Self-consistent relaxation theory of collective ion dynamics in Yukawa one-component plasmas under intermediate screening regimes

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The self-consistent relaxation theory is employed to describe the collective ion dynamics in strongly coupled Yukawa classical one-component plasmas. The theory is applied to equilibrium states corresponding to intermediate screening regimes with appropriate values of the structure and coupling parameters. The information about the structure (the radial distribution function and the static structure factor) and the thermodynamics of the system are sufficient to describe collective dynamics over a wide range of spatial scales, namely, from the extended hydrodynamic to the microscopic dynamics scale. The main experimentally measurable characteristics of the equilibrium collective dynamics of ions—the spectrum of the dynamic structure factor, the dispersion parameters, the speed of sound, and the sound attenuation—are determined within the framework of the theory without using any adjustable parameters. The results demonstrate agreement with molecular dynamics simulations. Thus a direct realization is presented of the key idea of statistical mechanics: for the theoretical description of the collective particle dynamics in equilibrium fluids it is sufficient to know the interparticle interaction potential and the structural characteristics. Comparison with alternative or complementary theoretical approaches is provided.

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I. INTRODUCTION

Collective dynamics determines essential physical properties of a many-particle system, including the sound propagation, the heat capacity, and the mass and heat transfer. If we consider a crystalline solid as a system of interacting particles, as it is customarily done in statistical mechanics, then the concept of phonons is applied to describe the collective dynamics of such systems [1], and qualitative results can be achieved if the interparticle interaction potential and the structural characteristics (the lattice type and the lattice constant) are initially known. However, the extension of the concept of phonons to collective particle dynamics in equilibrium classical liquids is somewhat misleading or dubious. Instead of this, in the case of liquids the time correlation function formalism appears to be sufficiently efficient [2]. This formalism serves as a suitable basis for various theories that are proposed for reproducing collective and single-particle dynamics in liquids such as the generalized hydrodynamics [3], the viscoelastic theory [4,5], the mode-coupling theory [6], and others. Despite an impressive progress in the theoretical interpretation of currently available experimental results related to the collective dynamics in liquids [7–9], an appropriate theory is still missing, which could be based solely on an interaction potential and structural characteristics as input parameters [10,11].

It is remarkable that a model of many-particle systems, where particles interact through the Yukawa (screened-Coulomb, or Debye-Hückel) potential,

$$\phi(r) = \frac{Q^2}{r} \exp\left(-\frac{r}{\lambda_s}\right), \tag{1}$$

is a very suitable for the advancement and testing of such a theory. Here, Q is the effective particle charge and λ_s is the Debye screening length [12]. The interparticle interaction defined by Eq. (1) reproduces the repulsion of point ions neutralized by the (electronic) background, and such an interaction corresponds to the case of the classical one-component plasma (OCP) called the Yukawa-OCP [13–16]. If the microscopic structure is known (for example, in terms of the pair distribution function of the particles), then the simple analytical form of the Yukawa potential allows one to find expressions for the internal and free energies, the internal pressure, the shear stress, and also to determine the system virial equation of state [3]. Note that the Yukawa-OCP is of interest not only from the point of view of the fundamental issues of liquid matter physics, but it has also remarkable applications in various physical situations, including interiors of neutron stars and white dwarfs, dusty plasmas, ultracold plasmas, and colloidal suspensions [17–24].

The dynamic structure factor $S(k, \omega)$ (k being the wave number and ω being the frequency) contains complete information about the collective particle movements in a many-particle system. This quantity is experimentally measurable by inelastic scattering of light, neutrons, and x rays. On the other hand, the dynamic structure factor can be directly calculated from known particle trajectories, which were initially determined by experimental methods or by means of molecular dynamics (MD) simulations. In addition, the quantity $S(k, \omega)$ is the Fourier transform in time of the density-density correlation function $F(k, t)$ known also as

the intermediate scattering function [3]. Therefore it is usually possible to compute $S(k,\omega)$ theoretically, and a direct comparison of theoretical and experimental results for the dynamic structure factor can verify the validity and quality of a theory suggested to describe the collective dynamics of system particles.

The dynamic properties of the Yukawa-OCP in the intermediate screening regime, i.e., with the finite screening lengths in interparticle interactions, are characterized by the presence of propagating waves, manifested in the dynamic structure factor spectra as a shifted-frequency doublet. This feature is symmetric and typical for dense classical liquids. The dispersion of these collective excitations is similar to that usually observed in equilibrium dense liquids and is completely different from those characteristic for the Coulomb systems, i.e., when in Eq. (1) the screening length λ_s tends to infinity. A remarkable feature of the collective dynamics of the Yukawa-OCP is the practically absent zero-frequency Rayleigh mode in the extended hydrodynamic wave-number range. This mode is associated with the nonpropagating isobaric entropy fluctuations [1]. In the present paper we wish to demonstrate that all main characteristics of the classical Yukawa-liquid collective dynamics for the whole wave-number range and in the intermediate screening regime can be determined in a self-consistent manner within the relaxation (microscopic) theory.

II. THEORETICAL FORMALISM

The simplest way to treat an experimental scattering law $S(k,\omega)$ is to fit this spectrum by a linear combination of some model functions whose parameters are identified with some physical parameters. However, physically justified reasons for such a fit can be given for two limiting cases only: the low-k (long-range) hydrodynamic and the high-k (short-range) free-particle dynamics limits. There is an alternative to these fittings.

Any scattering law $S(k,\omega)$ at a fixed k can be characterized by a set of its frequency moments

$$\langle\omega^{(l)}(k)\rangle = \frac{1}{\rho}\int_{-\infty}^{\infty}\omega^l\, S(k,\omega)\, d\omega, \quad l = 0,\ 1,\ 2,\ \ldots, \tag{2}$$

usually called the sum rules, where ρ is the particle concentration. The dimension of the lth-order frequency moment depends on its order l and it is $(\textit{frequency})^l$. Therefore, it is more convenient to use the set of frequency parameters defined by the ratios of the moments:

$$\begin{aligned}
\Delta_1(k) &= \frac{\langle\omega^{(2)}(k)\rangle}{\langle\omega^{(0)}(k)\rangle}, \quad \Delta_2(k) = \frac{\langle\omega^{(4)}(k)\rangle}{\langle\omega^{(2)}(k)\rangle} - \frac{\langle\omega^{(2)}(k)\rangle}{\langle\omega^{(0)}(k)\rangle},\\
\Delta_3(k) &= \frac{[\langle\omega^{(6)}(k)\rangle\langle\omega^{(2)}(k)\rangle - (\langle\omega^{(4)}(k)\rangle)^2]\langle\omega^{(0)}(k)\rangle}{\langle\omega^{(4)}(k)\rangle\langle\omega^{(2)}(k)\rangle\langle\omega^{(0)}(k)\rangle - (\langle\omega^{(2)}(k)\rangle)^3},\\
&\ldots,
\end{aligned} \tag{3}$$

all having the same dimensions of the frequency squared. In a classical system the dynamic structure factor is an even function of frequency so that its odd-order moments vanish and the nth-order frequency parameter $\Delta_n(k)$, where $n = 1, 2, 3, \ldots$, can be expressed in terms of only even-order moments up to a $2n$th-order one: $\langle\omega^{(2)}(k)\rangle, \langle\omega^{(4)}(k)\rangle, \ldots, \langle\omega^{(2n)}(k)\rangle$. It is remarkable that the frequency parameters can be determined independently and exactly in terms of the microscopic characteristics. In particular, for the first frequency parameter due to the fluctuation-dissipation theorem one has that

$$\Delta_1(k) = \frac{\omega_p^2}{3\Gamma}\frac{(ka)^2}{S(k)}, \tag{4a}$$

while the second frequency parameter can be written as

$$\Delta_2(k) = \Delta_1(k)[3S(k) - 1] + \omega_p^2 D(k), \tag{4b}$$

with (some details are provided in the Supplemental Material [25])

$$\begin{aligned}
D(k) = \int_0^\infty \frac{\exp(-\kappa x)}{3x}&[(2(\kappa x)^2 + 6\kappa x + 6)j_2(kax)\\
&+ (\kappa x)^2(1 - j_0(kax))]g(x)dx,
\end{aligned}$$

where

$$S(k) \equiv \langle\omega^{(0)}(k)\rangle = 1 + \frac{4\pi\rho}{k}\int_0^\infty r[g(r) - 1]\sin(kr)dr$$

is the static structure factor, $\omega_p = \sqrt{4\pi Q^2\rho/m}$ is the plasma frequency, $a = \sqrt[3]{3/(4\pi\rho)}$ is the Wigner-Seitz radius, $\Gamma = Q^2/(k_B T a)$ is the coupling parameter, $\kappa = a/\lambda_s$ is the structure parameter, $x = r/a$ is the dimensionless spacial variable, $j_n(x)$ are the spherical Bessel functions, and $g(x)$ is the radial distribution function. Generally speaking, the expression for the nth-order frequency parameter $\Delta_n(k)$ at $n \geqslant 2$ contains an integral expression with the interparticle potential and the distribution function for n particles.

The higher the order of the frequency moment (or the relaxation parameter), the more high-frequency properties of the spectrum it captures. The set of these moments (and the relaxation parameters) uniquely matches a specific spectrum at a fixed k. Therefore it is reasonable to expect that the scattering law can be expressed in terms of the relaxation parameters as a functional. Based on the set of the dynamic variables,

$$\mathbf{W}(k) = \{W_0(k),\ W_1(k),\ W_2(k),\ W_3(k),\ W_4(k)\}, \tag{5}$$

interrelated by the following recurrent relations,

$$\begin{aligned}
W_{j+1}(k) &= \frac{dW_j(k)}{dt} + \Delta_j(k)W_{j-1}(k),\\
\Delta_j(k) &= \frac{\langle|W_j(k)|^2\rangle}{\langle|W_{j-1}(k)|^2\rangle}, \quad W_{-1}(k) \equiv 0, \quad j = 0,\ 1,\ 2,\ \ldots,
\end{aligned}$$

where the initial variable $W_0(k) = \rho_k$ defines the local density fluctuations, the self-consistent relaxation theory provides the dynamic structure factor in terms of the first four relaxation parameters, $S(k,\omega) \propto \mathcal{F}[S(k),\ \Delta_1(k),\ \Delta_2(k),\ \Delta_3(k),\ \Delta_4(k)]$, where $\mathcal{F}[\ldots]$ means an algebraic expression [34,35]. The exact equation for the dynamic structure factor $S(k,\omega)$, obtained on the basis of the self-consistent relaxation theory, can be found in Refs. [31,36,37] (see, for example, Eq. (42) in Ref. [31]). We notice that the relaxation theory belongs to the theoretical schemes, where the known infinite chain of integrodifferential equations for the time correlation functions of variables from

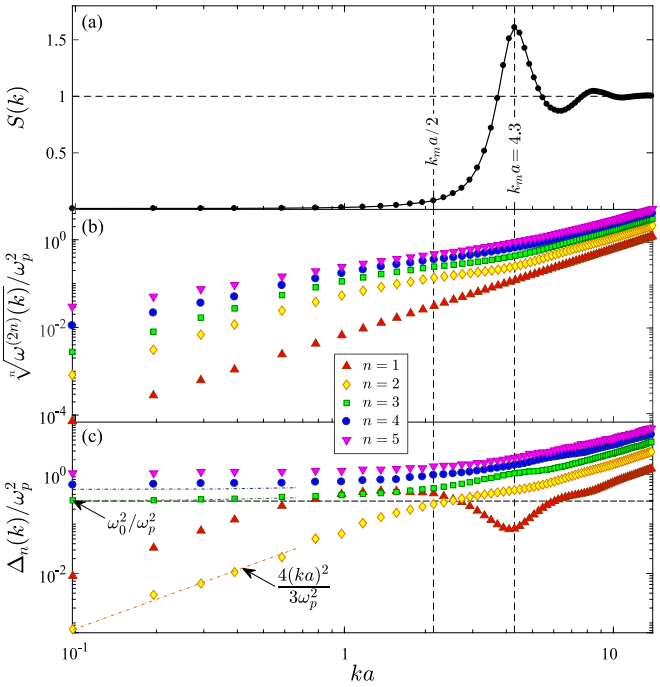

FIG. 1. Wave-number dependence of some characteristics evaluated by means of molecular dynamics simulations for the Yukawa-OCP at the thermodynamic state with $\Gamma = 50$ and $\kappa = 1$. (a) Dots connected by the solid line represent the static structure factor $S(k)$, where the location of the main peak is marked by $k_m a$; and $k_m a/2$ corresponds to the first pseudo-Brillouin zone boundary. (b) Reduced frequency moments. (c) Frequency parameters scaled by ω_p^2. Low-k asymptotic forms shown by straight lines. For $\Delta_1(k)$ it follows from Eq. (4a), for $\Delta_2(k)$ it can be obtained taking into account the results of the quasilocalized charge approximation (QLCA) [48–52], and for the parameters $\Delta_3(k)$ and $\Delta_4(k)$ they are obtained empirically.

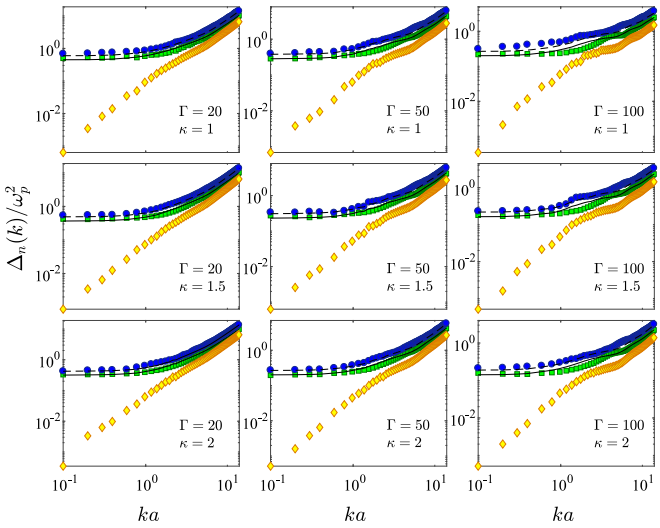

FIG. 2. Wave-number dependence of the scaled frequency parameters $\Delta_2(k)/\omega_p^2$ (yellow diamonds), $\Delta_3(k)/\omega_p^2$ (green squares), and $\Delta_4(k)/\omega_p^2$ (dark blue circles) obtained by molecular dynamics simulations of the Yukawa-OCP for nine thermodynamic states and some combinations of Γ and κ. Solid and dashed lines correspond to relations (6a) and (6b), respectively.

the set $\mathbf{W}(k)$ is solved in a self-consistent way as, for example, in the self-consistent mode-coupling theory [38–42], and no approximations of these time correlation functions by any model functions with free parameters are required [43]. This also becomes possible when the entire infinite set of sum rules (2) [or (3)] is known [31,36,44–46]. In the case we consider here, the theoretical procedure is nonperturbative, which is especially appropriate for the description of the systems we are dealing with here. The main ideas of the theory are to take advantage of the correspondence between the timescales of a sequence of relaxation processes associated with the dynamical variables from the set $\mathbf{W}(k)$ and of the fact that the timescales themselves are evaluated through the frequency parameters as $\tau_n(k) = \Delta_n^{-1/2}(k)$ [47]. The description is based solely on the assumption that relaxation processes, determined by the energy flow, and by more subtle physical effects that are determined through the derivatives of the energy current with respect to time, occur on higher-order timescales $\tau_n(k)$ which become asymptotically equal at large n. In the case of classical equilibrium fluids independently of the interaction range of the fluid particles, this condition is sufficient to find the dynamic structure factor as well as other characteristics of the collective dynamics of particles. However, for specific systems one can expect to find additional interrelations between frequency parameters, which will cause corresponding modifications in the relaxation theory.

The equilibrium molecular dynamics simulations[1] of the Yukawa-OCP for $\Gamma = 20$, 50, 100 and $\kappa = 1$, 1.5, 2 reveal no simple correlation between the frequency parameters $\Delta_1(k)$ and $\Delta_2(k)$, and, therefore, it is not possible to simplify Eq. (4b). Nevertheless, there is a correspondence between $\Delta_2(k)$, $\Delta_3(k)$, and $\Delta_4(k)$ for the extended range of the wave-number variation, which is clearly seen from the defined k dependence of these frequency parameters (Figs. 1 and 2):

$$\Delta_3(k) = \tfrac{3}{2}\Delta_2(k) + \omega_0^2, \tag{6a}$$

$$\Delta_4(k) = \tfrac{4}{3}\Delta_3(k) = 2\Delta_2(k) + \tfrac{4}{3}\omega_0^2, \tag{6b}$$

with

$$\omega_0^2 = \frac{2\omega_p^2}{\sqrt{\Gamma\kappa}}.$$

Relations (6) express the higher-order relaxation parameters $\Delta_3(k)$ and $\Delta_4(k)$ in terms of the parameter $\Delta_2(k)$. These relations are similar, in a sense, to the representation of the three- and four-particle distribution functions in terms of the pair correlation function—the radial distribution function of particles. Further, relations (6) satisfy the

[1]The equilibrium molecular dynamics simulations of the Yukawa-OCP for $\Gamma = 20$, 50, 100 and $\kappa = 1$, 1.5, 2 were carried out using the computational package LAMMPS [S. Plimpton, J. Comput. Phys. **117**, 1 (1995)]. The simulation cell contained 64 000 particles interacting with the Yukawa potential, and periodic boundary conditions were applied to the cell in all directions. The evolution of the system corresponding to the NVT ensemble was monitored. The particle motion equations were integrated in accordance with the Verlet algorithm with a time integration step $\tau = 0.01/\omega_p$.

Cauchy-Bunyakovsky-Schwarz inequalities for the frequency moments [29,30]:

$$\frac{\langle\omega^{(2)}(k)\rangle}{\langle\omega^{(0)}(k)\rangle} \leqslant \frac{\langle\omega^{(4)}(k)\rangle}{\langle\omega^{(2)}(k)\rangle}, \quad \frac{\langle\omega^{(4)}(k)\rangle}{\langle\omega^{(0)}(k)\rangle} \leqslant \frac{\langle\omega^{(8)}(k)\rangle}{\langle\omega^{(4)}(k)\rangle}, \quad \frac{\langle\omega^{(6)}(k)\rangle}{\langle\omega^{(4)}(k)\rangle} \leqslant \frac{\langle\omega^{(8)}(k)\rangle}{\langle\omega^{(6)}(k)\rangle}. \tag{7}$$

Notice that these inequalities warrant the correct mathematical structure and properties of our results, e.g., the positiveness of the dynamic structure factor and of the decrement of the collective modes, etc. Besides, their fulfillment implies the compliance of the present approach with the fundamental requirements. Taking relations (6) into account, the self-consistent relaxation theory yields the dynamic structure factor in the form

$$S(k,\omega) = \frac{\rho S(k)}{\pi} \frac{2\Delta_2(k)\sqrt{A_3(k)}}{\omega^6 + A_1(k)\omega^4 + A_2(k)\omega^2 + A_3(k)}, \tag{8}$$

where

$$A_1(k) = 3\omega_0^2 - \frac{\Delta_2(k)}{2} - 2\Delta_1(k),$$
$$A_2(k) = [\Delta_1(k) - 2\Delta_2(k)]^2 - 6\Delta_1(k)\omega_0^2,$$
$$A_3(k) = \frac{3}{2}\Delta_1^2(k)\big[3\Delta_2(k) + 2\omega_0^2\big].$$

Some remarkable points associated with relations (6) and Eq. (8) are to be pointed out. First, relations (6) can provide a correct result for the high-k free-particle dynamics limit with $\Delta_2(k) \gg \omega_0^2$ and the following recurrence relation:

$$\Delta_{n+1}(k) = \frac{n+1}{n}\Delta_n(k), \quad n = 1,\ 2,\ 3,\ \ldots, \tag{9}$$

which exactly corresponds to the dynamic structure factor of the Gaussian form,

$$S_{\mathrm{fmp}}(k,\omega) = \sqrt{\frac{\rho^2}{2\pi\Delta_1(k)}}\exp\left(-\frac{\omega^2}{2\Delta_1(k)}\right). \tag{10}$$

Note that Eq. (10) reproduces the dynamic structure factor spectrum for the regime of "a free-moving particle" [3]. Second, according to Eq. (8), the shape of $S(k,\omega)$ at a fixed k is determined by the bicubic polynomial in the variable ω. Analysis of (8) allows one to obtain the dispersion equation for the high-frequency quasiacoustic mode:

$$s^3 + B(k)s^2 + \left[\Delta_1(k) + \frac{8}{5}\Delta_2(k)\right]s + B(k)\Delta_1(k) = 0,$$
$$B(k) = \frac{4\sqrt{A_3(k)}}{5\Delta_1(k)}. \tag{11}$$

Solution of this equation yields $s(k) = \pm i\omega_c(k) - \delta(k)$ with the dispersion for the high-frequency peak of the dynamic structure factor,

$$\omega_c(k) = \sqrt{3}\big(\sqrt[3]{Z(k) - q(k)} + \sqrt[3]{Z(k) + q(k)}\big), \tag{12}$$

the low-k asymptotes of this dispersion,

$$v_s\, k = \lim_{k\to 0}\omega_c(k) = \lim_{k\to 0}\sqrt{\frac{6\big[(\Delta_1(k) + 2\Delta_2(k))^2 - \Delta_1(k)\omega_0^2\big]}{4\Delta_1(k) + \Delta_2(k) - 6\omega_0^2}}, \tag{13}$$

and the dispersion for the sound decrement,

$$\delta(k) = \sqrt[3]{Z(k) + q(k)} - \sqrt[3]{Z(k) - q(k)} - \frac{B(k)}{3}, \tag{14}$$

where

$$Z(k) = \sqrt{p^3(k) + q^2(k)},$$
$$p(k) = \frac{\Delta_1(k)}{12} + \frac{4}{75}\big[\Delta_2(k) - \omega_0^2\big],$$
$$q(k) = \frac{B(k)}{600}\left[25\Delta_1(k) - 12\Delta_2(k) + \frac{16\omega_0^2}{3}\right],$$

and v_s is the sound velocity.

The spectral density $C_L(k,\omega)$ for the longitudinal current correlation function is also determined by the dynamic structure factor $S(k,\omega)$:

$$C_L(k,\omega) = \frac{\omega^2}{S(k)\Delta_1(k)}S(k,\omega). \tag{15}$$

Then, taking into account relation (8), one can obtain directly the analytical expression for the spectral density $C_L(k,\omega)$ and find the dispersion relation $\omega_L(k)$ for the longitudinal acousticlike excitations:

$$\omega_L(k) = \sqrt{C_+(k) + C_-(k) - \frac{A_1(k)}{6}} \tag{16}$$

with

$$C_\pm(k) = \sqrt[3]{\frac{A_3(k)}{4} - \frac{A_1^3(k)}{216} \pm \sqrt{\frac{A_3^2(k)}{16} - \frac{A_3(k)A_1^3(k)}{432}}}.$$

Since the parameters $\Delta_1(k)$ and $\Delta_2(k)$ can be calculated analytically by means of Eqs. (4a) and (4b), respectively, fitting is not necessary to compute the dynamic structure factor $S(k,\omega)$ and all other characteristics of the collective particle dynamics.

III. NUMERICAL RESULTS

Now we check to which extent the theoretical formalism is consistent with the molecular dynamics simulation data and results of alternative theoretical approaches. Several theoretical models are known that have been suggested earlier to describe the collective dynamics of Yukawa classical one-component plasmas [10,27,29,30,53–56]. An accurate theoretical description has been provided earlier by the theory based on the method of frequency moments (FM's)—the FM theory (for details, see Refs. [10,30]). This FM theory yields the expression for the dynamic structure factor $S(k,\omega)$ in the form of a linear-fractional transformation of the Nevanlinna parameter function (NPF) possessing specific mathematical properties, which guarantee the satisfaction of an imposed set of sum rules or power frequency moments automatically and independently of the NPF model. In Refs. [10,30], the NPF

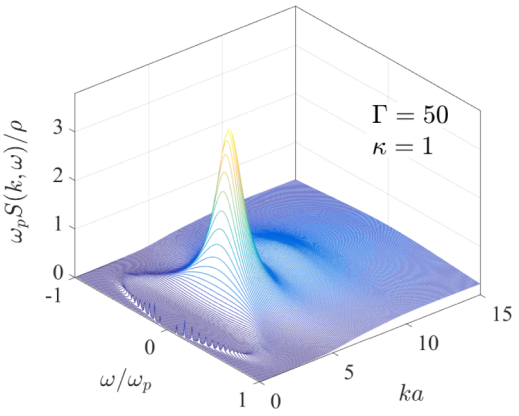

FIG. 3. Dynamic structure factor vs wave number ka and frequency ω/ω_p at the thermodynamic state with $\Gamma = 50$ and $\kappa = 1$ evaluated from Eq. (8). Note that the radial distribution function $g(r)$ generated on the basis of independent molecular dynamics simulations is used as a sole input parameter to compute the dynamic structure factor via Eq. (8).

determined by the relaxation frequency parameters $\Delta_1(k)$ and $\Delta_2(k)$ was found on the basis of physical considerations, and it leads to an expression for $S(k,\omega)$, similar to Eq. (8). Remarkably, at certain conditions, Eq. (8) transforms into the dynamic structure factor $S(k,\omega)$ of FM theory given in the above papers exactly. Details of the interrelation between the present relaxation and the moment self-consistent theoretical approaches are provided in the Supplemental Material [25].

For the thermodynamic state with $\Gamma = 50$ and $\kappa = 1$, the first maximum of the static structure factor $S(k)$ is located at the wave number $k_m = 4.3\, a^{-1}$ [see Fig. 1(a)]. The basic features of the microscopic collective dynamics appear at the wave numbers $k \in (0; k_m)$. This can be seen from Fig. 3, which presents the results predicted by Eq. (8) for this thermodynamic state—the scaled dynamic structure factor $\omega_p S(k,\omega)/\rho$ as a function of the scaled wave number ka and frequency ω/ω_p. The Brillouin doublet in $\omega_p S(k,\omega)/\rho$ is seen as symmetric maxima located at nonzero frequencies for the wave numbers up to $k \simeq 4.0\, a^{-1}$.

In Fig. 4 we show the scaled dynamic structure factor $\omega_p S(k,\omega)/\rho$ computed within the self-consistent relaxation theory with Eq. (8) for the fixed scaled wave numbers $ka =$ 0.29, 2.53, and 4.28 at the thermodynamic conditions of the Yukawa-OCP with $\Gamma = 20$ and 100, and $\kappa = 1$, 1.5, and 2. For these thermodynamic conditions and wave numbers, the self-consistent relaxation theory reproduces the MD simulation results quite accurately and describes all the spectral features. At small wave numbers $k < k_m/2$ corresponding to an extended hydrodynamic range, the spectra of $S(k,\omega)$ contain just a high-frequency Brillouin component. With the wave number k increase starting from the values comparable with $k_m/2$, the zero-frequency Rayleigh component emerges and becomes pronounced, while the high-frequency Brillouin component disappears. As it is seen, Eq. (8) provides sometimes even better agreement with the MD simulation results than the FM theory. In Fig. 5 we present results characterizing the capability of the theory to correctly reproduce the high-frequency Yukawa-OCP dynamics. It stems from Fig. 5 (top panel) that Eqs. (12) and (14) describe the MD simulations results for the dispersions characteristics $\omega_c(k)$ and $-\delta(k)$ as well. From the low-k asymptotes $\omega_c(k \to 0) \simeq v_s k$ and $\delta(k \to 0) \simeq -\Gamma_s k^2$, it is possible to determine the sound velocity v_s and the sound attenuation coefficient Γ_s.

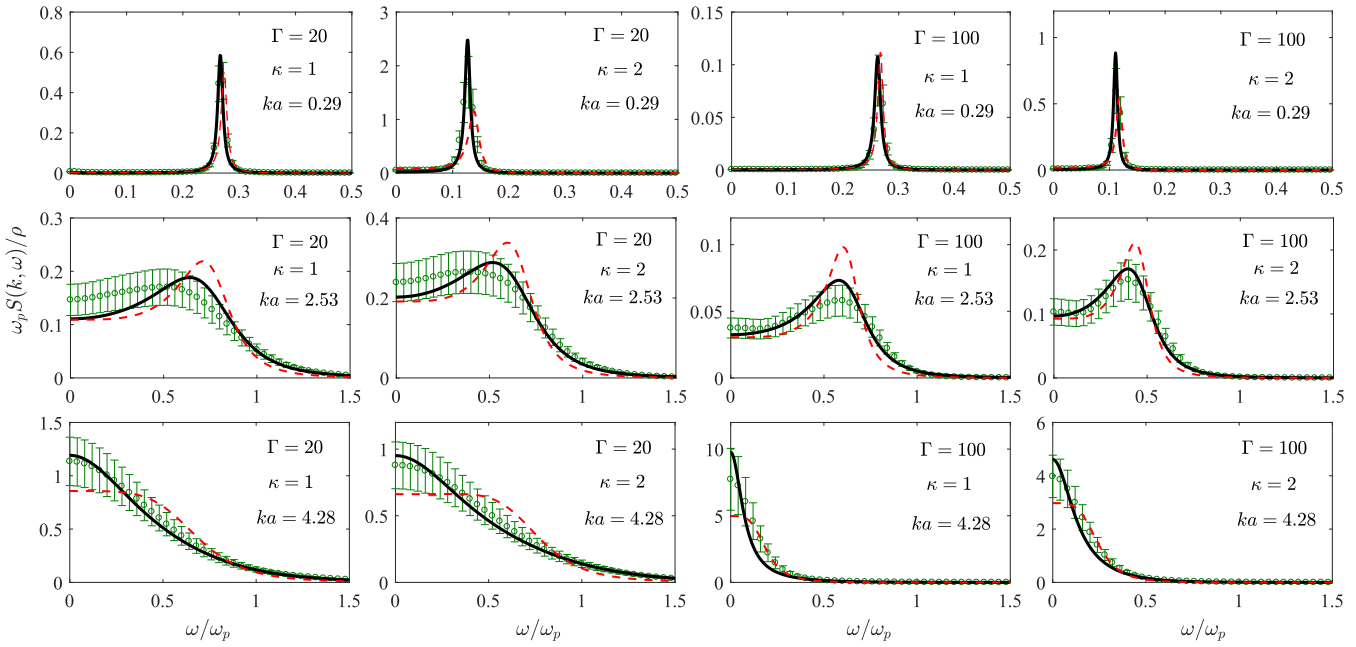

FIG. 4. Dynamic structure factor spectra, multiplied by the plasma frequency, for the thermodynamic states at various values of Γ and κ and at the various wave numbers. Here theoretical results from Eq. (8), shown by black solid lines, are compared with molecular dynamics (MD) simulation data given by green circles and with results of the FM theory [10] presented by red dashes lines.

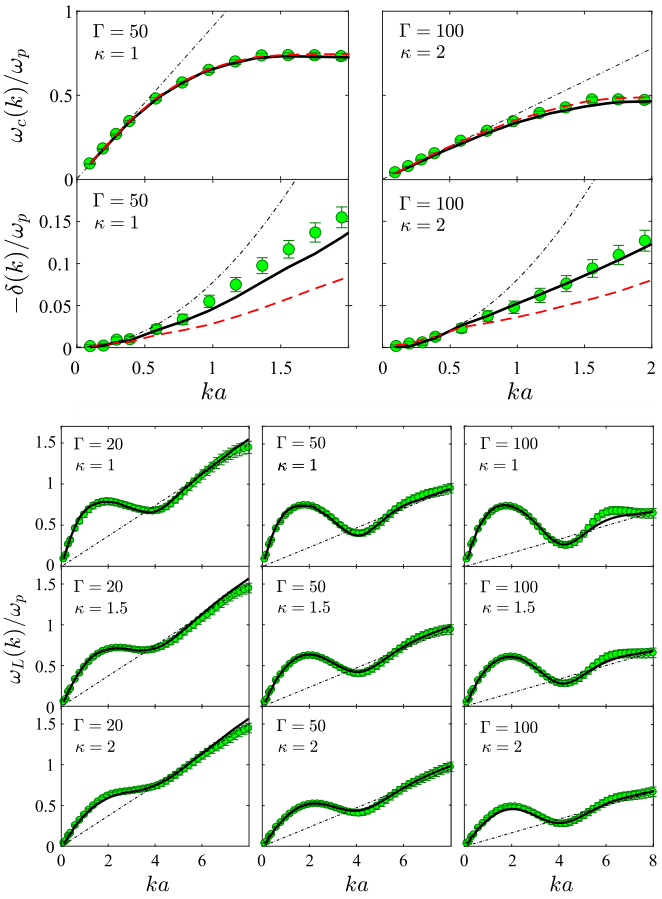

FIG. 5. (Top panel) Dispersions of the Brillouin peak frequency $\omega_c(k)$ and of the sound dumping coefficient $-\delta(k)$ scaled by the plasma frequency ω_p; the results are given for the thermodynamic states ($\Gamma = 50$, $\kappa = 1$) and ($\Gamma = 100$, $\kappa = 2$). Black solid lines are theoretical results with Eq. (12) for $\omega_c(k)$ and with Eq. (14) for $-\delta(k)$; red dashed lines depict results of FM theory [10] and green circles represent MD simulation data. Dash-dotted lines correspond to the asymptotic results $\omega_c(k) \sim c_s k$ and $-\delta(k) \sim \Gamma_s k^2$. (Bottom panel) Dispersion curves for longitudinal collective excitations evaluated from Eq. (16) (solid curves) and from MD simulations (green circles) for nine various thermodynamic (Γ, κ) states. Straight lines correspond to $\omega_L(k) \sim (a/\sqrt{3\Gamma})k$.

For the conditions pointed out in Fig. 5 (top panel), we found $v_s/(\omega_p a) = 0.938$ and $\Gamma_s/(\omega_p a^2) = 0.078$ for $\Gamma = 50$, $\kappa = 1$, and $v_s/(\omega_p a) = 0.39$, and $\Gamma_s/(\omega_p a^2) = 0.083$ for $\Gamma = 100$, $\kappa = 2$. We can conclude that the theory with Eq. (16) allows one to compute the dispersion curves $\omega_L(k)$ for the longitudinal collective excitations in a wide range of variation of the system parameters. Full correspondence between the theoretical and the MD simulation results for the dispersion $\omega_L(k)$ is seen in Fig. 5 (bottom panel), where our results for nine different (Γ, κ) combinations are given. The proposed theoretical description with Eq. (16) properly reproduces the low-k asymptotic forms and the roton minima located at $ka \simeq 4.3$ under the above condition. In full agreement with the simulation results, the theory indicates a smoothing of the roton minimum with a decrease in the parameter Γ and with an increase in κ, so that the roton minimum is practically absent when $\Gamma = 20$ and $\kappa = 2$. The extremum condition for the dispersion $\omega_L(k)$ is

$$\frac{\partial A_3(k)}{\partial k} = \omega_L^4(k)\frac{\partial A_1(k)}{\partial k}. \tag{17}$$

Then, with the known static structure factor $S(k)$ for a specific combination (Γ, κ), it is possible to accurately predict the location of the maximum and roton minimum on the dispersion curve $\omega_L(k)$. For example, at $\Gamma = 50$ and $\kappa = 1.5$, the maximum of $\omega_L(k)$ is at $ka = 1.95$, whereas the minimum is at $ka = 4.3$. Note that the position of the maximum in the dispersion $\omega_L(k)$ approximately coincides with the first pseudo-Brillouin zone boundary $k = k_m/2$, which corresponds to the transition range from the collective particle dynamics to the dynamics within an area formed by the neighboring particles. Moreover, the dispersion law $\omega_L(k)$ for all considered pairs (Γ, κ) demonstrate correct asymptotic forms at large wave numbers into the regime of a free-particle dynamics: $\omega_L(k) = \sqrt{2/(3\Gamma)}\omega_p ka$.

IV. CONCLUSIONS

It is shown that the self-consistent relaxation theory can be applied to describe the collective dynamics of ions in a strongly coupled classical one-component Yukawa plasma. For the intermediate screening regime of this system, when the interparticle interaction is realized on a finite scale, a correspondence between the sum rules is found which directly gives analytical expressions for the main characteristics of the collective dynamics, determined through the static structure factor and without any adjustment to the dynamic data. The present approach generates correct results within the range of parameters, where relations (6) are satisfied. Precisely, accurate results are produced for the Yukawa-OCP states with the values of the coupling and structure parameters varying in the ranges $\Gamma \in [20; 100]$ and $\kappa \in [1; 2]$, where the central (Rayleigh) peak is not pronounced. We emphasize that this study does not cover the states of the system corresponding to the weak coupling regime with the coupling parameter $\Gamma \sim 1$ or smaller and to the Coulomb system with $\kappa \to 0$.

The presented theory is an alternative to the FM theory presented recently [10]. Both approaches are nonperturbative, and a strong correspondence between them is elucidated. Energy dissipation processes in the system under scrutiny are taken into account in these two theoretical constructions so that they might be considered generalizations of the quasilocalized charge approximation [49]. Conclusions with respect to the analyticity of the system direct dielectric function envisaged in [32] and elaborated in [33] are confirmed (details are provided in the Supplemental Material [25]).

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