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Dynamic collision frequency of Kelbg-pseudopotential-modelled plasmas

Abstract. The simulation data [1,2] on the dynamic collision frequency (DCF) of hydrogen-like plasmas modelled with the Kelbg pseudopotential are treated within the theory of moments with local constraints. Additionally, the correlational sum rule which is the second power frequency moment of the external conductivity real part is taken into account to express the DCF in terms of the Nevanlinna parameter function. The validity of the suggetsed analytic form of the latter is tested against the simulation data, while the sum rules are calculated using the Kelbg potential and the Ornstein-Zernike hypernetted-chain equations.
Keywords:strongly coupled plasma, method of moments with local constraints, sum rule, Nevanlinna function, dynamic collision frequency.

Introduction

As it is known, the classical method of moments gives reliable resultson the reconstruction of some physical quantities such as the dynamic structure factor [3,4], i.e., the function that must obey some mathematical properties [5] satisfing sum rules and correct assymptotic behavior. Additioanlly, this method can be completed by local constraints, [6-8] and [9]. Based on [1, 2] here we try to reconstruct the dynamic collision frequencies using this latter method of moments with local constraints. But as you will see there is a problem occur which we will discuss about it further.

We are interested in strongly coupled hydrogen-like plasmas which exist in stellar like stars interior [10] and can be detected in the devices of thermonuclear fusion [11].We consider the simulation resultswhere the modified Kelbg potential is used [2].

In the first part of the paper we introduce the approach and then apply it to the simulated physical quantity.

The mathematical background

Consider the mixed Löwner-Nevanlinna problem [6-8], see also Ref. [12] for the matrix version of the problem.

Problem 1. Given a set of real numbers $(c_0,\dots,c_{2n})$*, a finite set of points* $(t_1,\dots,t_p)$ *on the real axis, and a set of complex numbers* $(w_1,\dots,w_p)$ *with non-negative imaginary parts, find a positive function* $f(t), t\in R$ *such that*

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

and

$$w_s = \lim_{\varepsilon\downarrow 0}\int_{-\infty}^{\infty}\frac{f(t)dt}{t-t_s-i\varepsilon},\ \ s=1,..,p.\ . \qquad (2)$$

The Problem 1 is a mixture of the truncated Hamburger moment problem with the Löwner-type interpolation problem in the class of Nevanlinna functions[13].

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 mixed problem solution
Solvability and contractive functions

Assume that the set of moments is definite-positive and that truncated Hamburger moments problem is solvable [6-8] and that there exists an infinite set of non-negative measures g on the real axis such that

$$\int_{-\infty}^{\infty} t^k dg(t) = c_k,\ k = 0,1,\dots,2n. \quad (3)$$

Then the formula

$$\int_{-\infty}^{\infty} \frac{d\sigma(t)}{t-z} = -\frac{E_{n+1}(z)+\zeta(z)E_n(z)}{D_{n+1}(z)+\zeta(z)D_n(z)},\quad Imz > 0,\quad n = 0,1,2,\dots \quad (4)$$

according to Nevanlinna's theorem, establishes a one-to-one correspondence between the set of all measures $g(t)$ satisfying (3) and the Nevanlinna functions $\zeta(z) \in \mathfrak{R}$, i.e., functions which are analytic in the half-plane $Imz > 0$, continuous on its closure $Imz = 0$, having in $Imz \geq 0$ a positive imaginary part and such that $\lim_{z\to\infty}\zeta(z)/z = 0,\ Imz > 0$.

Polynomials $\{D_k\}_0^{n+1}$ form an orthogonal system with respect to each g-measure satisfying (3) and can be found by the Gram-Schmidt procedure applied to the basis $\{1, t, t^2, \dots, t^{n+1}\}$, while $\{E_k\}_0^{n+1}$ is the corresponding set of conjugate polynomials [7]. Notice that the zeros of each orthogonal polynomial $D_k(z)$ are real and by virtue of the Schwarz-Christoffel identity [7] the zeros of $D_{k-1}(z)$ alternate with the zeros of $D_k(z)$ as well as with the zeros of $E_{k-1}(z)$.

To meet the constraints (2) it is enough now to substitute into the right hand side of (4) any function $\zeta(z)$ which satisfies the following conditions:

$$\xi_s = \zeta(t_s) = -\frac{w_s D_{n+1}(t_s)+E_{n+1}(t_s)}{w_s D_n(t_s)+E_n(t_s)},\ s = 1,..,p. \quad (5)$$

Note that $Im\xi_s > 0$. Thus Problem 1 reduces to

Problem 2 Given a finite number of distinct points $t_1,\dots,t_p$ of the real axis and a set of complex numbers $w_1,\dots,w_p$ with positive imaginary parts, find the set of functions $\zeta(z) \in \mathfrak{R}$continuous in the closed upper half-plane which satisfy conditions (5).

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

$$\zeta(z) = i\,\frac{1+\theta(z)}{1-\theta(z)}, \quad (6)$$

where

$$\theta(z) = \frac{\zeta(z)-i}{\zeta(z)+i} \quad (7)$$

is a holomorphic function on the upper half-plane with *contractive* values, i.e. $|\theta(z)| \leq 1,\ Imz > 0$. Therefore Problem 2 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 3 Given a finite number of distinct points $t_1,\dots,t_p$ of the real axis and a set of points $\lambda_1,\dots,\lambda_p$,

$$\lambda_s = \frac{\xi_s - i}{\xi_s + i},\ |\lambda_s| \leq 1,\ s = 1,\dots,p. \quad (8)$$

find a set of functions $\theta \in \mathfrak{B}$such that

$$\theta(t_s) = \lambda_s,\ s = 1,\dots,p. \quad (9)$$

Problem 3 is a limiting case of the Nevanlinna-Pick problem [7,13] with interpolation nodes on the real axis. Its solvability for any interpolation data $\lambda_1,\dots,\lambda_p$ inside the unit circle was actually proven in Ref. [14]. 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 $|\lambda_s| = 1$.

We describe below an algorithm of solution of Problem 3 when all $|\lambda_s| < 1$, which is a simple modification of the Schur algorithm. An alternative algorithm, similar to the Lagrange method of the interpolation theory, can be applied if some or even all $|\lambda_s| = 1$[8].

Schur algorithm

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

$$\theta(z) = \frac{\phi(z)+\lambda_1}{\overline{\lambda_1}\phi(z)+1}\ , \tag{10}$$

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

$$\phi(z) = \frac{z-t_1}{z-\overline{t_1}}\chi(z)\ ,$$

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

Here we carry out the reconstruction procedure using the non-rational functions, in particular, using the function suggested in Ref. [8]

$$\phi(z) = \theta_1(z)\exp\left\{\frac{\alpha}{\pi i}\int_{t_1-1}^{t_1+1}\frac{1+tz}{t-z}\ln|t-t_1|\frac{dt}{t^2+1}\right\} := \theta_1(z)u_1(z), \tag{11}$$

with a unique free parameter $\alpha \in (0,1)$. Here θ_1 is any function from $\mathfrak{B}$ such that

$$\theta_1(t_s) = \lambda_s' = \frac{1}{u_1(t_s)}\frac{\lambda_s-\lambda_1}{1-\overline{\lambda_1}\lambda_s},\ s = 2,\ldots,p. \tag{12}$$

Such a choice of $\theta_1(z)$ guarantees the verification of all of the conditions (9). Hence Problem 3 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 (12). 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 $t_{s+1},\ldots,t_p$ according to (12), permits to obtain some solution of Problem 3. Observe that contrary to the Nevanlinna-Pick problem with nodes in the open upper half-plane, our Problem 3 is always solvable if the values of the function to reconstruct are contractive at the nodes of interpolation.

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

$$\theta(z) = \frac{a(z)\mu(z)+b(z)}{c(z)\mu(z)+d(z)}, \tag{13}$$

where the elements of the matrix of the linear fractional transformation (13) are non-rational functions constructed as above and $\mu(z)$ runs the subset of all functions from $\mathfrak{B}$ satisfying the condition $\mu(t_p) = \lambda_p^{(p-1)}$. This matrix can be calculated as

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{s=1}^{p-1}\begin{pmatrix} u_s(z) & \lambda_s^{(s-1)} \\ \overline{\lambda_s^{(s-1)}}u_s(z) & 1 \end{pmatrix}, \tag{14}$$

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 (13) is just $\mu(z) \equiv \lambda_p^{(p-1)}$.

Hence, if initial parameters $\lambda_1,\ldots,\lambda_p$ in Problem 3 are strictly contractive, then among the solutions of this problem there are non-rational functions of the type we consider.

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.

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

$$c_k = \int_{-\infty}^{\infty} t^k f(t)dt \ , \quad k = 0,1,\dots,2n \ , \quad n = 1,2,\dots, \qquad (15)$$

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

$$w_s = \varphi(t_s) = P.V.\int_{-\infty}^{\infty} \frac{f(t)dt}{t-t_s} + i\pi f(t_s) \ . \quad (16)$$

In all cases we considered, we used only three non-zero moments, $n = 2$, and three interpolation, $p = 3$; the latter principal value integrals were computed numerically and the orthogonal polynomials were calculated directly:

$$\begin{aligned} D_0(z) &= 1, \quad D_1(z) = z, \quad D_2(z) = z^2 - \omega_1^2, \\ D_3(z) &= z(z^2 - \omega_2^2), \quad E_0(z) \equiv 0, \quad E_1(z) = c_0, \\ E_2(z) &= c_0 z, \quad E_3(z) = c_0(z^2 - \omega_2^2 + \omega_1^2) \end{aligned}$$

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

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

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

we made use of the Shannon entropy

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

maximization procedure [15], where the density $F(\alpha,t)$ is the one reconstructed within the algorithm, i.e., the imaginary part (divided by π) of the model function obtained by the Schur-algorithm procedure. The density $F(\alpha,t)$ has no real poles and is positive over the whole real axis, hence it is quite easy to solve the maximization procedure equation: $d\mathfrak{S}(\alpha)/d\alpha = 0$.

Results and conclusions

To check the quality of the above reconstruction techniquewe used the simulation data of [2] to obtain the dynamic collision frequency. Particularly for $\Gamma = 1, \mathrm{T} = 350\,000\,K$ three experimental points were used: $\mathrm{t}_1 = 0.4$; $\mathrm{t}_2 = 1$; $\mathrm{t}_3 = 1.2$. Since the imaginary part of DCF takes negative values it was decided to carry out the comparison for the real part of the DCF and the loss function which is mathematically corect fot the method of moments. Precisely, we applied the Nevanlinna theorem to the DCF, and expressed it in terms of the Nevanlinna parameter function $\zeta(\omega;k)$ reconstructed by the above algorithm. The numerical results were compared to the simulation data of [2] and the data are presented is figures 1 and 2. In all figures the the thick lines correspond to our results, ω_p is the plasma frequency.

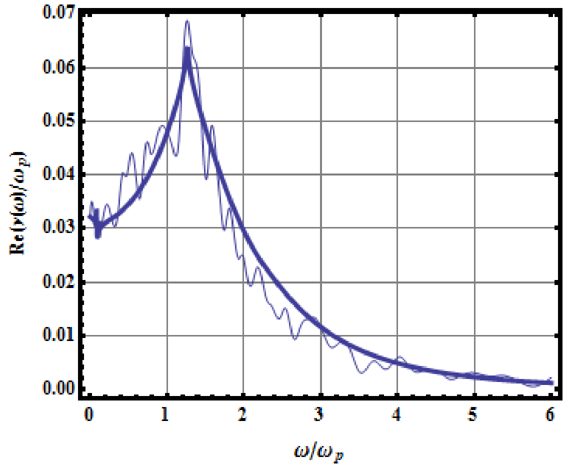
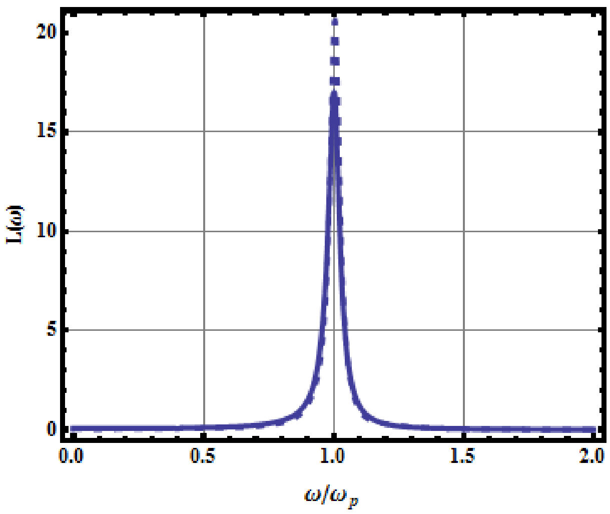


Figure 1 –The real part of the dynamical collision frequency in comparison with the simulation data of [2] at Γ=1, T=350 000 K



We can conclude that an algorithm presented here per mits to obtain, at least in the cases we consider, a quantitative agreement between the simulation data on the plasma DCF and loss functions reconstructed by a few integral characteristics, the power moments and the local constraints.

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