number density. Thus,

$$C_2(k) = \frac{1}{\pi}\int_{-\infty}^{\infty}\omega^2\mathcal{L}(k,\omega)\,d\omega = \omega_p^2 := 4\pi e^2\sum_a\frac{Z_a^2 n_a}{m_a}, \tag{3.24}$$

where ω_p is the system plasma frequency.

The 4^{th} moment

Similarly, see Appendix IV for details,

$$\begin{aligned}\ddot{\rho}_{\mathbf{k}} &= \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \left(\hat{K}+\hat{W}\right)\right] = \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{K}\right]+\frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{W}\right] = \\ &= \frac{-e\hbar^2}{\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a^2}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)^2 a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} + \\ &\quad + \frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{p}}{}'\frac{Z_a}{m_a}\left(\mathbf{p}\cdot\mathbf{k}\right)\frac{\zeta_{ab}(p)}{p^2}n^b_{-\mathbf{p}}n^a_{\mathbf{k}+\mathbf{p}}\ .\end{aligned}$$

Remember that the double prime means that the there is only one $a \neq b$ contribution and that the value $\mathbf{q} = \mathbf{0}$ is omitted.

Then, according to (3.11),

$$\begin{aligned} C_4(k) &= \int_{-\infty}^{\infty} \omega^4 \mathcal{L}(k,\omega)\, d\omega = C_4^K(k) + C_4^W(k) = \\ &= \pi e^2 \hbar^2 k^4 \sum_a \frac{Z_a^2 n_a}{m_a^3} + 8\pi e^2 k^2 \sum_a \frac{Z_a^2 n_a E_T^a}{m_a^2} + \end{aligned}$$

$$+\frac{16\pi^2 e^4}{V} \sum_{a,b,\mathbf{q}\neq\mathbf{0}} \frac{Z_a}{m_a} \zeta_{ab}(q) \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(\frac{Z_b}{m_b} \left\langle n^b_{-\mathbf{k}-\mathbf{q}} n^a_{\mathbf{k}+\mathbf{q}} \right\rangle - \frac{Z_a}{m_a} \left\langle n^b_{-\mathbf{q}} n^a_{\mathbf{q}} \right\rangle \right). \tag{3.25}$$

The average partial kinetic energy

$$E_T^a = \frac{m_a}{2} \left\langle v_a^2 \right\rangle = \frac{3}{2\beta} \frac{F_{3/2}(\eta_a)}{D_a^{3/2}},$$

where

$$F_\nu(\eta) = \int_0^\infty \frac{x^\nu}{\exp(x-\eta)+1} dx$$

is the order-ν Fermi integral, and $\eta_a = \beta\mu_a$ the dimensionless chemical potential of the subsystem a, which should be determined by the normalization condition

$$F_{1/2}(\eta_a) = \frac{2}{3} D_a^{3/2},$$

$$D_a = \beta E_{Fa} = \beta \frac{m_a v_{Fa}^2}{2} = \beta \frac{\hbar^2 k_{Fa}^2}{2m_a} = \beta \frac{\hbar^2 \left(3\pi^2 n_a\right)^{2/3}}{2m_a},$$

being the degeneracy parameter. Notice that in a classical case $F_{3/2}(\eta \to -\infty) \simeq D^{3/2}$.

We omit in the latter sum (3.25) the $\mathbf{q} = \mathbf{0}$ contribution, but the contribution which corresponds to $\mathbf{q} = -\mathbf{k}$ is present. This "singular" contribution equals

$$C_{4s}^W(k) = 16\pi^2 e^4 \sum_{a,b} \zeta_{ab}(k) \frac{Z_a Z_b}{m_a m_b} n_a n_b.$$

The rest, which is the correlation contribution, equals

$$C_{4c}^W(k) =$$

$$= 16\pi^2 e^4 {\sum_{a,b,\mathbf{q}}}' \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{ab}(q) \sqrt{n_a n_b} \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(\frac{Z_a Z_b}{m_a m_b} S_{ab}(\mathbf{k}+\mathbf{q}) - \frac{Z_a^2}{m_a^2} S_{ab}(q) \right) = \tag{3.26}$$

$$= 16\pi^2 e^4 \sum_a \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{Z_a^2}{m_a^2} \zeta_{aa}(q)\, n_a \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(S_{aa}(\mathbf{k}+\mathbf{q}) - S_{aa}(q) \right) +$$

$$+16\pi^2 e^4 \sum_{a\neq b} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{ab}(q) \sqrt{n_a n_b} \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(\frac{Z_a Z_b}{m_a m_b} S_{ab}(\mathbf{k}+\mathbf{q}) - \frac{Z_a^2}{m_a^2} S_{ab}(q) \right) =$$

$$= C_{4c}^{Ws}(k) + C_{4c}^{Wd}(k),$$

where

$$\begin{aligned} C_{4c}^{Ws}(k) &= 16\pi^2 e^4 \sum_a \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{Z_a^2}{m_a^2} \zeta_{aa}(q)\, n_a F_a(q), \\ F_a(q) &= \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(S_{aa}(\mathbf{k}+\mathbf{q}) - S_{aa}(q) \right), \end{aligned}$$

and

$$\begin{aligned} C_{4c}^{Wd}(k) &= 16\pi^2 e^4 \sum_{a\neq b} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{ab}(q) \sqrt{n_a n_b} F_{ab}(q), \\ F_{ab}(q) &= \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(\frac{Z_a Z_b}{m_a m_b} S_{ab}(\mathbf{k}+\mathbf{q}) - \frac{Z_a^2}{m_a^2} S_{ab}(q) \right). \end{aligned}$$

Here $S_{ab}(q)$ is the partial static structure factor which can be calculated by different numerical methods like the method of Ornstein - Zernike, the method of molecular dynamics, Monte - Carlo, etc. [22], or evaluated analytically using the method of temperature Green functions [23, 24].

Now we carry out integration over the angular variables (in a homogeneous system the result cannot depend on the direction of the vector $\mathbf{k}$) and thus simplify the same and different species contribution to the correlation part of the fourth moment. Let

$$Z_{ab}(q) = \int_{q-k}^{q+k} \zeta_{ab}(p) \left(q^2 - k^2 - p^2 \right)^2 \frac{dp}{qk^3 p}.$$

Then

$$C_{4c}^{Ws}(k) = 16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{aa}(q) \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(S_{aa}(\mathbf{k}+\mathbf{q}) - 1 \right) -$$

$$-16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{aa}(q) \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(S_{aa}(q) - 1 \right) =$$

$$= 16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int \frac{d\mathbf{p}}{(2\pi)^3} \zeta_{aa}(|\mathbf{p}-\mathbf{k}|) \frac{((\mathbf{p}-\mathbf{k})\cdot\mathbf{k})^2}{k^2 (\mathbf{p}-\mathbf{k})^2} \left(S_{aa}(p) - 1 \right) -$$

$$-16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{aa}(q) \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} (S_{aa}(q) - 1) =$$

$$= 16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int \frac{d\mathbf{q}}{(2\pi)^3} G_a(\mathbf{q}) (S_{aa}(q) - 1),$$

$$G_a(\mathbf{q}) = \zeta_{aa}(|\mathbf{q}-\mathbf{k}|) \frac{((\mathbf{q}-\mathbf{k})\cdot\mathbf{k})^2}{k^2 |\mathbf{q}-\mathbf{k}|^2} - \zeta_{aa}(q) \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2};$$

Hence,

$$C_{4c}^{Ws}(k) = 16\pi^2 e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int_0^\infty q^2 (S_{aa}(q) - 1)\, dq \int_{-1}^{1} \frac{G_a(q,s)\, ds}{(2\pi)^2}$$

with

$$G_a(q,s) = \zeta_{aa}\left(\sqrt{q^2 + k^2 - 2qks}\right) \frac{(qks - k^2)^2}{k^2 (q^2 + k^2 - 2qks)} - \zeta_{aa}(q)\, s^2,$$

or

$$C_{4c}^{Ws}(k) = e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int_0^\infty q^2 (S_{aa}(q) - 1) \left(Z_{aa}(q) - \frac{8\zeta_{aa}(q)}{3} \right) dq.$$

Notice that in the case of the pure Coulomb interaction,

$$C_{4c}^{Ws}(k) = e^4 \sum_a \frac{Z_a^2 n_a}{m_a^2} \int_0^\infty q^2 (S_{aa}(q) - 1)\, f(q,k)\, dq$$

with

$$f(q,k) = \frac{10}{3} - 2\frac{q^2}{k^2} + \frac{(q^2 - k^2)^2}{qk^3} \ln\left| \frac{q+k}{q-k} \right|,$$

so that the standard expression for the same-species correlation correction [6] is recovered.

Similarly,

$$C_{4c}^{Wd}(k) = 16\pi^2 e^4 \sum_{a\neq b} \int \frac{d\mathbf{q}}{(2\pi)^3} \zeta_{ab}(q) \sqrt{n_a n_b} F_{ab}(q),$$

$$F_{ab}(q) = \frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2} \left(\frac{Z_a Z_b}{m_a m_b} S_{ab}(\mathbf{k}+\mathbf{q}) - \frac{Z_a^2}{m_a^2} S_{ab}(q) \right),$$

so that

$$C_{4c}^{Wd}(k) = e^4 \sum_{a\neq b} \frac{Z_a}{m_a} \sqrt{n_a n_b} \int_0^\infty q^2 S_{ab}(q) \left(\frac{Z_b}{m_b} Z_{ab}(q) - \frac{8}{3} \frac{Z_a}{m_a} \zeta_{ab}(q) \right) dq,$$

and if we have species with significantly different charge-to-mass ratios, the different-species correction equal to $\omega_p^4 H = \omega_p^4 h_{ei}(0)/3$, $h_{ei}(0) = g_{ei}(0) - 1$, $g_{ei}(r)$ being the electron-ion radial distribution function [6], is also recovered.

Higher order moments

In the same way, higher order moments can be calculated, e.g. in model Coulomb systems with the effective potential (3.14) different from the bare Coulomb one. But in purely Coulomb systems containing species of different masses, the sixth and higher-order moments diverge [21]. This takes place because the corresponding explicit expressions contain uncompensated contributions like

$$\sum_{\mathbf{q}} \left\langle n^a_{\mathbf{q}} n^a_{-\mathbf{q}} \right\rangle = \infty.$$

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

$$\mathcal{L}(k, |\omega| \to \infty) \simeq A(k) / |\omega|^\gamma ,$$

then due to the divergence of the sixth moment and the convergence of the fourth one (3.25), we conclude that $5 < \gamma \leq 7$.

In a completely ionized plasma for $\omega \geq (\beta\hbar)^{-1}$ 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 ([25], and also, e.g., [27]) 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 $\omega \gg (\beta\hbar)^{-1}$ [26], lead to the following asymptotic form of $\mathrm{Im}\,\epsilon(k,\omega)$ in a completely ionized (for simplicity,hydrogen-like) plasma [21]:

$$\mathrm{Im}\,\epsilon\left(\mathbf{k}, \omega \gg (\beta\hbar)^{-1}\right) \simeq \frac{4\pi A_0}{\omega^{9/2}} \left(1 - \frac{\omega_T}{\omega} + \cdots\right), \qquad (3.27)$$

where

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

$n_i = Z n_e$. The main term of (3.27) was obtained by Perel' and Eliashberg [28]. One of our aims is to specify (3.27) taking into account the sum rules (3.1). Notice that even the main term of the plasma dielectric function asymptotic behavior (3.27) is still discussed in literature, producing sometimes even contradictory results [29].

Chapter 4

One-component plasmas

Introduction

The classical one-component plasma (OCP) might be considered a test-tube for the modelling of strongly interacting Coulomb systems [30], see also [31] and [32] for more recent reviews. OCP is often employed as a simplified version of real physical systems ranging from electrolytes and charged-stabilized colloids [33], laser-cooled ions in cryogenic traps [34] to dense astrophysical matter in white dwarfs and neutron stars [35]. 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 [36].

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

$$\Gamma = \beta \left(Ze\right)^2 / a \ . \tag{4.1}$$

Here β^{-1} stands for the temperature in energy units, Ze designates the ion charge, and $a = \left(3/4\pi n\right)^{1/3}$ is the Wigner-Seitz radius, n being the number density of charged particles. For $\Gamma \gtrsim 1$ the interaction effects determine the physical properties of the OCP.

The investigation of OCPs using the classical method of moments

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 found by computer simulations (see [31] and [32]). Moreover, molecular dynamics (MD) as well as other simulations can provide valuable information on the dynamic structure factor (DSF), $S(k,\omega)$ and other dynamic characteristics.

In this Section, the OCP dynamic properties are studied by the moment approach based on sum rules and other exact relations, see [37], [38] and references therein and comparison is made with the simulation data of Hansen, McDonald, and Pollock [39] and of Wierling, Pschiwul and Zwicknagel [32]. The results of alternative theoretical methods, the quasi-localized charge approximation (QLCA) [40, 41], [31], the visco-elastic approximation (VEA) [42, **?**], and the recurrence relation (RR) technique, [43, 32], are considered as well.

Precisely, the aim of this Section is threefold. First, we use the method of moments to study the OCP dispersion plasmon frequency, $\omega_L(k)$, the corresponding decay decrement, $\delta_L(k)$, and the dynamic local-field correction (DLFC), $G(k,\omega)$. Second, we compare our results on the dynamic structure factor to the MD simulation data of [39] and pay special attention to onset of the so called negative dispersion of the plasmon mode in strongly coupled OCPs by determining the range of the coupling parameter Γ within which the derivative $d\omega_L(k)/dk$ changes its sign. And third, we crosscheck our results against the theoretical methods mentioned above. In particular, we note that the plasmon decay rate cannot be studied within the QLCA approach due to its intrinsic nature and, to the best of our knowledge, its k-dependence was not referred to in the literature as yet. We also show how the VEA and RR results for the DLFC and the DSF can be retrieved and partly extended within the sum rule or moment approach.

Mathematical background

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

$$S_\nu(k) = \frac{1}{n}\int_{-\infty}^{\infty} \omega^\nu S(k,\omega)\, d\omega, \quad \nu = 0,1,2,3,4. \qquad (4.2)$$

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

The method of moments is, generally speaking, capable of handling any number of convergent sum rules. In two-component plasmas, though, all higher order frequency moments diverge which can be attributed to and understood [44] from the exact asymptotic form of the imaginary part of the dielectric function [28]. 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 (4.2) are the only convergent even order frequency sum rules. However, the ambiguity of higher-order frequency moments [42], 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.

As we know [3], the analytic prolongation of the positive function of frequency, DSF, onto the upper half-plane $\mathrm{Im}\, z > 0$, constructed by means of the Cauchy integral formula,

$$S(k,z) = \frac{1}{n}\int_{-\infty}^{\infty} \frac{S(k,\omega)}{\omega - z} d\omega, \tag{4.3}$$

admits the asymptotic expansion

$$S(k, z \to \infty) \simeq -\frac{S_0\,(k)}{z} - \frac{S_2\,(k)}{z^3} - \frac{S_4\,(k)}{z^5} - \mathrm{o}\left(\frac{1}{z^5}\right), \quad \mathrm{Im}\, z \geq 0. \tag{4.4}$$

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

$$S_2\,(k) = \omega_0^2\,(k) = \omega_p^2 \left(\frac{k^2}{k_D^2}\right) = \omega_p^2 \left(\frac{q^2}{3\Gamma}\right), \tag{4.5}$$

and

$$S_4\,(k) = \omega_p^2 \omega_0^2\,(k) \left\{1 + \frac{3k^2}{k_D^2} + U\,(k)\right\} = \omega_p^2 \omega_0^2\,(q) \left\{1 + \frac{q^2}{\Gamma} + U\,(q)\right\}. \tag{4.6}$$

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

$$U\,(q) = \frac{1}{4\pi^2 n} \int_0^{\infty} \left[S\,(k') - 1\right] f\,(k';k)\, k'^2 dk' = \frac{1}{3\pi} \int_0^{\infty} \left[S\,(p) - 1\right] f\,(p;q)\, p^2 dp,$$

where

$$f\,(p;q) = \frac{5}{6} - \frac{p^2}{2q^2} + \left(\frac{p^3}{4q^3} - \frac{p}{2q} + \frac{q}{4p}\right) \ln\left|\frac{q+p}{q-p}\right|, \quad q = ka,\ p = k'a.$$

This 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 [45] the following limits hold

$$U(k \to \infty) = \frac{2}{3}(g(0) - 1) = -\frac{2}{3}, \qquad (4.7)$$

$$U(k \to 0) \simeq \frac{2}{15}\frac{\langle\phi(k)\rangle}{\phi(k)} := \frac{2}{15}\frac{k^2}{k_0^2}, \qquad (4.8)$$

where, by virtue of Parseval's theorem,

$$\begin{aligned} \langle\phi(k)\rangle &= \frac{4\pi(Ze)^2}{k_0^2} = \int \phi(k)[S(k) - 1]\frac{d\mathbf{k}}{(2\pi)^3 n} = \\ &= \int \phi(r)[g(r) - 1]\, d\mathbf{r}, \end{aligned}$$

is the average interaction energy between two ions with

$$\phi(k) = 4\pi(Ze)^2/k^2\ , \quad \phi(r) = (Ze)^2/r\ .$$

As we know, the Nevanlinna formula of the classical theory of moments expresses the response function [2, 37]

$$S(k, z) = -\frac{1}{n}\frac{\mathrm{E}_3(z; k) + Q_2(k, z)\,\mathrm{E}_2(z; k)}{\mathrm{D}_3(z; k) + Q_2(k, z)\,\mathrm{D}_2(z; k)} \qquad (4.9)$$

in terms of a Nevanlinna class function $Q_2 = Q_2(k, z) \in \mathfrak{R}_0$, which we model here as

$$Q(k, z) = \frac{i}{\tau(k)} + 2z\int_0^\infty \frac{du(t)}{t^2 - z^2} \qquad (4.10)$$

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

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

Furthermore, the polynomials $\mathrm{D}_j(z; k)$, $j = 0, 1, 2, 3$, orthogonal with respect to the distribution density $S(k, \omega)$ and their conjugate counterparts $\mathrm{E}_j(z; k)$, $j = 0, 1, 2, 3$ are once more determined as

$$E_j(z; k) = \int_{-\infty}^\infty \frac{D_j(\omega; k) - D_j(z; k)}{\omega - z} S(k, \omega)\, d\omega, \qquad j = 0, 1, 2, 3:$$

$$\begin{aligned} &\mathrm{D}_0(z; k) = 1, \quad \mathrm{D}_1(z; k) = z, \quad \mathrm{D}_2(z; k) = z^2 - \omega_1^2(k), \\ &\mathrm{D}_3(z; k) = z^3 - z\omega_2^2(k), \quad \mathrm{E}_0(z; k) \equiv 0, \quad \mathrm{E}_1(z; k) = S_0(k), \quad (4.11) \\ &\mathrm{E}_2(z; k) = S_0(k)\, z, \quad \mathrm{E}_3(z; k) = S_0(k)\left[z^2 + \omega_1^2(k) - \omega_2^2(k)\right]. \end{aligned}$$

The frequencies $\omega_1(k)$ and $\omega_2(k)$ in Eq. (4.11) are defined by the respective ratios of the moments $S_\nu(k)$ [37], and, thus, are determined by the system static characteristics:

$$\omega_1^2 = \omega_1^2(k) = S_2(k)/S_0(k), \quad \omega_2^2 = \omega_2^2(k) = S_4(k)/S_2(k). \tag{4.12}$$

The DSF is therefore found from (4.3) as

$$\begin{aligned} S(k,\omega) &= \frac{n}{\pi} \lim_{\eta \downarrow 0} \operatorname{Im} S(k, \omega + i\eta) \\ &= \frac{n}{\pi} \frac{S(k)\,\omega_1^2\left(\omega_2^2 - \omega_1^2\right) \operatorname{Im} Q_2(k,\omega)}{\left[\omega\left(\omega^2 - \omega_2^2\right) + \operatorname{Re} Q_2(k,\omega)\left(\omega^2 - \omega_1^2\right)\right]^2 + \left[\operatorname{Im} Q_2(k,\omega)\right]^2\left(\omega^2 - \omega_1^2\right)^2}. \end{aligned} \tag{4.13}$$

In the present work we *approximate* the Nevanlinna interpolation function $Q_2(q,z)$ by its *static value* $i\tau^{-1}(k) = Q_2(k,0)$, where the "relaxation time" is selected to reproduce an exact static value of the dynamic structure factor in (4.13):

$$\tau(k) = \frac{\pi S(k,0)}{nS(k)} \frac{\omega_1^2(k)}{\omega_p^2 \Delta(k)}. \tag{4.14}$$

Alternatives in determination of the relaxation time were discussed in [46] (Ch. 9). Note that

$$\Delta(k) := \frac{\omega_2^2(k) - \omega_1^2(k)}{\omega_p^2} > 0 \tag{4.15}$$

due to the Cauchy-Schwarz inequality, see Appendix IV. Once more, it is important that the DSF (4.13), since $Q_2(q,z) \in \mathfrak{R}_0$, obeys the correct asymptotic expansion (4.4) and, hence, satisfies the sum rules (4.2) by construction, regardless of the form of the Nevanlinna parameter function $Q_2(k,z)$. On the other hand, this means that the asymptotic expansion (4.4) holds for any adequate choice of the function $Q_2(k,z)$.

Within the approximation described above we adopt,

$$\frac{S(k,\omega)}{S(k,0)} = \frac{\omega_1^4}{\left[\omega^2 - \omega_1^2(k)\right]^2 + \left[\left(\omega^2 - \omega_2^2(k)\right)\omega\tau(k)\right]^2}. \tag{4.16}$$

The static characteristics, i.e., $S(k,0)$, $S(k)$ together with the moments $S_2(k)$, $S_4(k)$, 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 hyper-netted chain (HNC) approximation or to be taken directly from the MD simulation data on the DSF. Straightforward comparison of the data obtained from (4.16) with the simulation data is transferred to Sect. 4. Note that the DSF (4.16) contains an exact static value, $S(k,0)$.

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

$$S(k,\omega) = \frac{\mathcal{L}(k,\omega)}{\pi\beta\phi(k)} \tag{4.17}$$

so that the moments (4.2) are proportional, for a given value of the wave number, to the corresponding moments of the loss function

$$\mathcal{L}(k,\omega) = -\frac{\operatorname{Im}\epsilon^{-1}(k,\omega)}{\omega}, \tag{4.18}$$

in the following way:

$$S_\nu(k) = \frac{k^2}{k_D^2} C_\nu(k), \quad \nu = 0,2,4: \tag{4.19}$$

$$C_\nu(k) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^\nu \mathcal{L}(k,\omega)\, d\omega, \quad \nu = 0,2,4. \tag{4.20}$$

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

Since we have constructed the DSF on the basis of the Nevanlinna formula, we, thus, obtain for the IDF [37]:

$$\epsilon^{-1}(k,z) = 1 + \frac{\omega_p^2(z+Q_2)}{z(z^2-\omega_2^2)+Q_2(z^2-\omega_1^2)}, \quad z = \omega + i0^+, \tag{4.21}$$

where, the Nevanlinna parameter function $Q_2 = Q_2(k,z)$ coincides with that of (4.9) due to relation (4.17).

The aim of the following Section is to compare expression (4.16) to those stemming from the visco-elastic approximation [42, 24] and the continued-fraction approach.

Alternative theoretical approaches

VEA

It is well known that the VEA is based on the random-phase approximation (RPA) for the polarization operator and interpolates between the dynamic local-field correction (DLFC) and the RPA itself [24]. Consider, first, the RPA polarization operator (a simple loop)

$$\Pi(k,\omega) = \beta n(1+\zeta Z(\zeta)), \quad \zeta = \frac{\omega}{k}\sqrt{\frac{\beta m}{2}} + i0^+.$$

Here

$$Z(\zeta) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \frac{\exp(-t^2)}{t-\zeta} dt \tag{4.22}$$

is the plasma dispersion function [47]. Note that the following expansions hold:

$$Z(\zeta \to 0) \simeq i\sqrt{\pi}\exp\left(-\zeta^2\right) - 2\zeta\left(1 - \frac{2}{3}\zeta^2 + \frac{4}{15}\zeta^4 - \cdots\right), \quad (4.23)$$

$$Z(\zeta \to \infty) \simeq i\sqrt{\pi}\exp\left(-\zeta^2\right) - \zeta^{-1}\left(1 + \frac{1}{2\zeta^2} + \frac{3}{4\zeta^4} + \cdots\right). \quad (4.24)$$

When the coupling effects come to play, the DLFC amends the RPA form of the IDF as follows:

$$\epsilon^{-1}(k,\omega) = 1 - \frac{\phi(k)\,\Pi(k,\omega)}{1 - \phi(k)\left(G(k,\omega) - 1\right)\Pi(k,\omega)}. \quad (4.25)$$

A direct comparison of Eqs. (4.21) and (4.25) leads to the following expression for the DLFC:

$$G(k,\omega) = A(k,\omega) + \frac{\Delta(k)}{1 + \frac{\omega}{Q(k,\omega)}}, \quad (4.26)$$

which, in the static approximation $Q(k,\omega) = i\tau^{-1}(k)$ we employ, simplifies to

$$G(k,\omega) = A(k,\omega) + \frac{\Delta(k)}{1 - i\tau\omega} = \frac{B(k,\omega) - i\tau\omega A(k,\omega)}{1 - i\tau\omega}. \quad (4.27)$$

Right above the following notations are utilized:

$$A(k,\omega) = 1 + \frac{1}{\phi(k)\,\Pi(k,\omega)} + \frac{\omega^2 - \omega_2^2}{\omega_p^2}, \quad B(k,\omega) = A(k,\omega) + \Delta(k) .$$

Due to the Kramers-Kronig relation,

$$\epsilon^{-1}(k,\omega) = 1 - \frac{1}{\pi}\int_{-\infty}^{\infty}\mathcal{L}(k,\omega')\,\frac{\omega' d\omega'}{\omega' - z}, \quad z = \omega + i0^+,$$

$$S(k) = S_0(k) = \frac{k^2}{k_D^2}C_0(k) = \frac{k^2}{k_D^2}\left[1 - \epsilon^{-1}(k,0)\right], \quad (4.28)$$

so that the correct value of the static local-field correction (SLFC), $B(k,0) = G(k,0) := G(k)$ is automatically obtained from (4.26). Moreover, by virtue of (4.28), the SLFC is directly related to the SSF:

$$G(k) = 1 + \frac{k^2}{k_D^2}\left[1 - \frac{1}{S(k)}\right]. \quad (4.29)$$

Another static characteristic we employed was the static value of the DSF, $S(k,0)$. Since the asymptotic behavior of the DLFC as $\omega \to 0$ is difficult to predict for strongly coupled systems, we had to consider

$S(k,0)$ to be an input parameter determined on the basis of the simulation data together with the SSF $S(k)$.

The influence of the SLFC on the static properties of dense and cold electronic liquids (the interaction potential, the static conductivity, etc.) within the STLS model [24] has recently been studied in detail in [48].

It follows from (4.24) that $A(k,\omega\to\infty)\simeq -U(k)$ asymptotically. Thus, we recover the VEA, which is an interpolation between the asymptotic values of the DLFC at $\omega=0$ and $\omega\to\infty$:

$$G^{VEA}(k,\omega)=\frac{B(k,0)-i\tau\omega A(k,\infty)}{1-i\tau\omega}=\frac{G(k)+i\tau\omega U(k)}{1-i\tau\omega}. \quad (4.30)$$

But expression (4.27) might be considered as an extension of the VEA equivalent to representation (4.16) and

$$\epsilon^{-1}(k,\omega)=1+\frac{\omega_p^2(\omega\tau+i)}{\omega\tau(\omega^2-\omega_2^2)+i(\omega^2-\omega_1^2)}, \quad (4.31)$$

stemming from (4.21) with $Q_2=i\tau^{-1}$. Observe also that Eq. (4.30) coincides with Eq. (2.159) of [24] if we identify the Nevanlinna static parameter $\tau(k)$ as the generalized visco-elastic relaxation time $\tau_m(k)$ and observe that, by Eq. (2.146) of [24], $U(k)=-I(k)$.

As further shown in Sect. 4, numerical results obtained from Eqs. (4.16) and (4.31) coincide, within the computational error, with those found from Eqs. (4.25), (4.26), and (4.27).

It is relevant to note that the model expression for the DSF (4.16) coincides formally with that obtained within the same VEA in [46]. Such a coincidence takes place because the adjustable parameters of the general hydrodynamics approach [46] were chosen to satisfy the same number of convergent frequency moments of the DSF. The difference between these two expressions lies in that the OCP hydrodynamic characteristics, which, of course, describe the dissipation processes in the system, acquire, within the moment approach, some specific definitions, see below, (4.40, 4.41).

Generally speaking, the hydrodynamic characteristics like the kinematic viscosity, the adiabatic sound velocity, and the thermal conductivity, for which there exist generic expressions in terms of the specific limiting values of the correlation functions of the hydrodynamic current longitudinal component, can presumably be determined by numerical simulations only.

The choice of the Nevanlinna parameter function, a non-phenomenological component of the moment approach, might seem to be as arbitrary as that of the memory function form and its parameters, see, e.g., [46]. Nevertheless, here we manage to relate all parameters involved in (4.16) to measurable quantities, like the zero-frequency value of the DSF. Although, for more realistic systems like two-component plasmas [44], the Nevanlinna parameter function can further be specified by taking into account some details of the energy dissipation processes [28].

A remark on the continued-fraction approach

As it is mentioned above, we compare our theoretical results to two data sets, [39] and [32]. The theoretical approach employed in [32] was the method of recurrence relations [43], closely related to the method of continued fractions, which, in turn, is equivalent to the classical moment method we apply. Indeed, it is easy to see that expression (4.21) for the response function

$$\chi(k,z) = \epsilon^{-1}(k,z) - 1 = \frac{\omega_p^2(z+Q)}{z(z^2-\omega_2^2)+Q(z^2-\omega_1^2)}, \quad z = \omega + i0^+, \tag{4.32}$$

is equivalent to the truncated continuous-fraction form [32] (the so-called J-fraction, for a recent review, see [49]):

$$\chi(k,z) := \epsilon^{-1}(k,z) - 1 = \chi(k,0)\left(1 - \cfrac{z}{z - \cfrac{\omega_1^2}{z - \cfrac{\omega_2^2-\omega_1^2}{z+Q}}}\right) \tag{4.33}$$

with the same Nevanlinna parameter function $Q_2 = Q_2(k,z)$, $\chi(k,0) = \epsilon^{-1}(k,0) - 1$. Of course, representation (4.33) satisfies the sum rules (4.20) independently of the choice of the function $Q_2 = Q_2(k,z)$. Nevertheless, the form of the DLFC employed in [32], is equivalent to the VEA expression (4.30) but without any limitation to small wavelengths.

Plasma modes

Approximate solution to the dispersion relation If, in a complete accord with the Landau damping, the decay rate of the plasma mode is assumed exponentially small, then, the poles of (4.31) lead to the existence of two modes in the system, i.e. the diffusion, unshifted, mode at $\omega_{us} = 0$ and the plasmon modes at $\omega_L = \pm\omega_2(k)$. From the mathematical point of view, such an assumption implies the incorporation of the so-called canonical solution to the moment problem [50] for the DSF:

$$S(k,\omega) = \omega_0^2\left\{\left(\frac{1}{\omega_1^2} - \frac{1}{\omega_2^2}\right)\delta(\omega) + \frac{1}{2\omega_2^2}\left[\delta\left(\omega+\omega_2^2\right) + \delta\left(\omega-\omega_2^2\right)\right]\right\}, \tag{4.34}$$

which generalizes the Feynman approximation for the DSF used in [46] (Ch.7) and, thus, justifies the VEA.

Eq. (4.34) makes the Landau-Placzek ratio,

$$R_{LP}\left(k\right)=\frac{\omega_2^2-\omega_1^2}{\omega_1^2}>0$$

a measurable quantity. Note that if the plasma isothermal compressibility is introduced as $\kappa=n\left(\partial n/\partial p\right)_\beta$, with p being the pressure, the compressibility sum rule then states that

$$G\left(k\rightarrow 0\right)=\frac{k^2}{k_D^2}\left(1-\frac{\beta n}{\kappa}\right), \tag{4.35}$$

hence, due to (4.8),

$$R_{LP}\left(k\rightarrow 0\right)\simeq\frac{k^2}{k_D^2}\left(3-\frac{n\beta}{\kappa}+\frac{8\pi k_D^2}{15k_0^2}\right). \tag{4.36}$$

On the other hand, in the classical limit one gets for any frequency,

$$\lim_{k\rightarrow\infty}G\left(k,\omega\right)=1-g\left(0\right)=1, \tag{4.37}$$

$$R_{LP}\left(k\rightarrow\infty\right)\simeq 2. \tag{4.38}$$

Further, if the decay decrements are assumed to be finite but small enough, then, the dispersion relation

$$\omega\tau(\omega^2-\omega_2^2)+i(\omega^2-\omega_1^2)=0 \tag{4.39}$$

can approximately be solved to give simple estimates for the decrements of the two collective modes, respectively, as

$$\delta_{us}\left(k\right)=-\frac{\omega_1^2\left(k\right)}{\tau\left(k\right)\omega_2^2\left(k\right)}, \tag{4.40}$$

$$\delta_L\left(k\right)=-\frac{\omega_p^2\Delta\left(k\right)}{2\tau\left(k\right)\omega_2^2\left(k\right)}. \tag{4.41}$$

Both decrements determined above are obviously negative.

Finally, by construction, the sum of the intensities of all three peaks equals $S\left(k\right)$, i.e., satisfies the *elastic sum rule.*

One serious drawback of the above approximate solution to the dispersion equation is that it is unable to predict the appearance of the "negative" dispersion, i.e. physical conditions under which the derivative $d\omega_L\left(k\right)/dk$ first vanishes and, then, turns negative. To specify these conditions it is necessary to study the dispersion relation in a more strict manner.

Exact solution of the dispersion relation Dispersion relation (4.39) can be solved exactly using the Cardano formulas. Let $w = \exp\left(\frac{2\pi i}{3}\right) = \left(-\frac{1}{2} + \frac{1}{2}i\sqrt{3}\right)$ and introduce the following parameters:

$$Z^3 = \sqrt{-\left(\frac{\omega_2^2}{3} - \frac{1}{9\tau^2}\right)^3 - \frac{1}{4\tau^2}\left(-\frac{\omega_2^2}{3} + \omega_1^2 + \frac{2}{27\tau^2}\right)^2},$$

$$X = \sqrt[3]{Z^3 - \frac{i}{2\tau}\left(-\frac{\omega_2^2}{3} + \omega_1^2 + \frac{2}{27\tau^2}\right)},$$

$$Y = \sqrt[3]{-\frac{i}{2\tau}\left(-\frac{\omega_2^2}{3} + \omega_1^2 + \frac{2}{27\tau^2}\right) - Z^3}.$$

Then, the exact solutions of the dispersion relation, i.e., the solution with the zero real part and two solutions with symmetric real parts, are:

$$\omega_{us} = -w^2 X - wY - \frac{i}{3\tau}, \tag{4.42}$$

$$\omega_L = -wX - w^2 Y - \frac{i}{3\tau}, \tag{4.43}$$

$$\omega_L' = -X - Y - \frac{i}{3\tau}. \tag{4.44}$$

The approximate solutions are naturally recovered

$$\omega_{us}(k) \simeq -\frac{i\omega_1^2(k)}{\tau(k)\,\omega_2^2(k)}, \tag{4.45}$$

$$\omega_L(k) \simeq \omega_2(k) - \frac{i\omega_p^2 \Delta(k)}{2\tau(k)\,\omega_2^2(k)}, \tag{4.46}$$

$$\omega_L'(k) \simeq -\omega_2(k) - \frac{i\omega_p^2 \Delta(k)}{2\tau(k)\,\omega_2^2(k)} \tag{4.47}$$

when, formally, $\tau(k) \to \infty$.

It is expected that the frequencies $\omega_L(k)$ (and $\omega_L'(k)$) correspond to the positions of the shifted peaks of the DSF [30].

Our results for the OCP collective modes are invalid in the long-wavelength limit only like those, for instance, of the VEA hydrodynamic approach [46]. Note that in the QLCA the direct thermal effects are dropped out, i.e., the corresponding dispersion relation for the plasmon mode lacks the classical Vlasov contribution [40], [41] (though in [45] this contribution was included as a result of the moment analysis without providing any detail or obtaining quantitative agreement with the simulation data) and the decrements of the collective modes are out of the scope of that theory.

Numerical results and conclusions

We have carried out a numerical analysis of the dispersion relation (4.43) based on the HNC results for the static characteristics and have confirmed that the derivative $d\omega_L(k)/dk$ vanishes at about $\Gamma = 9$ so that the negative dispersion takes place for higher values of the coupling parameter Γ.

We have also carried out an extensive comparison of our theoretical results with the simulation data of [39] and [32]. To do so we have used the graphic data presented in [39] and the numerical data of [32].

First of all we compare the theoretically predicted and simulated forms of the DSF (Figs. 2 - 8).

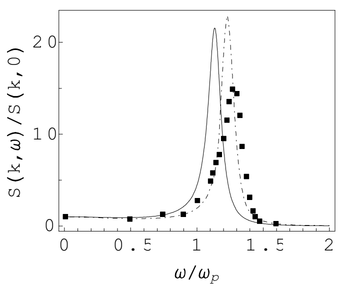

Fig. 2. The OCP normalized dynamic structure factor for $\Gamma = 0.993$ and $q = 0.6187$ in comparison with the simulation data of [39] (boxes). The solid line is constructed according to (4.16) with the values of the moments taken from [39] and/or calculated by the HNC method; the dot-dashed line is also constructed according to (4.16) but with the values of the moments obtained by direct integration of the graphic data of [39].

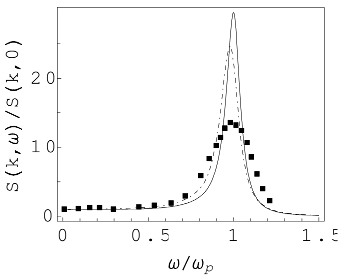

Fig. 3. Same as in Fig. 2 but for $\Gamma = 9.7$ and $q = 1.3835$.

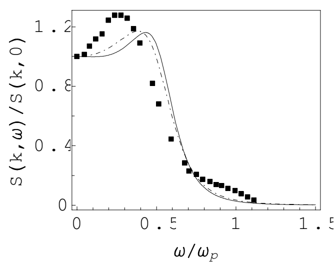

Fig. 4. Same as in Fig. 2 but for $\Gamma = 110.4$ and $q = 3.0937$.

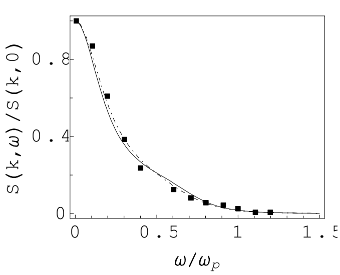

Fig. 5. Same as in Fig. 2 but for $\Gamma = 152.4$ and $q = 6.1837$.

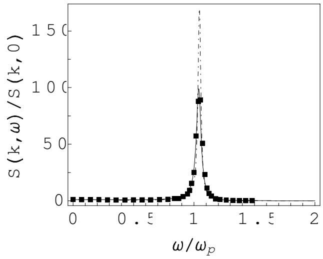

Fig. 6. The OCP normalized dynamic structure factor for $\Gamma = 2.0$ and $q = 0.49109$ in comparison with the simulation data of [32] (boxes). The solid line is constructed according to (4.16) with the values of the moments taken from [32] and/or calculated by the HNC method; the dot-dashed line is also constructed according to (4.16) but with the values of the moments obtained by direct integration of the graphic data of [32].

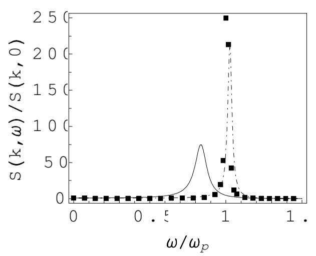

Fig. 7. Same as in Fig. 6 but for $\Gamma = 4.0$ and $q = 0.34725$.

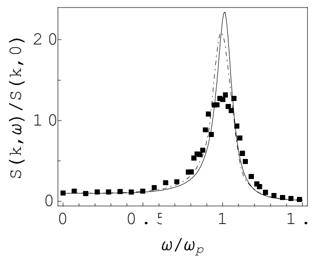

Fig. 8. Same as in Fig. 6 but for $\Gamma = 8.0$ and $q = 1.389$.

The simulation data have been processed in two different ways to calculate the static parameters (the frequencies $\omega_j^2(k)$, $j = 1, 2$, etc.). We have used either the static MD data presented in the above mentioned papers, or the data on the DSF itself to calculate the moments directly. In the latter case, care, of course, has been taken of the "tails" of the DSF, corresponding to high frequencies: the asymptotic behavior of the DSF according to (4.4) has been used, in a consistent way, to evaluate the high-frequency contributions to the moments.

In all figures we display the dimensionless DSF normalized to its zero-frequency value, $S(k,\omega)/S(k,0)$ vs. the dimensionless frequency ω/ω_p at fixed values of the dimensionless wave numbers $q = ka$ and at different values of the coupling parameter Γ, corresponding to the OCP liquid state. It is seen that a good quantitative agreement with the simulation data is gained, especially, for the positions of the unshifted peaks of the DSF, i.e., for the plasmon mode dispersion when the moments are calculated by direct integration of the DSF data.

In a few cases we have had to adjust the static values of the DSF within the numerical precision. In this context it is necessary to admit that the simulation data of [39], which are already 34 years old, proved to be somewhat inconsistent when we use the graphic data of [39] on the DSF to estimate the values of the power moments $\{S_\nu(k)\}_0^4$. They turn out quite different from the corresponding values provided in the paper.

Additionally, we present results for the dispersion relation of the Langmuir mode and the corresponding decay rates obtained by the exact and approximate solutions of the dispersion equation $\epsilon(k,\omega) = 0$ (Figs. 9-12).

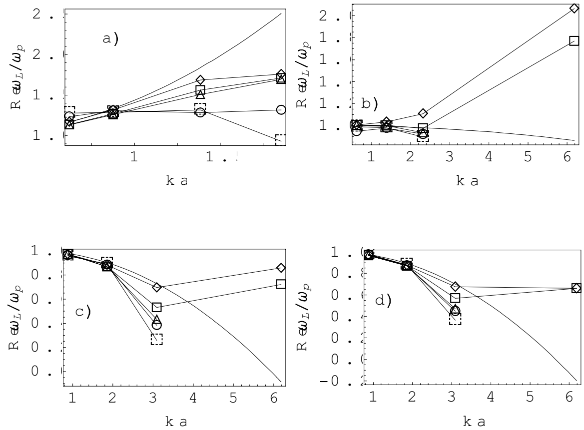

Fig. 9. The normalized plasmon frequency $\mathrm{Re}\,\omega_L(q)/\omega_p$ for four different values of Γ: a) $\Gamma = 0.993$; b) $\Gamma = 9.7$; c) $\Gamma = 110.4$; d) $\Gamma = 152.4$. Solid lines: VEA (4.48); diamonds: the approximate solution of the dispersion equation, $\mathrm{Re}\,\omega_L(q)/\omega_p = \omega_2(q)/\omega_p$; triangles: determined from the positions of the reconstructed DSF maxima with the values of the moments taken from [39]; circles: same as triangles but with the values of the moments obtained by direct integration of the graphic data of [39]; squares: the exact solution of the dispersion equation with the values of the parameters taken from [39]; dashed squares: determined from the positions of DSF maxima of the graphic data of [39].

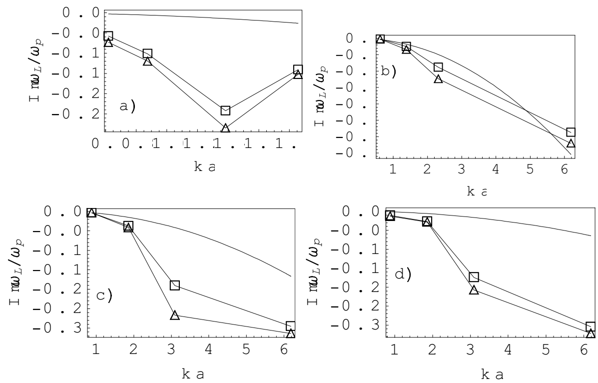

Fig. 10. The normalized plasmon decay rate $\mathrm{Im}\,\omega_L(q)/\omega_p$ for four different values of Γ: a) $\Gamma = 0.993$; b) $\Gamma = 9.7$; c) $\Gamma = 110.4$; d) $\Gamma = 152.4$. Solid lines: VEA (4.48); triangles: the approximate solution of the dispersion equation, (51); squares: the exact solution of the dispersion equation calculated using the data of [39].

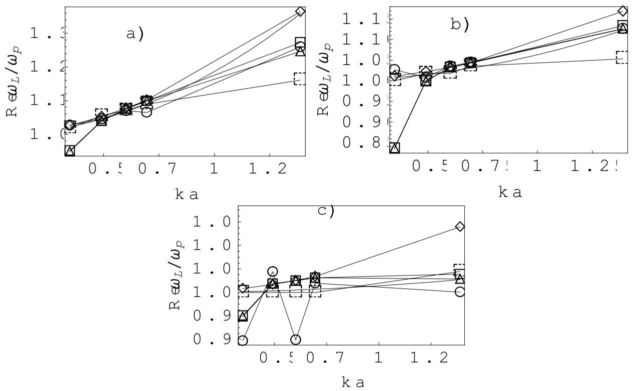

Fig. 11. Same as in Fig. 9 but using the data of [32] for three different values of Γ: a) Γ = 2; b) Γ = 4; c) Γ = 8.

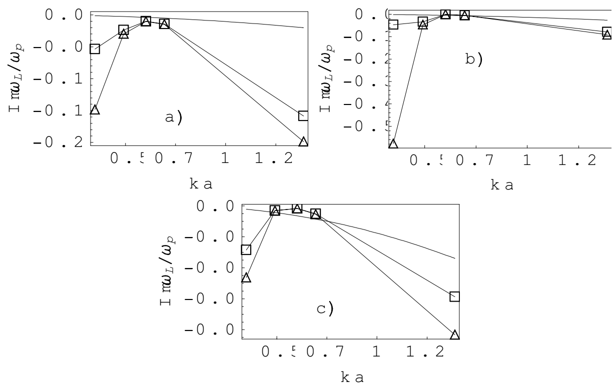

Fig. 12. Same as in Fig. 10 but using the data of [32], for three different values of Γ: a) $\Gamma = 2$; b) $\Gamma = 4$; c) $\Gamma = 8$.

These results on the dispersion are compared to the positions of the plasmon peaks of the DSF and to the prediction of the VEA estimate [51]:

$$\frac{\omega_L(q)}{\omega_p} = 1 + \frac{q^2}{2\Gamma}\left(1 + \frac{\delta_1}{3}\right) + i\delta_2\frac{q^2}{6\Gamma}, \tag{4.48}$$

$$\delta_1 = -\frac{6\Gamma}{25} - \frac{4\Gamma}{25}W_1\left(0.23\sqrt{\Gamma}\right),$$

$$\delta_2 = -\frac{4\Gamma}{25}W_2\left(0.23\sqrt{\Gamma}\right),$$

where

$$W(\xi) = W_1(\xi) + iW_2(\xi) = 1 + \frac{\xi}{\sqrt{2}}Z\left(\frac{\xi}{\sqrt{2}}\right),$$

and $Z(x)$ is defined in (4.22), [47].

Notice that no plasmon mode is observed on Fig. 4 for $\Gamma = 152.4$ and $q = 6.1837$. This is confirmed by our exact solution of the dispersion relation with the module of the imaginary part being only about a half of the real part of the solution, see Figs. 8 and 9 d).

Regarding the existence of negative dispersion due to interparticle correlations, we should note that the comparison of simulations results obtained in Ref. [39] and Ref. [32] is not conclusive at this point, since both show quantitatively different trends at large values of Γ. But even in the case of [32], we observe that the correlational energy term amounts to compensate the Vlasov thermal dispersion contribution at the highest value of the coupling. Nonetheless, we should outline here the good agreement achieved in any case by our theoretical approach, once the static characteristics have been computed through numerical simulations. We should also mention that the accuracy of our calculations for the dispersion in Fig. 11 c) might be affected by the fact that the maximum frequency available in the simulated spectra in [32] only reaches a value of 2.8 (compared to 6.5 for the other two cases). This might be applicable specially for the circles line in Fig. 11 c).

Within our approach we can also compute the effects of damping processes on the collective mode, which is given by the imaginary part of the zeros of the dispersion equation $\epsilon(k, \omega) = 0$. Our results show an increment of the modulus of the imaginary part of those zeros, as a function of k. This behavior is expected due to the existence of the well-known Landau damping mechanism, which dominates at those higher values of the wavevector. There are two additional main damping mechanisms, namely, collisional damping and diffusional damping. The latter is more relevant at small values of k. Fig. 12 points out the fact that there is a certain non-monotonic behavior of the damping as a function of k, which could be explained by a cancellation of those damping mechanisms at intermediate values of the wavenumber. In addition, we observe that higher values of the coupling parameter tend to counteract damping effects, probably due to the higher particle localization. Finally, it is evident that the usage of the VEA tends to underestimate notably the importance of damping processes. Again, this is not surprising, as this approximation does not describe dynamic screening adequately at intermediate frequencies.

Finally, for the reference, we present the values of the static parameter $S(q = ka, 0)$ we used in the present work, see Tables 2 and 3.

Table 2. The values of $S\,(q = ka, 0)$ taken from [39].

	$q = 0.6187$	$q = 0.8750$	$q = 1.3835$	$q = 1.8562$
$\Gamma = 0.993$	0.0133	0.0413	0.1059	0.1581
	$q = 0,6187$	$q = 1,3837$	$q = 2,315$	$q = 6,1873$
$\Gamma = 9.7$	$0,001$	0.0075	0.0763	0.3897
	$q = 0.8750$	$q = 1.8562$	$q = 3.0937$	$q = 6.1873$
$\Gamma = 110.4$	0.0003	0.0045	0.1220	1.003
	$q = 0.8750$	$q = 1.8562$	$q = 3.0937$	$q = 6.1873$
$\Gamma = 152.4$	0.0001	0.0045	0.1160	1.0733

Table 3. The values of $S\,(q = ka, 0)$ taken from [32].

	$q = 0.34725$	$q = 0.8750$	$q = 1.3835$	$q = 1.8562$	$q = 1.8562$
$\Gamma = 0.5$	0.007897	0.025195	0.040043	0.055783	0.145137
$\Gamma = 1$	0.002741	0.005957	0.022131	0.029141	0.097899
$\Gamma = 2$	0.001305	0.002572	0.013369	0.018699	0.059578
$\Gamma = 4$	0.000665	0.001557	0.011154	0.015553	0.036259
$\Gamma = 8$	0.000256	0.000509	0.001203	0.001343	0.009562

In conclusion, a fairly good agreement is obtained with numerous simulation data on the dynamic properties of strongly coupled one-component plasmas. The model expressions for the DSF or the DLFC characteristic for the VEA or the recurrence relation approach are incorporated into the moment scheme. This allows us to determine the abstract component of our approach based on phenomenologically sounded properties. Our results on the collective modes and their damping complement those found with other approaches. A more systematic set of simulation of this system could be interesting with the aim of studying the onset of negative dispersion and quantitative damping properties at long wavelengths. Our methods can be used to model dynamic properties of more complex Coulomb systems with high density of energy.

The investigation of OCPs using the method of moments with local constraints

The numerical procedure

Since we 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 of the moment problem. We use a finite, very small number of moments, which can be easily estimated numerically, i.e. we want to solve the truncated problem which, since the sought measure has a non-zero density, has infinitely many solutions.

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,

$$c_k = \int_{-\infty}^{\infty} t^k f(t) dt \ , \quad k = 0, 1, \ldots, 2n \ , \quad n = 1, 2, \ldots, \tag{4.49}$$

but also the values of the Nevanlinna function,

$$w_s = \varphi(t_s) = P.V. \int_{-\infty}^{\infty} \frac{f(t)dt}{t - t_s} + i\pi f(t_s) \ , \tag{4.50}$$

at the set of real points $(t_1, ..., t_p)$.

In all five cases we consider, the latter principal value integrals were computed numerically and the sets of orthogonal polynomials (**??**) were calculated directly, while the conjugate polynomials were generated using the recurrence relations stemming from the Liouville-Ostrogradsky (or Schwarz-Christoffel) identity (2.28).

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

$$u_s(z) = \exp\left\{ \frac{\alpha}{\pi i} \int_{t_s - 1}^{t_s + 1} \frac{1 + tz}{t - z} \ln|t - t_s| \frac{dt}{t^2 + 1} \right\} \ , \quad s = 1, 2, \ldots, p, \tag{4.51}$$

we made use of the Shannon entropy maximization procedure [20] (see Appendix IV) for the Shannon entropy

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

where the density $\psi(\alpha, t)$ is the one reconstructed within the algorithm, it is the imaginary part (divided by π) of the Nevanlinna model function obtained by the Schur-algorithm procedure. The density $\psi(\alpha, t)$ has no real poles and is positive over the whole real axis, hence it is quite easy to solve the maximization procedure equation: $d\mathfrak{S}(\alpha)/d\alpha = 0$.

Numerical data

To check the quality of the reconstruction technique we suggest, we carried out an extensive study of the present approach as applied to the simulation data of [32]. To carry out this comparison, we made use of the classical fluctuation-dissipation theorem to express the dynamic structure factor, $S(k,\omega)$ (DSF), in terms of the loss function (2.61):

$$S(k,\omega) = \frac{k^2}{4\pi\beta e^2}\frac{dG(\omega)}{d\omega}$$

so that, like in (4.13),

$$S(k,\omega) = \frac{n}{\pi}\frac{S(k)\,\omega_1^2\left(\omega_2^2-\omega_1^2\right)\operatorname{Im}Q(k,\omega)}{\left[\omega\left(\omega^2-\omega_2^2\right)+\operatorname{Re}Q(k,\omega)\left(\omega^2-\omega_1^2\right)\right]^2+\left[\operatorname{Im}Q(k,\omega)\right]^2\left(\omega^2-\omega_1^2\right)^2},$$

where

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

is the static structure factor. Notice that with the space dispersion taken into account, the moments $c_0(k)$, $c_2(k)$, and $c_4(k)$, and the frequencies

$$\omega_j = \omega_j(k) = \sqrt{c_{2j}(k)/c_{2(j-1)}(k)}, \qquad j = 1,2$$

were calculated numerically directly from the numerical data on the dynamic structure factor of [32].

The numerical results were compared to the simulation data of [32] on the dynamic structure factor and are summarized in the following figures 13-17. In all figures the squares correspond to the data of [32].

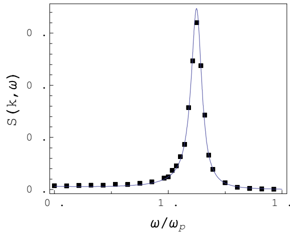

Fig. 13. The OCP dynamic structure factor at $\Gamma = 0.5$ and $ka = 0.34725$.

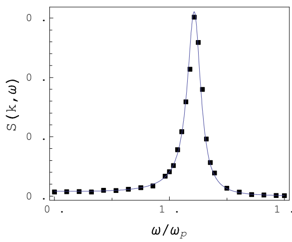

Fig. 14. As in Fig. 13, but for $\Gamma = 1$ and $ka = 0.49109$.

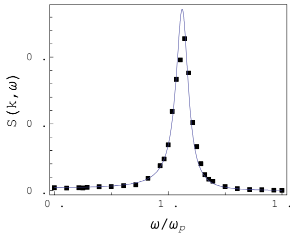

Fig. 15. As in Fig. 13, but for $\Gamma = 2$ and $ka = 0.60145$.

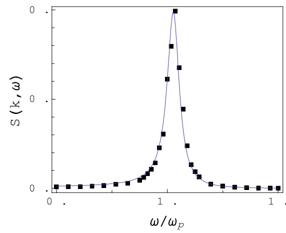

Fig. 16. As in Fig. 13, but for $\Gamma = 4$ and $ka = 0.6945$.

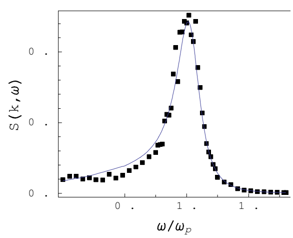

Fig. 17. As in Fig. 13, but for $\Gamma = 8$ and $ka = 1.389$. The discrepancy is within the simulation data precision.

The Langmuir mode

To study the characteristics of the plasmon mode we used the data on the Nevanlinna parameter function $Q_2(k,\omega)$ to solve the dispersion equation

$$z\left(z^2 - \omega_2^2(k)\right) + Q_2(k,z)\left(z^2 - \omega_1^2(k)\right) = 0. \qquad (4.52)$$

If the parameter function $Q_2(k,\omega)$ vanishes, the dispersion reduces to the frequency

$$\omega_2(k) = \sqrt{\omega_p^2 + \Omega^2(k)}, \qquad (4.53)$$

where the contribution $\Omega(k)$ accounts for the coupling in the system [44]. These results are presented in Figs. 18.

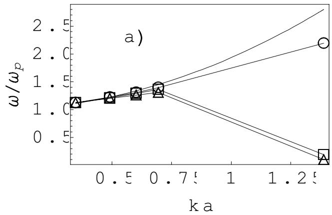

Fig. 18a. The plasmon dispersion relation for $\Gamma = 0.5$, i.e., the real part of the solution of the dispersion equation (4.52). The triangles represent the positions of the maxima of the DSF, the squares stand for the solutions of the dispersion equation (4.52), the circles correspond to $\omega_2(k)/\omega_p$ (4.53), and the solid line was calculated by the interpolation formulas of [51].

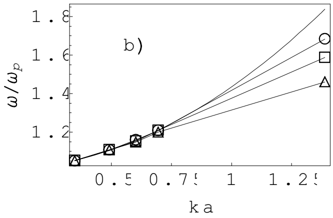

Fig. 18b. As in Fig. 18a, but for $\Gamma = 1.0$.

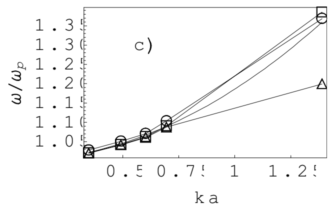

Fig. 18c. As in Fig. 18a, but for $\Gamma = 2.0$.

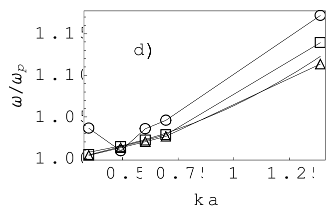

Fig. 18d. As in Fig. 18a, but for $\Gamma = 4.0$.

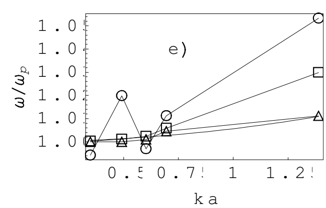

Fig. 18e. As in Fig. 18a, but for $\Gamma = 8.0$.

The solution of the dispersion equation (4.52) produced also the decay decrement of the Langmuir mode, the results are displayed in Fig. 19.

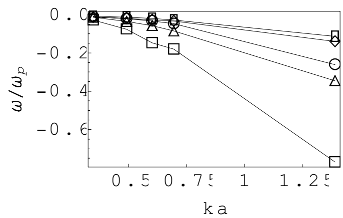

Fig. 19. The mode decrement, i.e., the imaginary part of the solution of the dispersion equation (4.52) for $\Gamma = 0.5$ (squares), $\Gamma = 1.0$ (triangles), $\Gamma = 2.0$ (circles), $\Gamma = 4.0$ (diamonds), and $\Gamma = 8.0$ (rectangles).

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

Chapter 5

Two-component plasmas

Let us know broaden the realm of application of the method of moments to more complex Coulomb systems. Consider the two-component completely ionized, usually, hydrogen-like plasmas.

The three-moment model vs. the generalized Drude-Lorentz model

First, if we take into account only the moments $\{C_0(k), 0, C_2\}$, the Nevanlinna formula immediately gives for the IDF:

$$\epsilon_{MM1}^{-1}(k,w) = 1 + \frac{\omega_p^2}{w^2 - \omega_1^2(k) + wQ_1(k,w)}, \quad \operatorname{Im} w > 0. \tag{5.1}$$

Claim 54 *We observe that in the long-wavelength approximation, when $\omega_1(k \to 0) \simeq \omega_p$, if we choose $Q_1(0,\omega) = i\nu(\omega)$, this expression (5.1) reduces to the generalized Drude-Lorentz model*

$$\epsilon_{gDL}^{-1}(0,\omega) = 1 + \frac{\omega_p^2}{\omega^2 - \omega_p^2 + i\omega\nu(\omega)} \tag{5.2}$$

often used in numerical simulations of dense plasmas, [52, 53]. Notice that the corresponding internal dynamic conductivity

$$\sigma^{int}(\omega) = \frac{\omega}{4\pi i}(\epsilon_{gDL}(0,\omega) - 1) = \frac{i\omega_p^2/4\pi}{\omega + i\nu(\omega)}$$

converts into the classical Drude-Lorentz model if we neglect the frequency dependence of the generalized (complex) collision frequency $\nu(\omega)$*, the static conductivity being equal to* $\omega_p^2/(4\pi\nu)$.

Exercise 55 *Prove the previous statement.*

The Nevanlinna parameter function $Q_N(k,w)$ for any moment problem of construction of a response function which satisfies $2N+1$ sum rules $\{C_0(k), 0, C_2, 0, \ldots, C_{2N}\}$, as well as the response function, i.e., the IDF, belongs to the Nevanlinna class of functions (i.e., it is analytic in the half-plane $\operatorname{Im} w > 0$ and possesses there a non-negative imaginary part) and, additionally, it is such that in the same half-plane $\lim_{w\to\infty} Q_N(k,w)/w = 0$. By virtue of the latter property of $Q_1(k,w)$, the model $\epsilon_{MM1}^{-1}(k,w)$ satisfies the sum rules $\{C_0(k), 0, C_2\}$ irrespectively of our choice of the parameter function $Q_1(k,w)$:

$$\epsilon_{MM1}^{-1}(k, w\to\infty) \simeq 1 + \frac{\omega_p^2}{w^2} + \cdots,$$

but, this cannot be said *a priori* about the model expression like (5.2). Certainly, for a constant collision frequency or with $Q_1(k,w) = Q_1(k, w=0) = ih(k)$, $h(k) > 0$, the fact that the loss function $\mathcal{L}_1(k,\omega) = \operatorname{Im}\epsilon_{MM1}^{-1}(k,\omega)/\omega$ has finite moments $\{C_0(k), 0, C_2\}$ can be easily checked by direct integration, but it is not clear from ([52, 53]) if with the Born dynamic collision frequency (**??**) the model (5.2) would satisfy these sum rules. In any case, neither (5.2), nor (5.1) satisfies the fourth sum rule $C_4(k)$.

The five-moment model

The loss function which corresponds to the IDF [6]

$$\epsilon_{MM2}^{-1}(k,w) = 1 + \frac{\omega_p^2 (w + Q_2(k,w))}{w(w^2-\omega_2^2) + Q_2(k,w)(w^2-\omega_1^2)}, \quad \operatorname{Im} w > 0, \tag{5.3}$$

possesses all five convergent power moments $\{C_0(k), 0, C_2, 0, C_4(k)\}$ by construction. Besides, without violating these sum rules, in a two-component plasma we can make use of the exact asymptotic form of the DF imaginary part obtained by Perel' and Eliashberg [28], and to model the parameter function $Q_2(k,w)$ as [1]

$$Q_2(k,w) = B(k)\sqrt{w}(1+i) + ih(k), \tag{5.4}$$

with

$$\begin{aligned} B(k) &= \frac{4\pi A_0}{\omega_p^2(\omega_2^2-\omega_1^2)} > 0, \\ A_0 &= \frac{2^{5/2}\pi}{3} n_e n_i \frac{Z^2 e^6}{(\hbar m)^{3/2}}, \\ h(k) &= \frac{\omega_2^2-\omega_1^2}{3\pi\Gamma\omega_1^4} \frac{\omega_p^2 k^2 a^2}{s(k,0)}. \end{aligned}$$

Observe that by virtue of the Cauchy-Schwarz inequality (see Appendix IV) $\omega_2^2 - \omega_1^2 > 0$ and that

$$s(k,0) = \frac{\omega_p}{n} S(k,0) \tag{5.5}$$

is the dimensionless charge-charge dynamic structure factor at $\omega = 0$; the values of $s(k,0)$ can be computed numerically, other approximations for the static contribution $h(k)$ can be constructed as well, e.g., if we know the static conductivity $\sigma^{int}(0,0)$ [6].

The expression (5.3) is virtually an interpolation (in the class of response functions) between the asymptotic expansion

$$\epsilon_{MM2}^{-1}(k, w \to \infty) \simeq 1 + \frac{\omega_p^2}{w^2} + \frac{\omega_p^2\omega_2^2(k)}{w^4} - \frac{4\pi A_0}{w^{9/2}}(1+i) + \mathrm{O}\left(\frac{1}{w^{11/2}}\right) \cdots, \tag{5.6}$$

[1] Notice that (5.4) maintains the parity of the papameter function on the real axis:

$$Q_2(k, \omega \in \mathbb{R}) = B(k)\sqrt{|\omega|}(sign(\omega) + i) + ih(k).$$

which satisfies the asymptotic form [28] (see also [21]):

$$\operatorname{Im} \epsilon \left(k, \omega \gg (\beta\hbar)^{-1}\right) \simeq \frac{4\pi A_0}{\omega^{9/2}}, \tag{5.7}$$

and some static characteristic of the system like $s(k, 0)$ [2]. This interpolation is carried out by the Nevanlinna parameter function $Q_N(k, z)$. The validity of the moment-generated models (5.3, 5.4) has been successfully compared to virtually all available real and simulation data as well as some theoretical approaches, see [6] and references therein.

Neither the extended RPA nor the extended Mermin model satisfy the asymptotic form (5.7), no fractional terms like $(\omega/\omega_p)^{-9/2}$ can appear within these approximations. Notice also that the real correction of the order $(\omega/\omega_p)^{-9/2}$ is negligible with respect to other real contributions in the asymptotic form (5.6), while the same order imaginary contribution is the largest.

Notice also that this exact asymptotic form implies the divergence of higher-order moments $C_{2l}(k)$ with $l \geq 2$ and that the interpolation form suggested in [54] for the dynamic local-field correction at $\beta = \infty$ and employed in [55] complies with it.

Finally, observe that, generally speaking, only the positivity of the loss function constructed by the moment method is guaranteed. The positivity of the loss function based on the Mermin model expression for the IDF is to be studied elsewhere. The violation of the positivity condition might produce erroneous conclusions with respect to the plasma stopping power.

[2]In a completely ionized plasma for $\omega \geq (\beta\hbar)^{-1}$ 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 ([25], and also, e.g., [27]) this circumstance permits to use the detailed equilibrium principle to express the imaginary part of the longitudinal dielectric function, $\operatorname{Im} \epsilon(k, \omega)$ of a completely ionized plasma, in terms of the bremsstrahlung cross-section.

Collective and static properties of model two-component plasmas

Let us employ now the method of moments to study the classical molecular dynamics [22] data on the charge-charge dynamic structure factor of two-component plasmas modelled in [56]. The convergent power moments of the imaginary part of the model system dielectric function are expressed in terms of its partial static structure factors and the latter are computed by the method of hypernetted-chains using the Deutsch effective potential, see below. High-frequency asymptotic behavior of the dielectric function is specified to include the effects of inverse bremsstrahlung [28].

Introduction

Classical molecular dynamics (MD) simulations of model two-component plasmas (TCP) were carried out in [56] many years ago. The system modelled in this pioneer work was a fully ionized strongly coupled hydrogen TCP of temperature T consisting of electrons ($a = e$, $Z_e = -1$) with the number density n and protons ($a = i$, $Z_i = +1$) with the same number density. The dynamic and static characteristics studied were the charge-charge dynamic structure factor, the species partial static structure factors and the static radial distribution functions, etc. Classical statistical averages were computed on the basis of the ergodic hypothesis while the quantum delocalization preventing the collapse were taken into account through the use of the Deutsch pair effective potential [57] arising from the quantum-diffraction effects,

$$\varphi_{ab}(r) = Z_a Z_b \frac{e^2}{r}\left(1 - \exp\left(-\kappa_{ab} r\right)\right), \quad a, b = e, i, \tag{5.8}$$

$$\kappa_{ab} = \sqrt{\frac{2\pi\mu_{ab}}{\beta\hbar^2}}, \quad \mu_{ab} = \left(m_a^{-1} + m_b^{-1}\right)^{-1},$$

where μ_{ab} is the reduced mass of an $a - b$ pair, without including the exchange or symmetry contribution, and β^{-1} is the temperature in energy units. The fact that the potentials (5.8) remain finite as $r \to 0$ is a consequence of the uncertainty principle and prevents the collapse to which we have already referred to. In the temperature range of interest

$$\kappa_{ii} a \gg 1, \quad a = \sqrt[3]{\frac{3}{4\pi n}}$$

being the Wigner-Seitz or the "ion sphere" radius. Thus the effective ion-ion interaction is virtually identical to the bare Coulomb potential at all separations.

The potential (5.8) was also employed to determine the static properties in the hypernetted-chain (HNC) approximation [22].

Since 1981, little effort was made to simulate this benchmark high-energy density system and study its static and dynamic properties. We mention a few related works: (i) the static electrical conductivity was studied in Refs. [58] and [59], (ii) the TCP dynamic characteristics in a different range of values of the wavenumber were investigated in [60].

The results of [56] were analyzed in [61] using the sum rules and other exact relations. An overall agreement with the MD results was obtained in [61] where the frequency moments of the imaginary part of the plasma (inverse) dielectric function, $\epsilon^{-1}(k,\omega)$, (the sum rules) were calculated there for the bare Coulomb potential.

Our aim is to reexamine the simulation data of [56] and the theoretical results of [61] within the moment approach and using the method of effective potentials to estimate the static characteristics of the TCP.

Mathematical details of the moment approach are provided in the next Section. A model Nevanlinna parameter function taking into account the fractional asymptotic form of the imaginary part of the system dielectric function is suggested and the convergent power moments of the loss function $-\operatorname{Im}\epsilon^{-1}(k,\omega)/\omega$ of the model system are calculated using the Deutsch effective potential and are computed by the method of hypernetted-chains using the same potential; for a recent review of the method of effective potentials see [62]. Numerical results and Conclusions are presented as well. The agreement with the MD data is shown to be good, and, simultaneously, important statistical characteristics of the model TCP in concern, like the probability to find both electron and ion at one point $[g_{ei}(0)]$, are determined, direct and exchange interaction contributions being compared.

The background

The MD results of [56] on the charge-charge dynamic structure factor $S_{zz}(k,\omega)$ were modelled in [61] using the moment approach which automatically takes into account the sum rules and other exact relations.

The starting point in the application of the method of moments [6] to the calculation of the system dynamic correlation function is the fluctuation-dissipation theorem (FDT) which relates the latter to the system dissipation characteristic, the Green function, whose power frequency moments, by virtue of the Kubo theory of linear response, can be directly expressed in terms of the static correlators of the time derivatives of the system observables. The latter can be related, using the system model Hamiltonian, to the system structural static correlation functions like the radial distribution functions or the static structure factors, and this is the only step of our approach where the system model interferes. Otherwise the relations we use are model-free. They are based on mathematical results which are not related to the physical details, i.e., the interaction potential. This permits to apply the moment approach to non-perturbative systems which lack small parameters, like the one we deal with here.

Indeed, in a classical Coulomb system the characteristic perturbation parameter is the potential energy of two charges at an average distance, i.e., the Wigner-Seitz radius a, divided by the characteristic kinetic energy or the system temperature:

$$\Gamma = \beta e^2/a.$$

The achievement of the work by Hansen and McDonald [56] was that the values of $\Gamma \gtrsim 1$ (precisely, $\Gamma = 0.5$ and $\Gamma = 2$) and $r_s = 0.4$ and $r_s = 1$, where

$$r_s = \frac{a}{a_B} = \frac{ame^2}{\hbar^2}$$

and a_B being the Bohr radius, were considered, which correspond to strongly coupled Coulomb systems or high-energy density (HED) matter. Under these conditions the Landau length, the Wigner-Seitz radius, and the Debye radius

$$\lambda_D = \frac{a}{\sqrt{3\Gamma}}$$

are of the same order of magnitude, so that no effective screening takes place: there is only one or less particles in the Debye sphere. Hence, standard theoretical treatments, e.g., the kinetic theory are not applicable, and we need alternative approaches like the one we make use of in the present work.

There is an additional dimensionless parameter which is commonly used to characterize the kind of statistical systems we deal with here. This is the so-called degeneracy parameter,

$$\theta^{-1} = D = \beta E_F = 1.84159\frac{\Gamma}{r_s}$$

which compares the Fermi energy of the system, E_F, to its thermal energy. For the thermodynamic conditions considered in Ref. [56] and here $D \gtrsim 1$, which means that strongly coupled two-component plasmas are intrinsically quantum statistical systems, and we might expect their physical properties to be greatly influenced by their quantum mechanical nature.

Nevertheless, due to the significant difficulties encountered in the analytical and computational modelling of these systems, it is a commonplace to use classical statistical approaches to investigate multicomponent plasmas. These classical approximations, like MD or HNC calculations, do require the application of potentials which effectively take into account the quantum mechanical nature of these systems, especially the quantum diffraction preventing the classical Coulomb collapse.

As we have said, the only step where the physical model under consideration appears explicitly in the method of moments is the modelling of the system Hamiltonian required to compute the frequency moments of the Green function (see Sect. 5). Strictly speaking, these calculations can be carried out following the laws of quantum statistical mechanics, and therefore no effective potential is needed. This means that the potential appearing in the Hamiltonian must be understood as the real interaction among charged particles at the microscopic level, which is, of course, the Coulomb potential.

However, our main aim here is to compare the static and dynamic characteristics obtained for the TCP with those of Ref. [56].

The mathematical background is that of the general framework of the method of moments. Thus, we work here to better assess the applicability of our approach. In this sense, the usage of the classical version of the FDT is justified:

$$S_{zz}\left(k,\omega\right)=\frac{\mathcal{L}\left(k,\omega\right)}{\pi\beta\phi\left(k\right)}, \tag{5.9}$$

where

$$\phi\left(k\right)=\frac{4\pi e^2}{k^2},$$

$$\mathcal{L}\left(k,\omega\right)=-\frac{\operatorname{Im}\epsilon^{-1}\left(k,\omega\right)}{\omega}$$

being the loss function of the system, which is assumed to be isotropic. The sum rules we employ are, as before, the power frequency moments of this loss function. Hence for the dynamic structure factor we obtain:

$$S_{zz}\left(k,\omega\right)=\frac{\omega_p^2}{\pi\beta\phi\left(k\right)}\frac{\left[\omega_2^2\left(k\right)-\omega_1^2\left(k\right)\right]Q_2\left(k,\omega\right)}{\left|\omega\left[\omega^2-\omega_2^2\left(k\right)\right]+Q_2\left(k,\omega\right)\left[\omega^2-\omega_1^2\left(k\right)\right]\right|^2}, \tag{5.10}$$

where the Nevanlinna parameter function is taken as in (5.4), instead of

$$Q_2(k,z)=ih\left(k\right),\quad h(k)=\frac{\omega_p^2}{\pi\beta\phi\left(k\right)}\frac{\omega_2^2-\omega_1^2}{S_{zz}(k,0)\omega_1^4}. \tag{5.11}$$

This is the approximation which was used as a basis of the analysis carried out in [61]. We wish to use it now combined with more precise values for the power moments calculated using the Deutsch potential [57], The approximation (5.11) is shown to be insufficient, i.e., within this approximation we fail to predict the values of the Langmuir collective mode frequency or the position of the lateral peak of the dynamic structure factor, and its width. The static values of the dynamic structure factor $S_{zz}(k,0)$ can be taken from Table IV of [56].

The expression for the (inverse) dielectric function and, hence, for the dynamic structure factor (4.17) with the Nevanlinna parameter function determined in (5.4), leads to the correct static value $S_{zz}(k,0)$ of the dynamic structure factor, satisfies all three sum rules (4.20), and also satisfies the exact relation (3.27).

The range of frequencies studied in [56] was about $(0, 2\omega_p)$, so that no data was obtained for the frequencies which satisfy the condition $\omega \gg (\beta\hbar)^{-1}$ or, equivalently,

$$\frac{\omega}{\omega_p} \gg \sqrt{\frac{r_s}{3\Gamma^2}}.$$

On the other hand, in spite of the classical approximations used here for comparison with Ref. [56], as we have discussed previously, the system we consider possesses an inherent quantum mechanical nature, and we may presume that the asymptotic form (3.27) is applicable to it.

Thus we reduce the determination of the dynamic structure factor to the knowledge of the static characteristics - the frequency moments $C_\nu(k)$, $\nu = 0, 2, 4$, see Sect. 5.

The latter were calculated [61] in terms of the static structure factors of both system species $S_{ab}(k)$ beyond the random-phase approximation with the inclusion of both electronic and ionic local-field corrections. These corrections were determined by means of the Ichimaru algorithm [64] in terms of the electronic one, which was found as an interpolation satisfying both the Kimball cusp condition and the compressibility sum-rule [65, 66] with the electronic equation of state taken from the numerical simulations [67]; the static structure factors were obtained using the method of temperature Green's functions.

The moments

The explicit form of the power moments $C_\nu(k)$, $\nu = 0, 2, 4$, for the bare Coulomb potential is known since long [6] (for details see Ref. [63]), they can be directly deduced fro the general results found in Section 3 when $\zeta(k) = 1$:

$$C_0(k) = \left[1 - \epsilon^{-1}(k,0)\right], \quad C_2(k) = \omega_p^2, \quad C_4(k) = \omega_p^4\left[1 + W(k)\right]. \tag{5.12}$$

The moment $C_0(k)$, as it was already commented, is related to the static dielectric function of the system, the second moment is actually the f-sum rule, which is independent of the system interactions. The correction in the fourth moment contains different contributions:

$$W(k) = K(k) + U(k) + H.$$

The first contribution stems from the kinetic term of the system Hamiltonian. In the classical case, this coincides with the known Vlasov contribution to the dispersion relation:

$$K(k) = 3\frac{k^2}{k_D^2}, \tag{5.13}$$

$k_D^2 = 4\pi n e^2 \beta$ being the square of the Debye wavenumber. Here, as in (5.12), we only account for the electronic subsystem, due to the large asymmetry between the masses of electrons and ions. We use expression (5.13) for comparison with the results of Ref. [56]. Nonetheless, due to the quantal nature of our system, it would be interesting to estimate quantitatively how the degeneracy would affect the dispersion law and the dynamic structure factor of the system through this kinetic contribution. In the quantum mechanical case, it can be recast as

$$K(k) = \frac{\langle v_e^2 \rangle k^2}{\omega_p^2} + \left(\frac{\hbar}{2m}\right)^2 \frac{k^4}{\omega_p^2}, \tag{5.14}$$

where the average of the square of the electron velocity is expressed as

$$\langle v_e^2 \rangle = \frac{3F_{3/2}(\eta)}{m\beta D^{3/2}}.$$

$$F_\nu(\eta) = \int_0^\infty \frac{x^\nu}{\exp(x-\eta)+1} dx$$

being the order-ν Fermi integral, and $\eta = \beta\mu$ the dimensionless chemical potential of the electronic subsystem, which should be determined by the normalization condition

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

The last two terms in the fourth moment correction term stem from the interaction contribution to the system Hamiltonian and are, therefore, dependent on the potential used. For the bare Coulomb potential we write:

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

$$H = \frac{1}{3} h_{ei}(0) = \frac{1}{3}\left(g_{ei}(0) - 1\right) = \frac{1}{6\pi^2 n} \int_0^\infty p^2 S_{ei}(p)\, dp,$$

where we have introduced

$$f(p,k) = \frac{5}{12} - \frac{p^2}{4k^2} + \frac{\left(k^2 - p^2\right)^2}{8pk^3} \ln\left|\frac{p+k}{p-k}\right|.$$

But for the sake of a better comparison with the MD results of Ref. [56], we recalculated here these moments using the model Hamiltonian with the Coulomb potential substituted by the model Deutsch effective potential. Then, the moment $C_2(k)$ (the f-sum rule) remains intact, the moment $C_0(k)$ changes together with the model system static dielectric function, and instead of $C_4(k)$ we have:

$$\widetilde{C}_4(k) = \omega_p^4 \left[1 + \widetilde{W}(k)\right], \tag{5.15}$$

where the "model" $\widetilde{W}(k)$ has the same kinetic contribution $K(k)$ (either classical or degenerate), but the interaction contributions are substituted by

$$\widetilde{U}(k) = \frac{1}{2\pi^2 n}\int_0^\infty p^2 \left(\widetilde{S}_{ee}(p) - 1\right) \widetilde{f}(p,k)\, dp \tag{5.16}$$

and

$$\widetilde{H} = \frac{\kappa_{ei}^2}{6\pi^2 n}\int_0^\infty \frac{p^2 \widetilde{S}_{ei}(p)}{p^2 + \kappa_{ei}^2} dp. \tag{5.17}$$

Here

$$\begin{aligned}\widetilde{f}(p,k) &= \frac{\kappa_{ee}^2}{4k^2} + \frac{\left(k^2 - p^2\right)^2}{8pk^3} \ln\left|\frac{p+k}{p-k}\right| - \\ &- \frac{\left(p^2 + \kappa_{ee}^2 - k^2\right)^2}{16pk^3} \ln\frac{(p+k)^2 + \kappa_{ee}^2}{(p-k)^2 + \kappa_{ee}^2} - \frac{\kappa_{ee}^2/3}{p^2 + \kappa_{ee}^2}.\end{aligned}$$

In addition, the model partial static structure factors $\widetilde{S}_{ab}(k)$ have been computed in the hypernetted-chain approximation using the Deutsch effective potential. This closes the algorithm of calculation of the static and dynamic characteristics of the system.

The results are discussed in the next two Sections.

Numerical results

Static characteristics

As it was mentioned, we calculated the static structure factors and the radial distribution functions in the hypernetted-chains approximation using the Deutsch effective potential (5.8), just as it was done in [56].

We present our data on the partial static structure factors in Tables I-IV. It is not surprising that the agreement we obtain with the values of the static characteristics given in Table V of [56], is within the computational precision. We add the corresponding values of the charge-charge static structure factor $S_{zz}(k)$. We calculated them from the static data:

$$S_{zz}(k) = S_{ii}(k) + S_{ee}(k) - 2S_{ie}(k) \tag{5.18}$$

and also as

$$S_{zz}(k) = \frac{1}{n}\int_{-\infty}^{\infty} S_{zz}(k,\omega)d\omega; \qquad (5.19)$$

i.e., as the zero-order frequency moment of the dynamic factor (5.10), these values coincide to the fourth digit.

The other two dimensionless even-order power moments of the dynamic structure factor (5.10) are defined as

$$S_\nu\left(k\right) = \frac{1}{n\omega_p^\nu}\int_{-\infty}^{\infty} \omega^\nu S_{zz}(k,\omega)d\omega, \quad \nu = 2,4, \qquad (5.20)$$

the latter being provided in Table IV. By virtue of the classical version of the FDT used here, the odd-order moments vanish due to the symmetry of (5.10).

These values may be used to determine the characteristic frequencies $\omega_1\left(k\right) = \sqrt{C_2\left(k\right)/\widetilde{C}_0\left(k\right)}$ and $\omega_2\left(k\right) = \sqrt{\widetilde{C}_4\left(k\right)/C_2\left(k\right)}$ which virtually coincide with their values calculated from the formulas (5.15), (5.16), and (5.17), but now differ significantly from the values given in Table VI of [61].

Notice that the static dielectric function and the moment $\widetilde{C}_0\left(k\right)$ is directly related to the charge-charge static structure factor (5.19) by the FDT (with subtraction) in the form

$$S_{zz}\left(k\right) = -\frac{k^2}{k_D^2}P.V.\int_{-\infty}^{\infty} \operatorname{Im}\epsilon^{-1}\left(k,\omega\right)\frac{d\omega}{\omega} = \frac{k^2}{k_D^2}\left(1 - \operatorname{Re}\epsilon^{-1}\left(k,0\right)\right),$$

Thus the moment $\widetilde{C}_0\left(k\right)$ was estimated as

$$\widetilde{C}_0\left(k\right) = \frac{k_D^2}{k^2}S_{zz}\left(k\right)$$

with the static structure factor $S_{zz}\left(k\right)$ also calculated in the hypernetted-chain approximation using the Deutsch effective potential (5.8).

Further, we display our results on the values of the partial radial distribution functions at zero separation, $g_{ee}(0)$ and $g_{ie}(0)$, computed using the effective potential (5.8) and also taking into account the symmetry effects in the electron-electron exchange contribution to the effective potential (while leaving other components unchanged):

$$\varphi_{ee}\left(r\right) = \frac{e^2}{r}\left(1 - \exp\left(-\kappa_{ee}r\right)\right) + \frac{\ln 2}{\beta}\exp\left(-\frac{r^2\kappa_{ee}^2}{\pi\ln 2}\right); \qquad (5.21)$$

for comparison we present also the values of $g_{ie}(0)$ calculated analytically in [68], see Table V.

In addition, we display the graphs for the three partial radial distribution functions for the conditions $\Gamma = 0.5$ and $r_s = 0.4$, calculated with the potential (5.8), Fig. 20. The curves in Fig.20 are virtually indistinguishable from those of Fig. 2 of Ref. [56].

Table I. Partial static structure factors at $\Gamma = 0.5$, $r_s = 0.4$ with the Deutsch effective potential without exchange (5.8).

$q = ka$	$S_{ii}(k)$	$S\_\{ie\}(k)$	$S_{ee}(k)$	$S_{zz}(k)^a$
0.767	0.5804	0.4387	0.6590	0.3620
1.074	0.6257	0.3600	0.7391	0.6448
1.381	0.6824	0.2813	0.8118	0.9316
1.534	0.7118	0.2455	0.8425	1.0634

[a] Calculated from (5.18) or (5.19).

Table II. Partial static structure factors at $\Gamma = 0.5$, $r_s = 1$ with the Deutsch effective potential without exchange (5.8).

$q = ka$	$S_{ii}(k)$	$S\_\{ie\}(k)$	$S_{ee}(k)$	$S_{zz}(k)^a$
0.767	0.6160	0.4606	0.6470	0.3418
1.074	0.6663	0.3943	0.7144	0.5922
1.381	0.7192	0.3275	0.7769	0.8412
1.534	0.7447	0.2952	0.8081	0.9624

[a] Calculated from (5.18) or (5.19).

Table III. Partial static structure factors at $\Gamma = 2$, $r_s = 1$ with the Deutsch effective potential without exchange (5.8).

$q = ka$	$S_{ii}(k)$	$S\_\{ie\}(k)$	$S_{ee}(k)$	$S_{zz}(k)^a$
0.767	0.5642	0.5821	0.7197	0.1198
1.074	0.5133	0.5001	0.7385	0.2516
1.381	0.5067	0.4275	0.7769	0.4286
1.534	0.5174	0.3940	0.7993	0.5288

[a] Calculated from (5.18) or (5.19).

Table IV. The fourth dimensionless power moment of $S_{zz}(k, \omega)$, according to (5.20), with the Deutsch effective potential without exchange (5.8). In the classical case, the kinetic contribution is approximated by the Vlasov term (5.13), whereas in the quantal case expression (5.14) is used.

	Classical			Quantal		
	$\Gamma = 0.5$	$\Gamma = 0.5$	$\Gamma = 2.0$	$\Gamma = 0.5$	$\Gamma = 0.5$	$\Gamma = 2.0$
$q = ka$	$r_s = 0.4$	$r_s = 1.0$	$r_s = 1.0$	$r_s = 0.4$	$r_s = 1.0$	$r_s = 1.0$
0.767	0.8845	0.9318	0.1403	1.1175	0.9966	0.1680
1.074	2.6028	2.6943	0.3294	3.6028	2.9856	0.4462
1.381	6.2193	6.3685	0.6644	9.3337	7.3169	1.0217
1.534	9.0728	9.2555	0.9073	14.1572	10.8366	1.4855

Table V. Zero-separation values of the partial radial distribution functions compared to the results of Ref. [68].

Γ	θ	r_s	$g_{ee}(0)^a$	$g_{ie}(0)^a$	$g_{ee}(0)^b$	$g_{ie}(0)^b$	$g_{ie}(0)^c$
0.1	0.1000	0.0184	0.9598	1.0684	0.7309	1.0474	1.0358
0.1	2.0000	0.3683	0.7569	1.5164	0.3868	1.5045	1.3478
0.5	0.4344	0.4000	0.6629	1.9865	0.3897	1.8874	1.4412
0.5	1.0860	1.0000	0.4707	3.5224	0.2500	3.2600	1.8963
1.0	0.1000	0.1842	0.7738	1.4979	0.6159	1.4276	1.2351

^{a} With Eq. (5.8). ^{b} With Eqs. (5.8) and (5.21). ^{c} Values from Ref. [68].

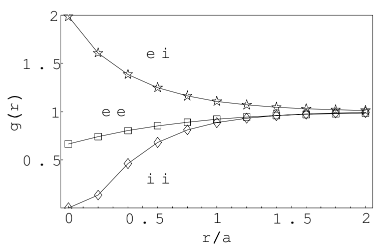

Fig. 20. The radial distribution functions $g_{ab}(r)$, $a, b = e, i$ for $\Gamma = 0.5$, $r_s = 0.4$, calculated with the potential (5.8). The solid lines are included to join the discrete points for a better visualization.

Dynamic characteristics

With all these efforts we have obtained a fairly good agreement with the simulation MD data on the dynamic structure factor. This agreement was quantitatively good, and it was better than that achieved in [61]. The introduction of the non-constant Nevanlinna parameter function (5.4) not only permitted to obtain better agreement in the position of the Langmuir peaks, but also lead to the adequate broadening (damping) of the Langmuir mode. In Figs. 21, 22 we present physically interesting results on the dispersion of the Langmuir mode. In this sense, it is interesting to calculate the complex solution for the dispersion equation $\epsilon(k,z) = 0$ explicitly in order to determine quantitatively the damping of the collective mode. From Eq. (5.10) we get the equation

$$z\left(z^2 - \omega_2^2\right) + Q_2\left(z^2 - \omega_1^2\right) = 0. \tag{5.22}$$

Due to the fact that the function $\epsilon^{-1}(k,z)$ must be analytic in the upper half-plane, the solution of the dispersion equation, $z(k)$, must possess a non-positive imaginary part, i.e., if $z(k) = \mathrm{Re}\, z(k) + i\, \mathrm{Im}\, z(k)$, then $\mathrm{Im} z \leq 0$. In particular, it is clear that for the approximation

$$Q(k,z) = i0^+ \tag{5.23}$$

we get for the (shifted) collective excitation the value of ω_2. However, for the model function (5.4), it is shown in Figs. 21 that $\mathrm{Re} z < \omega_2$, while the damping becomes more notorious, see Figs. 22.

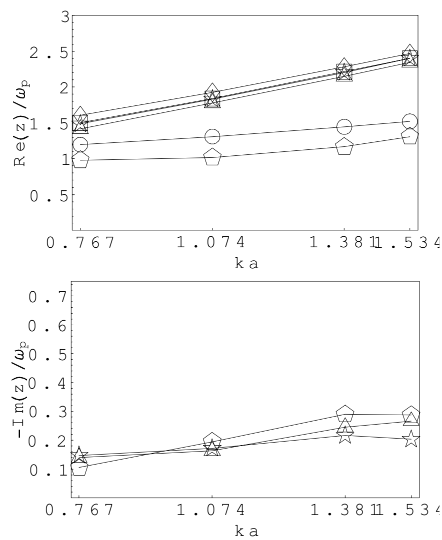

Fig. 21. Dispersion, $z(k) = \mathrm{Re} z(k) + i\mathrm{Im} z(k)$, for the collective excitation mode obtained from Eq. (5.22) in the classical approximation. The damped solution stemming from the model function (5.4) is compared to the undamped solution corresponding to the approximation (5.23). For expression (5.4): $\Gamma = 0.5$, $r_s = 0.4$ (triangles); $\Gamma = 0.5$, $r_s = 1$ (stars); $\Gamma = 2$, $r_s = 1$ (pentagons). For (5.23): $\Gamma = 0.5$, $r_s = 0.4$ (boxes); $\Gamma = 0.5$, $r_s = 1$ (diamonds); $\Gamma = 2$, $r_s = 1$ (circles). The solid lines are included to join the discrete points for a better visualization.

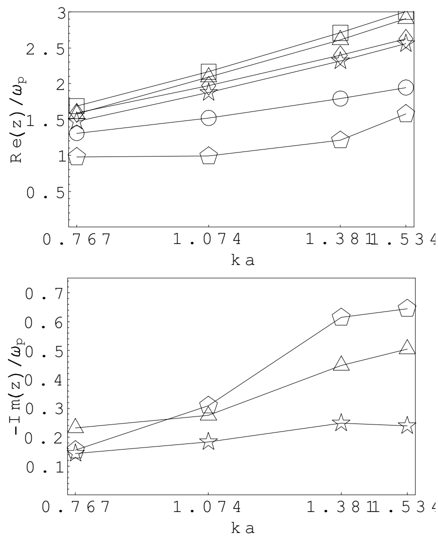

Fig. 22. Same as in Fig. 21, but for the quantal case. The degenerate kinetic term (5.14) is used, instead of the classical one (5.13).

We observe that in all cases, except for $\Gamma = 2$ and the lowest values of $q = ka$, the effects of degeneracy produce stronger positive dispersion, i.e., the Langmuir mode frequency become higher than ω_p. In addition, degeneracy or quantum mechanical characteristics of the effective interaction produce also stronger damping of the mode.

Indeed, at higher frequencies, we deal with shorter distances or shorter times, where the non-Coulomb nature of the effective potential and the wave nature of electrons become more pronounced.

Notice that these effects are reflected in the MD calculations using the Deutsch effective potential and are described in our calculations.

Conclusions

The agreement with the MD data on the dynamic structure factor and other dynamic characteristics of the model system, like the Langmuir collective mode dispersion, is improved with respect to the results obtained in [61], and, simultaneously, important statistical characteristics of the model TCP in concern, like the probability to find both electron and ion at one point $[g_{ei}(0)]$, are determined, importance of direct and exchange interactions being analyzed. The applicability of (5.14) and (5.4) are validated.

Since the static characteristics of the system (the static structure factors and the radial distribution functions) were computed with high precision in the way employed in [56], the reliability in the calculation of the zero- and four-order moments of the dynamic structure factor or the characteristic frequencies $\omega_1(k)$ and $\omega_2(k)$ is improved. These quantities are essential to estimate the position and damping of the plasma collective mode.

Another key ingredient for the good quantitative agreement achieved with the results of [56] with respect to the dispersion and decay of the Langmuir mode is the introduction of a non-constant Nevanlinna parameter function accounting for the exact high-frequency asymptotic of the system dielectric function. Further specification of this dynamic characteristic similar to the dynamic local-field correction in a TCP might be needed further.

We observed that for the Nevanlinna parameter function $Q_2 = Q_2(k, z)$ considered here, the value of the Langmuir frequency shifts from $\omega_2(k)$ closer to the plasma frequency, the effect which might be considered correct from the experimental point of view.

Further extension of the presented approach to model systems described by other effective potentials [60, 69] is planned.

Part III

Solutions of some exercises in Chapter 2

- Exercise 11. Directly from the Kramers-Kronig relations (2.4) and using the method of residues [1], we have:

$$\begin{aligned} n'(\omega) &= \frac{1}{\pi} P.V. \int_{-\infty}^{\infty} \frac{\Gamma}{(\omega' - u)^2 + \Gamma^2} \frac{d\omega'}{\omega' - \omega} = \\ &= 2i\Gamma \left\{ \frac{1}{2i\Gamma (u + i\Gamma - \omega)} + \frac{1}{2\left((\omega - u)^2 + \Gamma^2\right)} \right\} = \\ &= -\frac{1}{\omega - u - i\Gamma} + \frac{i\Gamma}{(\omega - u)^2 + \Gamma^2} = \\ &= \frac{u - \omega}{(\omega - u)^2 + \Gamma^2}; \end{aligned}$$

certainly, the same result stems from the answer of Exercise (**??**). Observe also that the complex response function

$$n(w = \omega + i\nu) = -\frac{1}{w - u + i\Gamma},$$

whose limiting value on the real axis $w = \omega$ equals

$$n\left(w = \omega + i0^+\right) = \frac{u - \omega}{(\omega - u)^2 + \Gamma^2} + \frac{i\Gamma}{(\omega - u)^2 + \Gamma^2}$$

can be found also as (close the integration path in the lower half-plane)

$$\begin{aligned} n(w) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{n''(\omega)\, d\omega}{\omega - w} = \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Gamma}{(\omega - u)^2 + \Gamma^2} \frac{d\omega}{\omega - w} = \\ &= \frac{-2i\Gamma}{2(-i\Gamma)(u - i\Gamma - w)} = -\frac{1}{w - u + i\Gamma}. \end{aligned} \tag{5.24}$$

The formula (5.24) is equivalent to the Kramers-Kronig relations (2.4). Observe that the unique pole of this complex refraction index is in the lower half-plane, as it should be for a response function.

- Exercise 38 We have to prove that

$$\int_{-\infty}^{\infty} D_n(x) D_m(x) d\sigma(x) = \delta_{nm} = \begin{cases} 1, & n = m, \\ 0, & n \neq m, \end{cases} \qquad n, m = 0, 1, 2.$$

It is obvious that

$$\int_{-\infty}^{\infty} D_0^2(x) d\sigma(x) = \int_{-\infty}^{\infty} \frac{d\sigma(x)}{\mu_0} = 1.$$

Further, since

$$
\begin{aligned}
D_1(x) &= \frac{x\mu_0 - \mu_1}{\sqrt{\mu_0\left(\mu_0\mu_2 - \mu_1^2\right)}}, \text{ and} \\
D_2(x) &= \frac{\left(\mu_0\mu_2 - \mu_1^2\right)x^2 + \left(\mu_1\mu_2 - \mu_0\mu_3\right)x + \left(\mu_3\mu_1 - \mu_2^2\right)}{\sqrt{\left(\mu_0\mu_2 - \mu_1^2\right)\Delta_2}},
\end{aligned}
$$

we have that

$$\int_{-\infty}^{\infty} D_2^2(x)d\sigma(x) =$$

$$= \frac{\left(\mu_0\mu_2 - \mu_1^2\right)\left(\mu_0\mu_2\mu_4 - \mu_2^3 - \mu_0\mu_3^2 - \mu_1^2\mu_4 + 2\mu_1\mu_2\mu_3\right)}{\left(\mu_0\mu_2 - \mu_1^2\right)\left(-\mu_2^3 - \mu_0\mu_3^2 - \mu_1^2\mu_4 + \mu_0\mu_2\mu_4 + 2\mu_1\mu_2\mu_3\right)} = 1;$$

$$\int_{-\infty}^{\infty} D_0(x)D_2(x)d\sigma(x) =$$

$$
\begin{aligned}
&= \int_{-\infty}^{\infty} \frac{\left(\mu_0\mu_2 - \mu_1^2\right)x^2 + \left(\mu_1\mu_2 - \mu_0\mu_3\right)x + \left(\mu_3\mu_1 - \mu_2^2\right)}{\sqrt{\mu_0}\sqrt{\left(\mu_0\mu_2 - \mu_1^2\right)\Delta_2}} d\sigma(x) = \\
&= \frac{\left(\mu_0\mu_2 - \mu_1^2\right)\mu_2 + \mu_1\left(\mu_1\mu_2 - \mu_0\mu_3\right) + \mu_0\left(\mu_3\mu_1 - \mu_2^2\right)}{\sqrt{\mu_0}\sqrt{\left(\mu_0\mu_2 - \mu_1^2\right)\Delta_2}} = 0;
\end{aligned}
$$

$$\int_{-\infty}^{\infty} D_1(x)D_2(x)d\sigma(x) = 0.$$

- Exercise 39 We start with $\mathrm{D}_0(t) = 1$, then

$$
\begin{aligned}
\mathrm{D}_1(t) &= t - \frac{\langle t, 1\rangle}{\|1\|^2}1 = t - \frac{\int_{-\infty}^{\infty} x d\sigma(x)}{\int_{-\infty}^{\infty} d\sigma(x)} = t - \frac{\mu_1}{\mu_0}, \\
\mathrm{D}_2(t) &= t^2 - \frac{\langle t^2, 1\rangle}{\|1\|^2}1 - \frac{\left\langle t^2, \left(t - \frac{\mu_1}{\mu_0}\right)\right\rangle}{\left\|t - \frac{\mu_1}{\mu_0}\right\|^2}\left(t - \frac{\mu_1}{\mu_0}\right) = \\
&= t^2 - \frac{\int_{-\infty}^{\infty} x^2 d\sigma(x)}{\int_{-\infty}^{\infty} d\sigma(x)} - \frac{\int_{-\infty}^{\infty}\left(x^3 - x^2\frac{\mu_1}{\mu_0}\right)d\sigma(x)}{\int_{-\infty}^{\infty}\left(x - \frac{\mu_1}{\mu_0}\right)^2 d\sigma(x)}t = \\
&= t^2 - \frac{\mu_2}{\mu_0} - \frac{\mu_3 - \frac{\mu_1}{\mu_0}\mu_2}{\mu_2 - \frac{\mu_1^2}{\mu_0}}t = t^2 - \frac{\mu_0\mu_3 - \mu_1\mu_2}{\mu_0\mu_2 - \mu_1^2}t - \frac{\mu_2}{\mu_0}, \text{ etc.}
\end{aligned}
$$

Notice that these vectors are all real and that

$$\int_{-\infty}^{\infty} D_n(x)D_m(x)d\sigma(x) = \int_{-\infty}^{\infty} D_m(x)D_n(x)d\sigma(x), \quad n, m = 0, 1, 2, \ldots.$$

We have the orthogonality as well:

$$\begin{aligned}\langle \mathrm{D}_0, \mathrm{D}_1\rangle &= \langle t,1\rangle - \langle t,1\rangle = 0;\\ \langle \mathrm{D}_0, \mathrm{D}_2\rangle &= \left\langle t^2,1\right\rangle - \left\langle t^2,1\right\rangle - \frac{\left\langle t^2, \left(t-\frac{\mu_1}{\mu_0}\right)\right\rangle}{\left\| t-\frac{\mu_1}{\mu_0}\right\|^2}\left\langle \left(t-\frac{\mu_1}{\mu_0}\right),1\right\rangle = 0;\\ \langle \mathrm{D}_1, \mathrm{D}_2\rangle &= \left\langle t^2, \left(t-\frac{\mu_1}{\mu_0}\right)\right\rangle - \frac{\langle t^2,1\rangle}{\|1\|^2}\left\langle 1, t-\frac{\mu_1}{\mu_0}\right\rangle - \left\langle t^2, \left(t-\frac{\mu_1}{\mu_0}\right)\right\rangle = 0,\end{aligned}$$

etc.

- Exercise 46 We have:

$$\sigma^{int}(z) = \frac{i\omega_p^2}{4\pi z}\frac{\left(1+\frac{i\tau\Omega^2}{z}\right)}{1+\frac{i\tau\Omega^2}{z}-\frac{\Omega^2}{z^2}} \underset{z\to\infty}{\simeq}$$

$$\frac{i\omega_p^2}{4\pi z}\left(1+\frac{i\tau\Omega^2}{z}\right)\left(1-\left(\frac{i\tau\Omega^2}{z}-\frac{\Omega^2}{z^2}\right)+\left(\frac{i\tau\Omega^2}{z}-\frac{\Omega^2}{z^2}\right)^2-\cdots\right) =$$

$$\frac{i\omega_p^2}{4\pi z}\left(1+\frac{\Omega^2}{z^2}-i\left(\frac{\Omega^4\tau}{z^3}-\frac{\Omega^6\tau}{z^5}\right)+\left(\frac{\Omega^4}{z^4}+\frac{2}{z^4}\Omega^6\tau^2\right)-\cdots\right) =$$

$$= \frac{i\omega_p^2}{4\pi z}+\frac{i\omega_p^2\Omega^2}{4\pi z^3}+\mathrm{o}\left(\frac{1}{z^3}\right).$$

Notice also that thus

$$\begin{aligned}\epsilon(z\to\infty) &= 1+\frac{4\pi i}{z}\left(\frac{i\omega_p^2}{4\pi z}+\frac{i\omega_p^2\Omega^2}{4\pi z^3}+\mathrm{o}\left(\frac{1}{z^3}\right)\right) =\\ &= 1-\frac{\omega_p^2}{z^2}-\frac{\omega_p^2\Omega^2}{z^4}+\mathrm{o}\left(\frac{1}{z^4}\right).\end{aligned}$$

- Exercise 52 Directly from the anticommutation relations (5.6 - **??**) we have

$$\begin{aligned}\left[a_{\mathbf{s}}^+a_{\mathbf{u}}, b_{\mathbf{r}}^+b_{\mathbf{t}}\right] &= a_{\mathbf{s}}^+a_{\mathbf{u}}b_{\mathbf{r}}^+b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\\ &= a_{\mathbf{s}}^+\left(-b_{\mathbf{r}}^+a_{\mathbf{u}}+\delta_{ab}\delta_{\mathbf{ur}}\right)b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\end{aligned}$$

$$\begin{aligned}&= -a_{\mathbf{s}}^+b_{\mathbf{r}}^+a_{\mathbf{u}}b_{\mathbf{t}}+\delta_{ab}\delta_{\mathbf{ur}}a_{\mathbf{s}}^+b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\\ &= -b_{\mathbf{r}}^+a_{\mathbf{s}}^+b_{\mathbf{t}}a_{\mathbf{u}}+\delta_{ab}\delta_{\mathbf{ur}}a_{\mathbf{s}}^+b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\\ &= -b_{\mathbf{r}}^+\left(-b_{\mathbf{t}}a_{\mathbf{s}}^++\delta_{ab}\delta_{\mathbf{st}}\right)a_{\mathbf{u}}+\delta_{ab}\delta_{\mathbf{ur}}a_{\mathbf{s}}^+b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\\ &= b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}}-\delta_{ab}\delta_{\mathbf{st}}b_{\mathbf{r}}^+a_{\mathbf{u}}+\delta_{ab}\delta_{\mathbf{ur}}a_{\mathbf{s}}^+b_{\mathbf{t}} - b_{\mathbf{r}}^+b_{\mathbf{t}}a_{\mathbf{s}}^+a_{\mathbf{u}} =\\ &= \delta_{ab}\left(\delta_{\mathbf{ur}}a_{\mathbf{s}}^+b_{\mathbf{t}}-\delta_{\mathbf{st}}b_{\mathbf{r}}^+a_{\mathbf{u}}\right).\end{aligned}$$

- Exercise 53 Take into account that

$$n^a_{\mathbf{q}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} a^+_{\mathbf{p}-\mathbf{q}} a_{\mathbf{p}} \ ,$$

and that

$$\begin{aligned} \left[a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}},\ \left(n^c_{\mathbf{p}} n^b_{-\mathbf{p}} - \delta_{cb} n_a\right)\right] &= \left[a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}},\ n^c_{\mathbf{p}} n^b_{-\mathbf{p}}\right] = \\ &= a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}} n^c_{\mathbf{p}} n^b_{-\mathbf{p}} - n^c_{\mathbf{p}} n^b_{-\mathbf{p}} a^+_{\mathbf{q}-\mathbf{k}} a_{\mathbf{q}} \ . \end{aligned}$$

Consider first

$$\begin{aligned} \left[a_{\mathbf{q}}, n^c_{\mathbf{p}}\right] &= a_{\mathbf{q}} \left(\frac{1}{\sqrt{V}} \sum_{\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}}\right) - \left(\frac{1}{\sqrt{V}} \sum_{\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}}\right) a_{\mathbf{q}} = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(a_{\mathbf{q}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(\left(\delta_{ac} \delta_{\mathbf{q},\mathbf{r}-\mathbf{p}} - c^+_{\mathbf{r}-\mathbf{p}} a_{\mathbf{q}}\right) c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(\delta_{ac} \delta_{\mathbf{q},\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} a_{\mathbf{q}} c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(\delta_{ac} \delta_{\mathbf{q},\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} + c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= \frac{\delta_{ac}}{\sqrt{V}} a_{\mathbf{q}+\mathbf{p}} \end{aligned}$$

and

$$\begin{aligned} \left[a^+_{\mathbf{q}-\mathbf{k}}, n^c_{\mathbf{p}}\right] &= a^+_{\mathbf{q}-\mathbf{k}} \left(\frac{1}{\sqrt{V}} \sum_{\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}}\right) - \left(\frac{1}{\sqrt{V}} \sum_{\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}}\right) a^+_{\mathbf{q}-\mathbf{k}} = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(a^+_{\mathbf{q}-\mathbf{k}} c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a^+_{\mathbf{q}-\mathbf{k}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(-c^+_{\mathbf{r}-\mathbf{p}} a^+_{\mathbf{q}-\mathbf{k}} c_{\mathbf{r}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a^+_{\mathbf{q}-\mathbf{k}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(-c^+_{\mathbf{r}-\mathbf{p}} \left(\delta_{ac} \delta_{\mathbf{q}-\mathbf{k},\mathbf{r}} - c_{\mathbf{r}} a^+_{\mathbf{q}-\mathbf{k}}\right) - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \left(-\delta_{ac} \delta_{\mathbf{q}-\mathbf{k},\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} + c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}-\mathbf{k}} - c^+_{\mathbf{r}-\mathbf{p}} c_{\mathbf{r}} a_{\mathbf{q}}\right) = \\ &= -\frac{1}{\sqrt{V}} \sum_{\mathbf{r}} \delta_{ac} \delta_{\mathbf{q}-\mathbf{k},\mathbf{r}} c^+_{\mathbf{r}-\mathbf{p}} = -\frac{\delta_{ac}}{\sqrt{V}} a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}} \ . \end{aligned}$$

Hence,

$$\left[a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\; n^c_{\mathbf{p}}n^b_{-\mathbf{p}}\right] = a^+_{\mathbf{q}-\mathbf{k}}\left(n^c_{\mathbf{p}}a_{\mathbf{q}}+\frac{\delta_{ac}}{\sqrt{V}}a_{\mathbf{q}+\mathbf{p}}\right)n^b_{-\mathbf{p}} - n^c_{\mathbf{p}}n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} =$$

$$= a^+_{\mathbf{q}-\mathbf{k}}n^c_{\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}+\frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}} - n^c_{\mathbf{p}}n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} =$$

$$= \left(n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}} - \frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}\right)a_{\mathbf{q}}n^b_{-\mathbf{p}}+\frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}}-n^c_{\mathbf{p}}n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} =$$

$$= n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}\left(n^b_{-\mathbf{p}}a_{\mathbf{q}}+\frac{\delta_{ab}}{\sqrt{V}}a_{\mathbf{q}-\mathbf{p}}\right) - \frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}+$$

$$+\frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}} - n^c_{\mathbf{p}}n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} =$$

$$= n^c_{\mathbf{p}}\left(n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}} - \frac{\delta_{ab}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}}\right)a_{\mathbf{q}}+\frac{\delta_{ab}}{\sqrt{V}}n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}-\mathbf{p}}-$$

$$-\frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}+\frac{\delta_{ac}}{\sqrt{V}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}} - n^c_{\mathbf{p}}n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}} =$$

$$= \frac{\delta_{ab}}{\sqrt{V}}\left(n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}-\mathbf{p}} - n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}}a_{\mathbf{q}}\right)+\frac{\delta_{ac}}{\sqrt{V}}\left(a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}} - a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}\right).$$

Part IV

Appendices

The integral (2.7)

Let us prove that

$$W_{r+is}(z) = \frac{iz^{r+is}}{\exp\left(\frac{\pi i(r+is)}{2}\right)\cos\left(\frac{\pi(r+is)}{2}\right)} \ .$$

Observe first that

$$\begin{aligned} W_{r+is}(z) &= \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{|x|^{r+is}\,dx}{x-z} = \\ &= \frac{1}{\pi}\left\{\begin{array}{l} x=-y, \\ dx=-dy, \end{array}\right. + \frac{1}{\pi}\int_{0}^{\infty}\frac{|x|^{r+is}\,dx}{x-z} = \\ &= -\frac{1}{\pi}\int_{0}^{\infty}\frac{y^{r+is}dy}{y+z} + \frac{1}{\pi}\int_{0}^{\infty}\frac{x^{r+is}dx}{x-z} = \\ &= \frac{2z}{\pi}\int_{0}^{\infty}\frac{x^{r+is}dx}{x^2-z^2} \ . \end{aligned}$$

Consider the contour integral with the closed integration path Γ , which consists of two segments $[\rho, R]$ of the real axis on two cut edges and two open circumferences C_ρ, $|z| = \rho$, and C_R, $|z| = R$, see Fig. # [1].

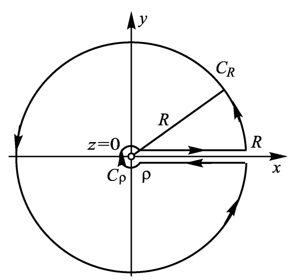

Fig. #. The integration path Γ.

By virtue of the main theorem of the theory of residues, for

$$\Phi(\zeta) = \frac{\zeta^{r+is}}{\zeta^2 - z^2} :$$

$$\oint_{\Gamma} \Phi(\zeta)\, d\zeta = \int_{\rho}^{R} \frac{x^{r+is} dx}{x^2 - z^2} + \int_{C_R^+} \Phi(\zeta)\, d\zeta + \int_{R}^{\rho} \Phi(\zeta)\, d\zeta +$$
$$+ \int_{C_\rho^-} \Phi(\zeta)\, d\zeta = 2\pi i \left\{ res\,(\Phi(\zeta))_z + res\,(\Phi(\zeta))_{-z} \right\}, \qquad (5.25)$$

the open circumference C_R is transited in the positive direction, i.e., anti-clockwise, while the open circumference C_ρ is transited in the negative direction.

Let us evaluate each contribution in the r.h.s. of (5.25):

$$\left| \int_{C_R^+} \frac{\zeta^{r+is} d\zeta}{\zeta^2 - z^2} \right| \le \frac{MR^r}{R^2} 2\pi R \underset{R\to\infty}{\longrightarrow} 0,$$

where

$$M > \frac{R^2}{|R^2 e^{2i\theta} - z^2|},\ 0 < \theta < 2\pi;$$

In the (third) integral over the lower edge of the cut $\zeta = xe^{2\pi i}$ $(x > 0)$ and $\zeta^r = x^r e^{2\pi i r}$. Hence,

$$\int_{R}^{\rho} \Phi(\zeta)\, d\zeta = -e^{2\pi i(r+is)} \int_{\rho}^{R} \frac{x^{r+is} dx}{x^2 - z^2}.$$

Finally, since in the vicinity of the point $z = 0$, for a sufficiently small radius ρ,

$$\frac{1}{|\rho^2 e^{2i\vartheta} - z^2|} < m,$$

$$\left| \int_{C_\rho^-} \Phi(\zeta)\, d\zeta \right| < m\rho^r 2\pi\rho \underset{\rho\to 0}{\longrightarrow} 0.$$

Now, taking $R \to \infty$ and $\rho \to 0$, we obtain:

$$\left(1 - e^{2\pi i(r+is)}\right) \int_{0}^{\infty} \frac{x^{r+is} dx}{x^2 - z^2} =$$

$$= 2\pi i \left\{ res\,(\Phi(\zeta))_z + res\,(\Phi(\zeta))_{-z} \right\} =$$
$$= 2\pi i \left(\frac{z^{r+is}}{2z} - \frac{(-z)^{r+is}}{2z} \right) = \frac{\pi i}{z} z^{r+is} \left(1 - e^{\pi i(r+is)}\right).$$

Thus,

$$W_{r+is}(z) = \frac{2z}{\pi} \int_{0}^{\infty} \frac{x^{r+is} dx}{x^2 - z^2} = 2iz^{r+is} \frac{1 - e^{\pi i(r+is)}}{1 - e^{2\pi i(r+is)}} =$$
$$= \frac{iz^{r+is}}{\exp\left(\frac{\pi i(r+is)}{2}\right) \cos\left(\frac{\pi(r+is)}{2}\right)}. \blacksquare$$

The Cauchy-Schwarz inequality in $\mathbf{L}^2$

states, for any pair of distribution densities, $f(\omega)$ and $g(\omega)$, that

$$\left| \int_{-\infty}^{\infty} f(\omega)\, g(\omega)\, d\omega \right|^2 \leq \int_{-\infty}^{\infty} |f(\omega)|^2\, d\omega \cdot \int_{-\infty}^{\infty} |g(\omega)|^2\, d\omega.$$

Choose $|g(\omega)| = \sqrt{\mathcal{L}(k,\omega)/\pi}$ and $|f(\omega)| = \omega^2 \sqrt{\mathcal{L}(k,\omega)/\pi}$ to get:

$$\begin{aligned} C_2^2 &= \left(\int_{-\infty}^{\infty} \omega^2 \mathcal{L}(k,\omega)\, \frac{d\omega}{\pi} \right)^2 \leq \left(\int_{-\infty}^{\infty} \omega^4 \mathcal{L}(k,\omega)\, \frac{d\omega}{\pi} \right) \cdot \left(\int_{-\infty}^{\infty} \mathcal{L}(k,\omega)\, \frac{d\omega}{\pi} \right) = \\ &= C_4(k)\, C_0(k)\,. \end{aligned}$$

Shannon entropy maximization

Imagine we want to reconstruct a distribution with the density $\exp\{-\Phi(t)\}$ such that

$$\int_{-\infty}^{\infty} \exp\{-\Phi(t)\}\,dt = 1 \tag{5.26}$$

Let $p(t) > 1$ be the approximate density such that

$$\int_{-\infty}^{\infty} p(t)\,dt = 1,$$

e.g., a rational density we want to be as close to $e^{-\Phi(t)}$ as possible. Then we can write:

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \exp\{-\Phi(t)\}\,dt = \\ &= \int_{-\infty}^{\infty} \exp\{-\Phi(t) - \ln p(t)\}\,p(t)\,dt. \end{aligned} \tag{5.27}$$

Due to the positivity of the latter integrand,

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \exp\{-\Phi(t)\}\,dt = \\ &= \int_{-\infty}^{\infty} \exp\{-\Phi(t) - \ln p(t)\}\,p(t)\,dt \geq \\ &\geq \exp\left\{-\int_{-\infty}^{\infty} [\Phi(t) + \ln p(t)]\,p(t)\,dt\right\}. \end{aligned} \tag{5.28}$$

If by definition

$$\langle f \rangle \equiv \int_{-\infty}^{\infty} f(t)\,p(t)\,dt,$$

we have from (5.27) and (5.28) that

$$1 \geq \exp\{-\langle \Phi(t) \rangle\} \exp\{S\}, \tag{5.29}$$

$$S = -\langle \ln p(t) \rangle \tag{5.30}$$

being the Shannon information entropy. Thus we have:

$$\langle \Phi(t) \rangle \geq S, \tag{5.31}$$

where equality corresponds to the exact coincidence between the reconstructed and the genuine distributions:

$$\int_{-\infty}^{\infty} \exp\{-\Phi(t) - \ln p(t)\}\,p(t)\,dt = 1$$

if and only if

$$p = e^{-\Phi}.$$

We conclude that the Shannon entropy (5.30) maximization is equivalent to the approximation improvement, though we are unable to control the quality of this improvement.

Notice also that the normalization condition (5.26) constitutes the first sum rule for the distribution to satisfy.

If the model distribution density $p(t)$ contains parameters, one can use different variational methods like the Rayleigh method, or, in case of having only numerical, not functional, parameters, even the Ritz method. The latter was used by us to obtain some of the numerical results described here.

Calculation of the loss function fourth power moment

Here we will provide details of calculations leading to (3.25), see Sect. 3. For the second derivative of the charge density operator we get from (3.10):

$$\ddot{\rho}_{\mathbf{k}} = \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{H}_0\right] = \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \left(\hat{K}+\hat{W}\right)\right] = \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{K}\right] + \frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{W}\right].$$

Consider first the "kinetic" contribution, using the result (3.21),

$$\begin{aligned}
\frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{K}\right] &= \frac{1}{i\hbar}\left[\frac{e\hbar}{i\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ \sum_{b,\mathbf{p}}\frac{\hbar^2p^2}{2m_b}b^+_{\mathbf{p}}b_{\mathbf{p}}\right] = \\
&= \frac{1}{i\hbar}\frac{e\hbar}{i\sqrt{V}}\frac{\hbar^2}{2}\sum_{a,b,\mathbf{q},\mathbf{p}}\frac{Z_a}{m_am_b}p^2\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\delta_{ab}\left[a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ b^+_{\mathbf{p}}b_{\mathbf{p}}\right] = \\
&= \frac{-e\hbar^2}{2\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a^2}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\left(q^2a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}}-(\mathbf{q}-\mathbf{k})^2a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}}\right) = \\
&= \frac{-e\hbar^2}{\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a^2}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)^2a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}};
\end{aligned}$$

Now,

$$\frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{W}\right] =$$

$$= \frac{1}{i\hbar}\left[\frac{e\hbar}{i\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ \frac{1}{2}\sum_{c,b,\mathbf{p}\neq\mathbf{0}}W_{cb}(p)\left(n^c_{\mathbf{p}}n^b_{-\mathbf{p}}-\delta_{cb}n_b\right)\right] =$$

$$\begin{aligned}
&= \frac{1}{i\hbar}\left[\frac{e\hbar}{i\sqrt{V}}\sum_{a,\mathbf{q}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ \frac{1}{2}\sum_{c,b,\mathbf{p}\neq\mathbf{0}}\frac{4\pi e^2}{p^2}\zeta_{cb}(q)\left(n^c_{\mathbf{p}}n^b_{-\mathbf{p}}-\delta_{cb}n_b\right)\right] = \\
&= -\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,c,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\frac{\zeta_{cb}(p)}{p^2}\left[a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}},\ \left(n^c_{\mathbf{p}}n^b_{-\mathbf{p}}-\delta_{cb}n_b\right)\right].
\end{aligned}$$

If we employ now the relation (3.22),

$$\frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{W}\right] = -\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,c,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\frac{\zeta_{cb}(p)}{p^2}\times$$

$$\times\left(\delta_{ab}\left(n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}-\mathbf{p}}-n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}}a_{\mathbf{q}}\right)+\delta_{ac}\left(a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}}-a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}\right)\right) =$$

$$= -\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,c,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\frac{\zeta_{cb}(p)}{p^2}\delta_{ab}\left(n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}-\mathbf{p}}-n^c_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}}a_{\mathbf{q}}\right)-$$

$$-\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,c,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\frac{\zeta_{cb}(p)}{p^2}\delta_{ac}\left(a^+_{\mathbf{q}-\mathbf{k}}a_{\mathbf{q}+\mathbf{p}}n^b_{-\mathbf{p}}-a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}\right)=$$

$$=-\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\left((\mathbf{q}+\mathbf{p})\cdot\mathbf{k}-\frac{k^2}{2}\right)-\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\right)\frac{\zeta_{ba}(p)}{p^2}n^b_{\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}+\mathbf{p}}a_{\mathbf{q}}-$$

$$-\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}\left(\left((\mathbf{q}-\mathbf{p})\cdot\mathbf{k}-\frac{k^2}{2}\right)-\left(\mathbf{q}\cdot\mathbf{k}-\frac{k^2}{2}\right)\right)\frac{\zeta_{ab}(p)}{p^2}a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}=$$

$$=\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{q},\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}(\mathbf{p}\cdot\mathbf{k})\frac{\zeta_{ab}(p)}{p^2}\left(a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}n^b_{-\mathbf{p}}+n^b_{-\mathbf{p}}a^+_{\mathbf{q}-\mathbf{k}-\mathbf{p}}a_{\mathbf{q}}\right)=$$

$$=\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}(\mathbf{p}\cdot\mathbf{k})\frac{\zeta_{ab}(p)}{p^2}n^b_{-\mathbf{p}}n^a_{\mathbf{k}+\mathbf{p}}.$$

And we are able to calculate the interaction contribution to the fourth moment:

$$C_4^W(k)=\frac{4\pi i}{\hbar k^2}\left\langle\left[\frac{1}{i\hbar}\left[\dot{\rho}_{\mathbf{k}},\ \hat{W}\right],\ \dot{\rho}_{-\mathbf{k}}\right]\right\rangle=\frac{4\pi i}{\hbar k^2}$$

$$\times\left\langle\left[\frac{4\pi e^3}{\sqrt{V}}\sum_{a,b,\mathbf{p}\neq\mathbf{0}}\frac{Z_a}{m_a}(\mathbf{p}\cdot\mathbf{k})\frac{\zeta_{ab}(p)}{p^2}n^b_{-\mathbf{p}}n^a_{\mathbf{k}+\mathbf{p}},\ \frac{ie\hbar}{\sqrt{V}}\sum_{c,\mathbf{s}}\frac{Z_c}{m_c}\left(\mathbf{s}\cdot\mathbf{k}+\frac{k^2}{2}\right)c^+_{\mathbf{s}+\mathbf{k}}c_{\mathbf{s}}\right]\right\rangle=$$

$$=-\frac{16\pi^2e^4}{k^2V}\sum_{a,b,c,\mathbf{s},\mathbf{p}\neq\mathbf{0}}\frac{Z_aZ_c}{m_am_c}\frac{\zeta_{ab}(p)}{p^2}\left\langle\left((\mathbf{p}\cdot\mathbf{k})\left(\mathbf{s}\cdot\mathbf{k}+\frac{k^2}{2}\right)\right)\times\right.$$

$$\left.\left(\delta_{ac}\left(n^b_{-\mathbf{p}}c^+_{\mathbf{s}-\mathbf{p}}c_{\mathbf{s}}-n^b_{-\mathbf{p}}c^+_{\mathbf{s}+\mathbf{k}}c_{\mathbf{s}+\mathbf{k}+\mathbf{p}}\right)+\delta_{bc}\left(c^+_{\mathbf{s}+\mathbf{k}+\mathbf{p}}c_{\mathbf{s}}n^a_{\mathbf{k}+\mathbf{p}}-c^+_{\mathbf{s}+\mathbf{k}}c_{\mathbf{s}-\mathbf{p}}n^a_{\mathbf{k}+\mathbf{p}}\right)\right)\right\rangle=$$

$$-\frac{16\pi^2e^4}{k^2V}\times$$

$$\times\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}}\frac{Z_a^2}{m_a^2}\frac{\zeta_{ab}(p)}{p^2}\left\langle\left((\mathbf{p}\cdot\mathbf{k})\left(\left(\mathbf{s}\cdot\mathbf{k}+\frac{k^2}{2}\right)-\left((\mathbf{s}-\mathbf{k}-\mathbf{p})\cdot\mathbf{k}+\frac{k^2}{2}\right)\right)\right)n^b_{-\mathbf{p}}a^+_{\mathbf{s}-\mathbf{p}}a_{\mathbf{s}}\right\rangle-$$

$$-\frac{16\pi^2e^4}{k^2V}\times$$

$$\times\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}}\frac{Z_aZ_b}{m_am_b}\frac{\zeta_{ab}(p)}{p^2}\left\langle(\mathbf{p}\cdot\mathbf{k})\left(\left(\mathbf{s}\cdot\mathbf{k}+\frac{k^2}{2}\right)-\left((\mathbf{s}+\mathbf{p})\cdot\mathbf{k}+\frac{k^2}{2}\right)\right)b^+_{\mathbf{s}+\mathbf{k}+\mathbf{p}}b_{\mathbf{s}}n^a_{\mathbf{k}+\mathbf{p}}\right\rangle=$$

$$\frac{16\pi^2e^4}{k^2V}\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}}\frac{Z_aZ_b}{m_am_b}\frac{\zeta_{ab}(p)}{p^2}\left\langle(\mathbf{p}\cdot\mathbf{k})^2\,b^+_{\mathbf{s}+\mathbf{k}+\mathbf{p}}b_{\mathbf{s}}n^a_{\mathbf{k}+\mathbf{p}}\right\rangle-$$

$$-\frac{16\pi^2e^4}{k^2V^2}\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}}\frac{Z_a^2}{m_a^2}\frac{\zeta_{ab}(p)}{p^2}\left((\mathbf{p}\cdot\mathbf{k})^2+(\mathbf{p}\cdot\mathbf{k})\,k^2\right)n^b_{-\mathbf{p}}a^+_{\mathbf{s}-\mathbf{p}}a_{\mathbf{s}}.$$

Notice that the angular average of $(\mathbf{p}\cdot\mathbf{k})$ vanishes! Hence,

$$C_4^W(k) = \frac{16\pi^2 e^4}{k^2 V}\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}} \frac{Z_a Z_b}{m_a m_b}\frac{\zeta_{ab}(p)}{p^2}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 b^+_{\mathbf{s}+\mathbf{k}+\mathbf{p}} b_{\mathbf{s}} n^a_{\mathbf{k}+\mathbf{p}}\right\rangle -$$

$$-\frac{16\pi^2 e^4}{k^2 V^2}\sum_{a,b,\mathbf{q},\mathbf{s},\mathbf{p}\neq\mathbf{0}} \frac{Z_a^2}{m_a^2}\frac{\zeta_{ab}(p)}{p^2}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 n^b_{-\mathbf{p}} a^+_{\mathbf{s}-\mathbf{p}} a_{\mathbf{s}}\right\rangle =$$

$$= \frac{16\pi^2 e^4}{k^2 V}\sum_{a,b,\mathbf{s},\mathbf{p}\neq\mathbf{0}} \frac{\zeta_{ab}(p)}{p^2}\left(\frac{Z_a Z_b}{m_a m_b}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 b^+_{\mathbf{s}+\mathbf{k}+\mathbf{p}} b_{\mathbf{s}} n^a_{\mathbf{k}+\mathbf{p}}\right\rangle - \frac{Z_a^2}{m_a^2}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 n^b_{-\mathbf{p}} a^+_{\mathbf{s}-\mathbf{p}} a_{\mathbf{s}}\right\rangle\right) =$$

$$= \frac{16\pi^2 e^4}{k^2 V}\sum_{a,b,\mathbf{p}\neq\mathbf{0}} \frac{\zeta_{ab}(p)}{p^2}\left(\frac{Z_a Z_b}{m_a m_b}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 n^b_{-\mathbf{k}-\mathbf{p}} n^a_{\mathbf{k}+\mathbf{p}}\right\rangle - \frac{Z_a^2}{m_a^2}\left\langle (\mathbf{p}\cdot\mathbf{k})^2 n^b_{-\mathbf{p}} n^a_{\mathbf{p}}\right\rangle\right).$$

Finally,

$$C_4^W(k) = \frac{16\pi^2 e^4}{V}\sum_{a,b,\mathbf{q}\neq\mathbf{0}} \zeta_{ab}(q)\frac{(\mathbf{q}\cdot\mathbf{k})^2}{k^2 q^2}\left(\frac{Z_a Z_b}{m_a m_b}\left\langle n^b_{-\mathbf{k}-\mathbf{q}} n^a_{\mathbf{k}+\mathbf{q}}\right\rangle - \frac{Z_a^2}{m_a^2}\left\langle n^b_{-\mathbf{q}} n^a_{\mathbf{q}}\right\rangle\right),$$

which reduces to (3.26) if we introduce the static partial structure factors

$$S_{ab}(q) = \frac{\left\langle n^b_{-\mathbf{k}-\mathbf{q}} n^a_{\mathbf{k}+\mathbf{q}}\right\rangle}{\sqrt{n_a n_b}}. \tag{5.32}$$

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