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ORIGINAL ARTICLE

Contributions to Plasma Physics

Sum rules and exact inequalities for strongly coupled one-component plasmas

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Several sum rules and other exact relations are employed to determine both the static and the dynamic properties of strongly coupled, partially and completely degenerate one-component plasmas. Emphasis is placed on the electron gas, both at zero and finite temperatures. The procedure is based on the self-consistent method of moments, recently developed in *Phys. Rev. Lett.*, 2017, 119, 045001, that provides a neat expression for the loss function valid at strong couplings. An input value of the method in its classical version is the static structure factor, whose accuracy is shown to insignificantly affect the resulting numerical data. Starting from the Cauchy-Bunyakovsky-Schwarz inequality, a criterion is proposed to verify the quality of various approaches to the evaluation of the static characteristics of one-component, strongly coupled plasmas.

KEYWORDS
method of moments, static and dynamic structure factors, sum rules

1 | INTRODUCTION

One of the great challenges of modern plasma physics is the analytical and numerical description of the transition from collision-less to collision-dominated regimes in different Coulomb systems as well as of the crossover from classical to Fermi liquid behaviour of dense plasmas.[1,2] This is especially true for warm and hot dense matter or strongly coupled plasmas characterized by a wide range of variation of temperature $T \in (10^4\text{–}10^7)$ K and the mass density $\rho \in (10^{-2}$ to $10^4)$ g/cm^3, thereby spanning a few orders of magnitude variation. Within such a broad range of physical conditions, various effects compete with one another at different scales and impede the construction of bridging gap theories capable of predicting static and dynamic properties of systems under investigation. The above-stated domain of plasma parameters is, of course, of high relevance to inertial fusion devices,[3] but it is, nowadays, over-reached by other advanced laboratory studies as evidenced, for instance, in research on ultracold plasmas.[4]

The focus of the present consideration is a one-component plasma that consists of a single particle species, say electrons, with the electric charge e, the mass m, and the number density n. The standard procedure is to introduce the following coupling and degeneracy parameters, respectively, as: $\Gamma = \beta e^2/a$ and $D = \theta^{-1} = \beta E_F$, where $\beta = (k_B T)^{-1}$ denotes the inverse temperature in energy units, $a = (4\pi n/3)^{-1/3}$ stands for the Wigner-Seitz radius, and $E_F = \hbar^2(3\pi^2 n)^{2/3}/2m$ designates the Fermi energy. Another dimensionless quantity appropriate for the description of one-component plasma is the Brueckner parameter, defined as follows:

$r_s = a/a_B$, where $a_B = \hbar^2/me^2$ signifies the first Bohr radius. Note that, for the domain of temperature and mass density mentioned above, the introduced dimensionless parameters vary in the following ranges: the coupling parameter $\Gamma \in (4.9 \times 10^{-3},\ 490)$, the degeneracy parameter $D \in (1.4 \times 10^{-3},\ 1.4 \times 10^{4})$, and the Brueckner parameter $r_s \in (6.5 \times 10^{-2}, 6.5)$.

On the one hand, the static and dynamic characteristics of strongly coupled plasmas are regularly simulated using first-principle physical approaches; see, for example.[2,5] On the other hand, the properties of weakly or even moderately coupled plasmas have been theoretically studied very well in the literature. In order to describe the transition from the ideal gas- to solid state-like behaviour of the system, it seems unavoidable to engage the fitting over a broader range of variation of Γ and/or D using few adjustable parameters.[6] In this case, however, some numerical data, for instance, the dynamic local-field correction, still remain unexplained theoretically.[7]

It is very well known that first-principle physical approaches are entirely based on equations of motion, classical or quantum mechanical, of particular physical systems that are finally reducible either to the set of Hamiltonian equations or to the many-body Schrödinger equation plus symmetrization. The quality and accuracy of the data obtained can be strictly verified by the so-called sum rules (e.g., for the dynamic structure factor [DSF]), which might be considered complementary conservation laws. To exactly satisfy them, it sometimes appears necessary to apply some additional adjustments, for example, by selecting a specific (Gaussian) memory function[8] in the Zwanzig-Mori time-propagator dynamic framework[9] or by partially ignoring them as is the case in the random-phase approximation (RPA), including its local-field and other corrected versions[10]; see ref. [11] for details. As is demonstrated below in this paper, another option is to use ab initio Monte Carlo simulation results on static characteristics of strongly coupled Coulomb systems[12] combined with the method of moments.

This paper particularly deals with an alternative mathematical approach capable of taking all the sum rules into account automatically. Distinguishing features of the physical system under investigation are then hidden in the sum rules that can be found independently and rigorously using the standard methods of quantum statistics within the Kubo linear response theory. This approach was first applied to strongly coupled plasmas more than 30 years ago[13,14] and was developed further in a series of works,[11,15–18] which were based on the classical monographs.[19,20] Final expressions essentially rely on Nevanlinna's solution[21] to the truncated Hamburger moment problem, consisting of the reconstruction of a non-negative continuous distribution density by its power moments. An infinite set of solutions of this problem is parameterized by the Nevanlinna parameter function (NPF), which has no particular physical meaning. Thus, the NPF is not a measurable quantity, and the quality of the whole approximation in the framework of the method of moments can be controlled by comparison with experimental results and numerical simulation data. It is important that the moment approach in general is equivalent to the continued fraction method.[22]

A new self-consistent version of the method of moments was recently proposed in ref. [23], where it was successfully applied to the direct determination of dynamic properties of one-component classical strongly coupled plasmas, and its validity was verified against available simulation data. The method itself contained no adjustable parameters, and its robustness was confirmed by applying several schemes to calculate the static structure factor (SSF), which was the input value and was shown to have minor influence on the dynamic properties themselves.

The aim of the present paper is twofold: (a) to check the possibility of extending the above-mentioned approach to partially or even completely degenerate one-component, strongly coupled plasmas (OCSCPs), for example, the paramagnetic uniform electron gas (PUEG),[24] and (b) to develop a criterion of validity of the SSF starting from the Cauchy-Bunyakovsky-Schwarz inequality.[11,25] It is worth mentioning that generalizations to other situations of physical interest, like magnetized and non-equilibrium plasmas, can be carried out within the matrix method of moments.[18,26]

The rest of the paper is organized in the following way. In Section 2, we first develop the self-consistent method of moments for the PUEG at zero and finite temperatures and, then, determine the DSF and the characteristics of the collective modes in order to verify them against the available theoretical predictions.[27] Section 3 is devoted to the Cauchy-Bunyakovsky-Schwarz inequality with the purpose of establishing a criterion on the validity of various schemes for calculating the SSF. Numerical results are presented in Section 4, and main inferences are summarized in the concluding Section 5.

2 | LOSS FUNCTION AND DSF

The keystone of the present version of the moment approach is the inverse plasma dielectric function, $\varepsilon^{-1}(\omega, q)$, which is the genuine response function for any dimensionless wavenumber $q = ka$ that yields the following positive even loss function of the frequency:

$$\mathscr{L}(x = \omega^2, q) = -Im\ \ \varepsilon^{-1}(\omega, q)/\omega.$$

It has to be admitted that only classical one-component systems were the focus of ref. [23], which means that the properties of the loss function and the DSF were actually equivalent in view of the fluctuation-dissipation theorem (FDT). However, it is not the case for the present consideration as partially and completely degenerate one-component plasmas are under scrutiny.

The fundamental blocks of the present approach are the so-called sum rules that constitute the loss function frequency moments defined as[1]:

$$C_\nu(q) = \frac{1}{\pi}\int_{-\infty}^{\infty} \omega^\nu \mathscr{L}(\omega^2, q) d\omega \ , \qquad \nu = 0, 2, 4, \tag{1}$$

and supplemented by *the semi-empirical observation* that the loss function should have, for an arbitrary q, an extremum at $x = \omega^2 = 0$, such that:

$$\left.\frac{d\mathscr{L}(x,q)}{dx}\right|_{x=\omega^2=0} = 0. \tag{2}$$

Note that the *Ansatz* (2) for the loss function was thoroughly tested in ref. [11] for quite a broad range of plasma parameters and various inter-particle interaction models, and its implication on the long-time behaviour of the density correlator in the ($\mathbf{r}$,t) space will be discussed elsewhere. It has to be stressed that the odd-order moments completely vanish in definition (1) as the loss function retains its evenness as a function of the frequency ω.

It is the power of the method of moments, together with the crucial assumption (2), that concisely reduces the description of all versatile dynamic properties of various types of plasmas to the knowledge of only two characteristic frequencies:

$$\omega_1(q) = \sqrt{C_2(q)/C_0(q)}, \qquad \omega_2(q) = \sqrt{C_4(q)/C_2(q)}, \tag{3}$$

defined via the loss function frequency moments $\{C_0(q), C_2(q), C_4(q)\}$ that are still to be independently determined.

Due to the Kramers–Kronig relations, the zeroth moment is determined by the static dielectric function $\epsilon(0, q)$, whereas the second moment simply represents the so-called f-sum rule. Thus, the square of the first characteristic frequency is found to be:

$$\omega_1^2(q) = \omega_p^2[1 - \epsilon^{-1}(0, q)]^{-1} \tag{4}$$

with $\omega_p^2 = 3e^2/ma^3$ being the plasma frequency squared.

It has been established—through the Kubo linear-response theory[28] and the second-quantization technique[14,18]—that, in a one-component Coulomb system of interest herein, the square of the second characteristic frequency reads as:

$$\omega_2^2(q) = \omega_p^2[1 + K(q) + U(q)], \tag{5}$$

to include the kinetic $K(q)$ and the coupling $U(q)$ contributions in the following form:

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

$$U(q) = \frac{1}{6\pi}\int_0^\infty p^2(S(p) - 1)\left(\frac{5}{3} - \frac{p^2}{q^2} + \frac{(p^2 - q^2)^2}{2pq^3}\ln\left|\frac{p+q}{p-q}\right|\right) dp. \tag{6}$$

Here, $S(q)$ denotes the SSF, and the μ-order Fermi integral is defined as:

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

with η being the dimensionless chemical potential of the electronic system determined by the normalization condition $I_{1/2}(\eta) = 2D^{3/2}/3$. It is therefore straightforward to infer that the moments of the loss function can be independently evaluated with an accuracy for which the SSF is known; for details, see refs [23] and [29].

It is rather interesting to stress that the following expansion holds in the hydrodynamic limit:

$$\omega_2^2(q \to 0) \simeq \omega_p^2\left[1 + \frac{q^2}{\Gamma}\left(\frac{F_{3/2}(\eta)}{D^{3/2}} + \frac{4u(\Gamma, r_s)}{45}\right) + O(q^4)\right], \tag{7}$$

where $u(\Gamma, r_s)$ stands for the reduced correlation energy[30] so that, at very large wavenumbers, the single-particle behaviour is exactly recovered as:

$$\omega_2^2(q \to \infty) \simeq \frac{\omega_p^2 q^4}{12 r_s}. \tag{8}$$

The original mathematical background of the present approach is called the truncated classical Hamburger problem of moments,[18,19] which is formulated as follows: reconstruct a positive function that is at least continuous on the whole real

[1]Note that $C_\nu(q) = \int_0^\infty x^{\frac{\nu-1}{2}} \mathscr{L}(x, q) dx$ are effectively Stieltjes fractional power moments.[19]

axis and whose first power moments are independently known. The function to be reconstructed hereafter is the loss function $\mathscr{L}(\omega, q)$, whose power frequency moments are strictly written out above. The subset of the infinite (except for some very particular specific cases[16]) set of solutions of the Hamburger problem, which is continuous on the real axis of frequency ω, is unilaterally parameterized by the NPF $R(\omega, q)$ via the Nevanlinna theorem[19,20] and the Nevanlinna formula (cf. Equation (59) in ref. [11]), wherefrom the loss function can be restored using the Sochocki–Plemelj–Dirac formula as:

$$\mathscr{L}(\omega^2, q) = \frac{\omega_p^2(\omega_2^2(q) - \omega_1^2(q))Im\ \ R(\omega, q)}{|\omega(\omega^2 - \omega_2^2(q)) + R(\omega, q)(\omega^2 - \omega_1^2(q))|^2}. \tag{9}$$

Like any response function, the NPF $R(\omega, q)$ must be analytical and possess a non-negative imaginary part in the upper half-plane Im $\omega > 0$, being at least continuous on its closure Im $\omega = 0$. In addition, the NPF $R(\omega, q)$ must obey the limiting condition:

$$\lim_{\omega\to\infty} \frac{R(\omega, q)}{\omega} = 0, \tag{10}$$

uniformly within any angle $\vartheta \leq \arg(\omega) \leq \pi - \vartheta$, $0 < \vartheta < \pi$, which ensures that all of the involved sum rules are automatically satisfied.

To proceed further, one has to justify the choice of the NPF $R(\omega, q)$, which has no specific physical meaning. It is apparent that the simplest mathematical approximation at hand is to replace the frequency-dependent NPF with its static value, how it was performed, for instance, in ref. [31] and in a series of other publications (see ref. [18] and references therein):

$$R(\omega, q) = R(0, q) = ih(q), \qquad h(q) > 0, \tag{11}$$

which converts (9) into

$$\begin{aligned} \left.\frac{\mathscr{L}(x = \omega^2, q)}{C_0(q)}\right|_{R=ih} &= \frac{\omega_1^2(q)(\omega_2^2(q) - \omega_1^2(q))h(q)}{\omega^2(\omega^2 - \omega_2^2(q))^2 + h^2(q)(\omega^2 - \omega_1^2(q))^2} \\ &= \frac{\omega_1^2(q)(\omega_2^2(q) - \omega_1^2(q))h(q)}{x(x - \omega_2^2(q))^2 + h^2(q)(x - \omega_1^2(q))^2}. \end{aligned} \tag{12}$$

Approximation (11) is certainly an imposed restriction on the class of the solutions to the Hamburger problem, and its further justification is assured by the comparison of the obtained results with those of real experiments and numerical simulations. In collision-less plasmas that are well described within the RPA and its local field-corrected extensions, approximation (11) should be modified, but it seems to work quite satisfactorily at least for classical[23] and partially degenerate OCSCPs.

As was earlier shown in ref. [18], the positive parameter $h(q)$ can be related to the static value of the "charge–charge" (DSF), $S(0, q)$. In virtue of the additional condition (2), the following explicit expression is readily obtained from (12) for the static value of the NPF in terms of the characteristic frequencies $\omega_1(q)$ and $\omega_2(q)$ [23]:

$$h(q) = h_0(q) = \frac{\omega_2^2(q)}{\sqrt{2}\omega_1(q)}, \tag{13}$$

thereby resulting in the neat expression for the loss function

$$\left.\frac{\mathscr{L}(\omega^2, q)}{C_0(q)}\right|_{R=ih_0} = \frac{\sqrt{2}\omega_1(q)\omega_2^2(q)(\omega_2^2(q) - \omega_1^2(q))}{2\omega^6 + \omega^4(\omega_2^2(q)/\omega_1^2(q))(\omega_2^2(q) - 4\omega_1^2(q)) + \omega_1^2(q)\omega_2^4(q)}, \tag{14}$$

that already contains no free parameters and, probably, represents the simplest theoretical dependence of the loss function on the frequency ω.

Expression (14) bears the following original sense. As soon as the SSF and the static value of the dielectric function are somehow known, it becomes possible to evaluate the characteristic frequencies $\omega_1(q)$ and $\omega_2(q)$ of the system under study, and then, formula (14) allows one to predict all the plasma dynamic properties in the strongly coupled regime. It has to be advocated that expression (14) can be verified for systems of various physical nature in which different effects might play an essential role. The only restrictions come from the finite number of moments taken into account in the solution of the truncated Hamburger problem as well as from the imposed behaviour of the loss function at zero frequency (2), finally leading to expression (13) of the NPF[23].

Equation (14) is the main result of the present research as the DSF, which is the central quantity of collective and dynamic effects, is determined by the loss function via:

$$S(\omega, q) = \frac{q^2 n}{3\pi\Gamma} B(\beta\hbar\omega)\mathscr{L}(\omega^2, q) = \frac{q^2 n}{3\pi\Gamma} \frac{\sqrt{2}\omega_1(q)\omega_2^2(q)\omega_p^2(\omega_2^2(q) - \omega_1^2(q))B(\beta\hbar\omega)}{2\omega_1^2(q)\omega^2(\omega^2 - \omega_2^2(q))^2 + \omega_2^4(q)(\omega^2 - \omega_1^2(q))^2}, \tag{15}$$

where $B(\beta\hbar\omega) = \beta\hbar\omega/[1 - \exp(-\beta\hbar\omega)]$ refers to the Bose factor. Note that, by virtue of (15), both dynamic functions $\mathscr{L}(\omega^2, q)$ and $S(\omega, q)$ behave in a similar way at low frequencies.

Taking into account the very well-known formula

$$\frac{1}{1 - \exp(-\beta\hbar\omega)} \underset{\beta=\infty}{=} \begin{cases} 1, & \omega \geq 0 \\ 0, & \omega < 0 \end{cases},$$

it is possible to conclude that

$$S(\omega \leq 0, q)|_{\beta=\infty} = 0, \tag{16}$$

that is, at exactly zero temperature, the DSF should vanish for the non-positive values of the frequency ω.

The DSF spectrum, that is, the zeros of the dispersion equation

$$\sqrt{2}z[z^2 - \omega_2^2(q)]\omega_1(q) + i\omega_2^2(q)[z^2 - \omega_1^2(q)] = 0 \tag{17}$$

provide direct information on the system (unshifted) diffusion $\omega_{\text{ush}}(q)$ and shifted (optical or acoustic-roton) $\omega_{\text{sh}}(q)$ modes that can now be analytically found as the exact solution of (17) (see refs [23] and [32]):

$$\begin{aligned} \omega_{\text{ush}}(q) &= -i\gamma(q) = -v^2X(q) - vY(q) - ih_0(q)/3, \\ \omega_{\text{sh}}(q) &= \omega(q) - i\delta(q) = -vX(q) - v^2Y(q) - ih_0(q)/3, \end{aligned} \tag{18}$$

where the intrinsically positive $\gamma(q)$ and $\delta(q)$ are simply the decrements of the corresponding collective modes, and the following notations are employed for the complex number $v = \exp(2\pi i/3)$ and for the complex functions $W(q) = -\omega_2^2(q)/3 + \omega_1^2(q) + 2h_0^2(q)/27$, $Z^3(q) = \sqrt{-(\omega_2^2(q)/3 - h_0^2(q)/9)^3 - (h_0(q)W(q)/2)^2}$, $Y(q) = \sqrt[3]{h_0(q)W(q)/2i - Z^3(q)}$, and $X = \sqrt[3]{h_0(q)W(q)/2i + Z^3(q)}$.

The latter result can be used to describe the collective mode behaviour in partially and completely degenerate OCSCPs, as was performed in ref. [23] for the classical OCPs.

3 | ON THE VALIDITY OF THE SSF

The frequency moments of the loss function employed above to reconstruct the latter are exact relations to be satisfied, like the conservation laws. In our approach, the knowledge of the characteristic frequencies depends significantly on the quality of the static data, that is, in general, the precision of our knowledge of both the static dielectric function and the SSF. Here, we suggest employing another exact relation, which is effectively the Cauchy–Bunyakovsky–Schwarz inequality, to check the validity of those static characteristics obtained within some theoretical approaches or fitting procedures. The above inequality in the context of the frequency moments was demonstrated in Appendix A of ref. [11]; it effectively reduces to the positivity of a function:

$$b(q) = [\omega_2(q) - \omega_1(q)]/\omega_{\text{p}} \geq 0. \tag{19}$$

The frequency $\omega_2(q)$ is directly determined by the SSF, see (5) and (6), and in classical systems, $\omega_1(q)$ is also related, via the FDT, to the SSF. Within a specific scheme of calculation of the above static characteristics, inequality (19) can be violated to clearly indicate their inapplicability to estimating the dynamic properties. We analyse several schemes for the evaluation of the SSF in dense classical plasmas from the viewpoint of fulfilment of inequality (19); see Section 4.2.

4 | NUMERICAL RESULTS

4.1 | Paramagnetic uniform electron gas

The purpose of this subsection is to evaluate the DSF (15) of a PUEG and to provide a comparison with the results of the non-equilibrium Green function simulations that essentially exploit the T-matrix self-energies with the vertex corrections [27]. Another goal is to study the dispersion characteristics (18) of the PUEG under the same conditions.

In order to proceed with the DSF (15) and the collective modes (18), only the characteristic frequencies $\omega_1(q)$ and $\omega_2(q)$ are needed. Comparing expression (14) with the loss function in the extended RPA that incorporates the static local field correction function (LFC) $G(0, q)$, it is straightforward to arrive at the following relation between the frequency $\omega_1(q)$ and the LFC $G(0, q)$:

$$\frac{\omega_1^2(q)}{\omega_p^2} = 1 + \frac{q^2}{3\Gamma\Pi_0(q)} - G(0, q), \tag{20}$$

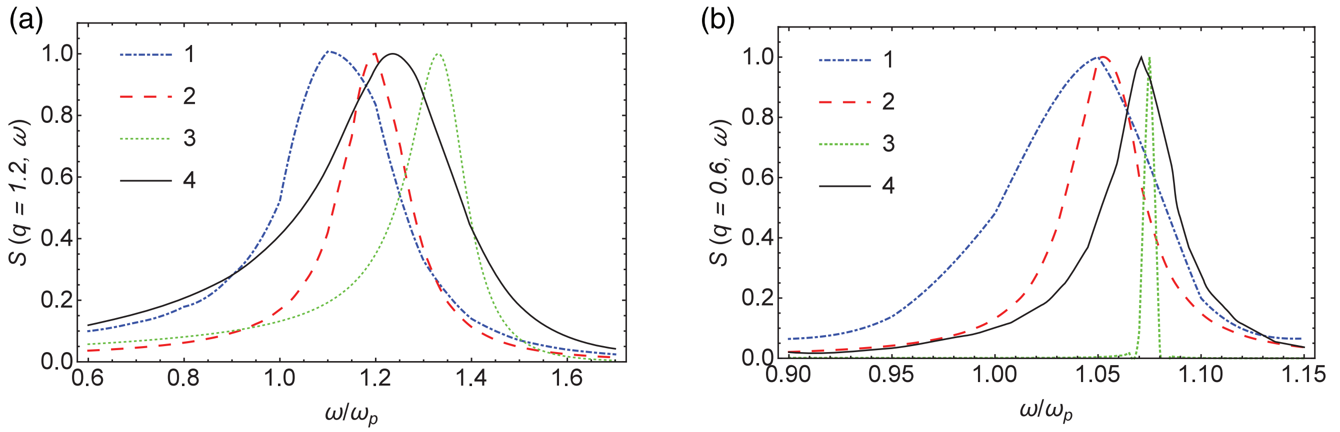

FIGURE 1 Dynamic structure factor for the correlated electron gas at $\theta = 0.69$ and $r_s = 4$ for (a) $q = 1.2$ and (b) $q = 0.6$. Dot-dashed line 1: Equation 15 taking into account the contributions of $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; dashed line 2: Equation 15 but neglecting the contributions from $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; dotted line 3: the standard RPA; solid line 4: (27). All curves are normalized to their DSF values at the maxima

where $\Pi_0(q)$ is the static polarization operator normalized to βn.

In the subsequent calculations, the following model is acquired for the LFC[33]:

$$G(0,q) = \left[\frac{1}{1-g(0)} + \frac{w}{q^2}\right]^{-1} \tag{21}$$

with $g(0)$ being the zero-separation value of the electronic radial distribution function[33], whereas the parameter w is calculated via the long-wavelength asymptote of the LFC as[33]:

$$w^{-1} = \frac{1}{3\Gamma}\left[1 - \beta\left(\frac{\partial P}{\partial n}\right)_\beta\right] \tag{22}$$

with the isothermal compressibility $(\partial P/\partial n)_\beta$ derived from the Monte Carlo fitting formula for the electron gas equation of state[34]. Note that Equations [20–22] virtually provide a concise expression for the SSF of the PUEG, which allows one to evaluate the second characteristic frequency $\omega_2(q)$ as well.

It has been demonstrated by the numerical calculations at $\theta = 0.69$ and $r_s = 4$ that the coupling contribution $U(q)$ to the characteristic frequency $\omega_2(q)$ is at least an order of magnitude lower than the kinetic contribution $K(q)$. This implies that, under those conditions, it might be sufficient to apply the quasi-RPA approximation[11] when the coupling contribution $U(q)$ together with the LFC function $G(0, q)$ are merely dropped out.

Finally, the numerical results for the DSF are presented in Figure 1 in comparison with the data obtained in ref. [27]. Three different calculation schemes have been applied: (a) Equation (15), taking into account the above stated contributions $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; (b) the same Equation (15) but neglecting the contributions from $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$, that is, estimating the latter frequencies in the quasi-RPA approximation; and (c) the RPA formula itself. Just a quick glance proves the robustness of the self-consistent moment approach as the discrepancy between the peak positions, corresponding to the two mentioned estimates of the characteristic frequencies, remains rather small and lies within 10% of the accuracy. It should be emphasized that the precision of the fitting formula for the equation of state could have influenced those results, but not significantly. In addition, the SSF has been employed to evaluate the LFC within the STLS scheme[30], but the resulting DSF differs substantially from the theoretical prediction of ref. [27].

Furthermore, the dispersion characteristics (18) of the PUEG have been evaluated under the same conditions of $\theta = 0.69$ and $r_s = 4$, and the results are shown in Figure 3a. Note that the decrement-to-frequency ratio remains rather small, such that the plasmon mode is only slightly decaying and, thus, can be observed experimentally.

In an attempt to describe the PUEG at zero temperature, the SSF from ref. [35] and the LFC function model from ref. [36] have been used, and the results are displayed in Figures 2 and 3b, respectively. Again, a fairly good agreement is found for the DSF, which vanishes at $\omega \leqslant 0$, whereas the plasmon dispersion undergoes no qualitative change in comparison with the non-zero temperature case.

It should be noted in closing that we have also tried to go beyond approximation [13] by assuming the following model for the NPF

$$R(\omega,q) = \frac{ih_0(q)}{\alpha + i(\alpha-1)\Xi(\omega)}, \tag{23}$$

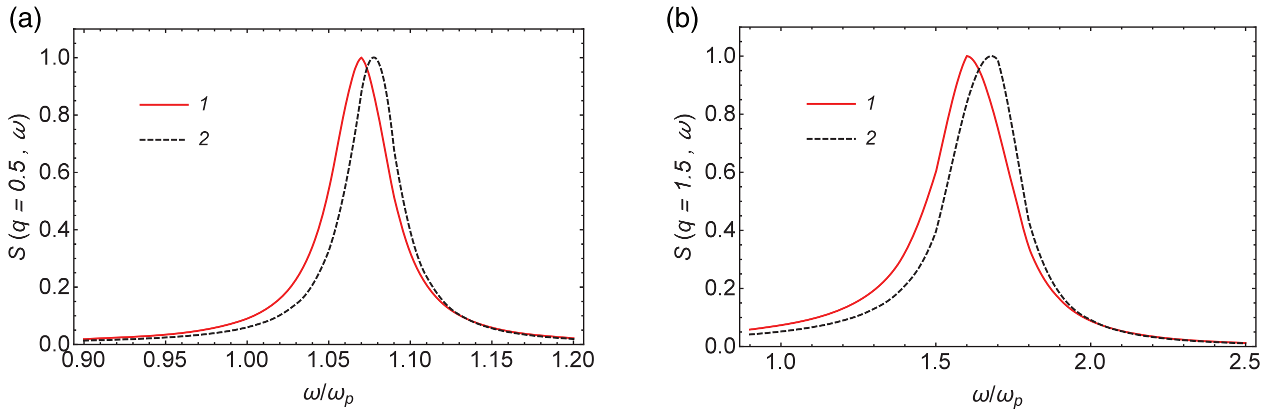

FIGURE 2 Dynamic structure factor for the electron gas at $T = 0$, $r_s = 1$, (a) $q = 0.5$, and (b) $q = 1.5$. *Solid line 1*: Equation 15 taking into account the contributions of $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; dashed line 2: Equation 15 but neglecting the contributions from $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$. All curves are normalized to their DSF values at the maxima

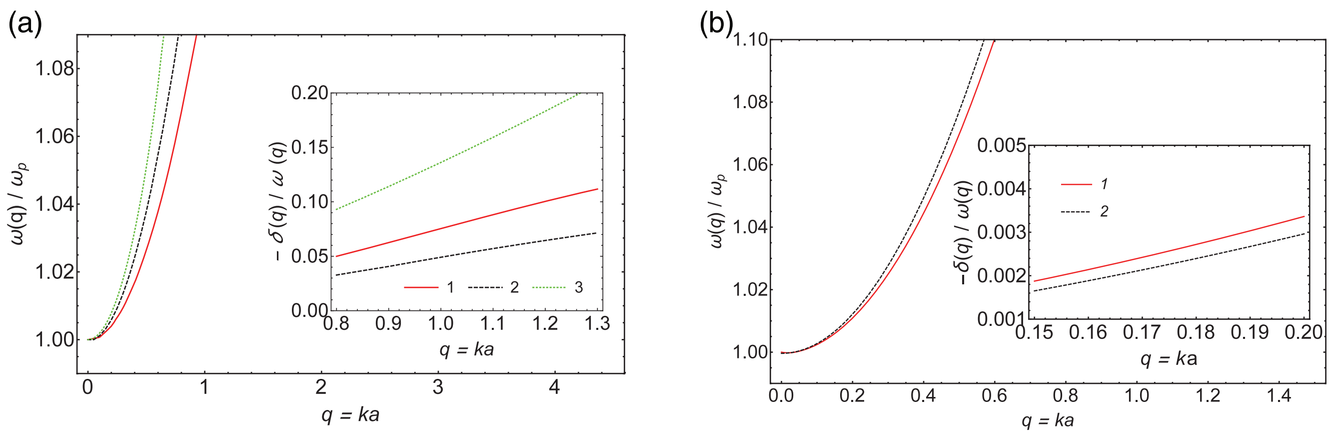

FIGURE 3 Plasmon mode dispersion and the plasmon frequency-to-decrement ratio of Equation 18 at (a) $\theta = 0.69$, $r_s = 4$ and (b) $T = 0$, $r_s = 1$. *Solid line 1*: Equation 18 taking into account the contributions of $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; *dashed line 2*: Equation 18 but neglecting the contributions from $G(0, q)$ and $U(q)$ to the frequencies $\omega_1(q)$ and $\omega_2(q)$; *dotted line 3*: the standard RPA

where the function $\Xi(z)$ is the Cauchy transform of the Fermi–Dirac distribution

$$\Xi(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{(1+\exp(\eta))dx}{(\exp(Dx^2)+\exp(\eta))(x-z)}.$$

Here, $z = (\omega + i0^+)/kv_F$ with $v_F = \sqrt{2E_F/m}$ being the Fermi velocity, while the parameter $\alpha \in (0, 1)$ could be determined by the maximization of the Shannon entropy. Numerical calculations demonstrate that the best agreement with the data of ref. [27] is archived for $\alpha \sim 0.99$, when expression (23) effectively reduces to the assumption (11).

4.2 | The Cauchy–Bunyakovsky–Schwarz inequality

In the context of satisfaction of the Cauchy-Bunyakovsky-Schwarz inequality (19), we have checked up to seven different static schemes of determination of the one-component, strongly coupled classical plasma SSF: the classical hyper-netted chain (HNC) approximation [37], the bridge function-corrected HNC by Ng [38], two different versions of the variational modified HNC Scheme,[39,40], and three different fitting procedures[41–43]; see Figure 4. It can be seen that two schemes of SSF calculation violate the Cauchy–Bunyakovsky–Schwarz inequality, which leads to the non-physical results for the DSF under these conditions. More relevant information can be found in ref. [29].

5 | CONCLUSIONS

In this paper, concise analytical expressions for the loss function and the DSF of the PUEG have been derived based on the self-consistent method of moments that, on the one hand, fulfils all of the exactly known sum rules and, on the other hand,

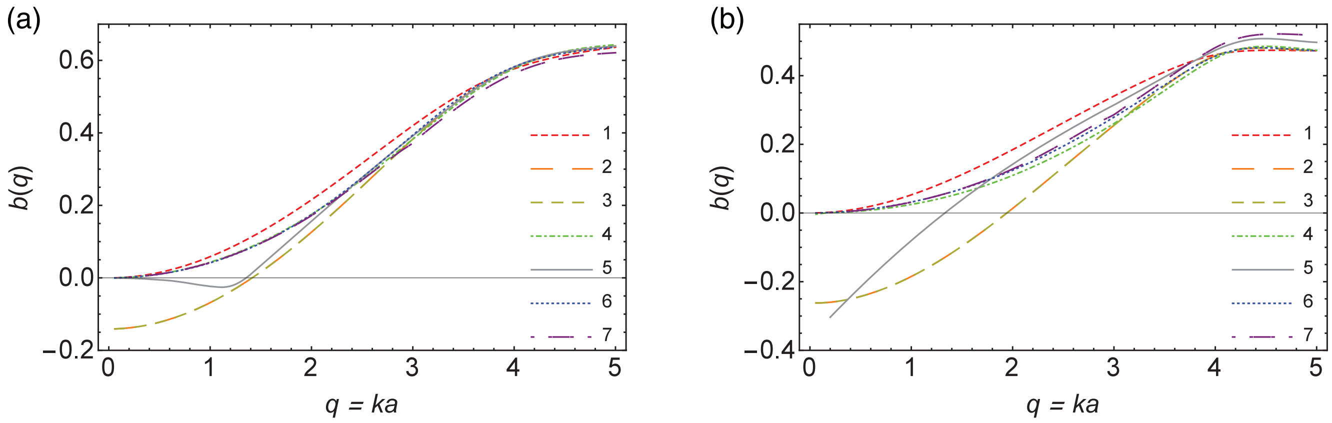

FIGURE 4 Function *b(q)* 19 for the classical Coulomb OCP at (a) $\Gamma = 20$, (b) $\Gamma = 80$. The static structure factors are calculated using the following numerical schemes: 1 - 37, 2 - 38, 3 - 39, 4 - 40, 5 - 41, 6 - 42, 7 - 43

imposes the existence of extremum at zero frequency. The obtained formulas allow one to predict the behaviour of dynamic properties of the system starting from the static characteristics.

The DSF has been evaluated for zero and finite temperatures to show that it weakly depends on the coupling contribution that appears in the fourth frequency moment of the loss function. The same inference has been made for the plasmon dispersion relation, and it has been proven that the decrement-to-frequency ratio remains rather small for not very large wavenumbers.

It is rather curious that the Cauchy–Bunyakovsky–Schwarz inequality yields a simple criterion for validity of the static characteristics. Seven different schemes for evaluating the SSF of strongly coupled, one-component classical plasmas have been tested using the aforementioned criterion, and some of them have failed to pass.

A plan has been made to proceed with the investigation of dynamic properties of the PUEGs based on the present results and the data of the quantum Monte Carlo simulations.[44] Different schemes for evaluating the SSF and their influence on the results of the dynamic characteristics of strongly coupled, one-component plasmas will also be scrutinized.

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