Self-Consistent Relaxation Theory of Collective Ion Dynamics in Yukawa One-Component Plasmas under Intermediate Screening Regimes

Anatolii V. Mokshin, Ilnaz I. Fairushin, and Igor M. Tkachenko

1Department of Computational Physics, Institute of Physics, Kazan Federal University, 420008 Kazan, Russia
2Departament de Matemàtica Aplicada, Universitat Politècnica de València, Camino de Vera s/n, 46022 Valencia, Spain
3Al-Farabi Kazakh National University, al-Farabi Av. 71, 050040 Almaty, Kazakhstan

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 is sufficient to describe collective dynamics over a wide range of spatial ranges, 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 simulation results. Thus a direct realization is presented of the key idea of statistical mechanics: for the theoretical description of the collective dynamics of equilibrium fluids it is sufficient to know the interparticle interaction potential and the structural characteristics. Comparison with alternative or complementary theoretical approaches is provided.

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 customary 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, 8], 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 system, where particles interact through the Yukawa (screened-Coulomb, or Debye-Hückel) potential

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

is a very suitable for the advancement and testing of such a theory. Here, $Q$ is the effective particle charge and $\lambda_s$ is the Debye screening length [12]. The inter-particle 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, 14]. 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, ultra-cold plasmas and colloidal suspensions [17, 24].

The dynamic structure factor $S(k, \omega)$ ($k$ being the wavenumber, and $\omega$ being the frequency) contains a 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 the one characteristic for the Coulomb systems, i.e., when in Eq. (1) the screening length $\lambda_s$ 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 wavenumber range. This mode is associated with the non-propagating 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 wavenumber range and in the intermediate screening regime can be determined in a self-consistent manner within the relaxation (microscopic) theory.

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

$$\langle \omega^l(k) \rangle = \frac{1}{\rho} \int_0^\infty \omega^l S(k,\omega) d\omega, \quad l = 0, 1, 2, \ldots, \quad (2)$$

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

$$\Delta_1(k) = \frac{\langle \omega^2(k) \rangle}{\langle \omega^0(k) \rangle}, \quad (3)$$

$$\Delta_2(k) = \frac{\langle \omega^4(k) \rangle - \langle \omega^2(k) \rangle^2}{\langle \omega^2(k) \rangle^2} - \langle \omega^2(k) \rangle^2, \quad (4a)$$

$$\Delta_3(k) = \frac{\langle \omega^6(k) \rangle - 2\langle \omega^4(k) \rangle \langle \omega^2(k) \rangle - \langle \omega^4(k) \rangle^2}{\langle \omega^4(k) \rangle^2} - \langle \omega^2(k) \rangle^2, \quad (4b)$$

with (some details are provided in the Supplemental Material [2]).

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

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

interrelated by the following recurrent relations

$$W_{j+1}(k) = \frac{dW_j(k)}{dt} + \Delta_j(k)W_{j-1}(k),$$

$$\Delta_j(k) = \frac{\langle W_j(k)^2 \rangle}{\langle \{W_{j-1}(k) \}^2 \rangle}, \quad W_{-1}(k) \equiv 0,$$

where...
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 \( \mathcal{F} \) 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]. 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 the set \( W(k) \) 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 non-perturbative, 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 time-scales of a sequence of relaxation processes associated with the dynamical variables from the set \( W(k) \), and of the fact that the time-scales 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 time-scales \( \tau_n(k) \) 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. (1b). Nevertheless, there is a correspondence between \( \Delta_3(k) \), \( \Delta_4(k) \) and \( \Delta_4(k) \) for the extended range of the wavenumber variation, that is clearly seen from the defined \( k \)-dependence of these frequency parameters (Figs. 1 and 2):

\[
\Delta_3(k) = \frac{3}{2} \Delta_2(k) + \omega_0^2, \tag{6a}
\]

\[
\Delta_4(k) = \frac{4}{3} \Delta_3(k) = 2 \Delta_2(k) + \frac{4}{3} \omega_0^2 \tag{6b}
\]

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

FIG. 1. Wavenumber 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 quasi-Brillouin zone boundary; (b) reduced frequency moments; (c) frequency parameters scaled by \( \omega_p^2 \). Low- \( k \) asymptotic forms shown by straight lines, for \( \Delta_4(k) \) it follows from Eq. (4a), for \( \Delta_2(k) \) it can be obtained taking into account the results of the quasi-localized charge approximation (QLCA) \([48],[52]\), and for the parameters \( \Delta_3(k) \) and \( \Delta_4(k) \) they are obtained empirically.
where the dynamic structure factor in the form into account, the self-consistent relaxation theory yields with the fundamental requirements. Taking relations (6) fulfillment implies the compliance of the present approach decrements of the collective modes, etc. Besides, their fullness of the dynamic structure factor and of the mathematical structure and properties of our results, e.g. the 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

\[ S(k, \omega) = \frac{\rho S(k)}{\pi} \frac{2\Delta_2(k) \sqrt{A_3(k)}}{\omega^3 + A_1(k)\omega^4 + A_2(k)\omega^2 + A_3(k)}. \]  

(8)

where

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

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:

\[ \Delta_{n+1}(k) = n + \frac{n}{n} \Delta_n(k), \quad n = 1, 2, 3, \ldots, \]  

(9)

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

\[ S_{\text{imp}}(k, \omega) = \sqrt{\frac{n^2}{2\pi \Delta_1(k)}} \exp \left( -\frac{\omega^2}{2\Delta_1(k)} \right). \]  

(10)

Note that Eq. (10) reproduces the dynamic structure factor spectrum for the regime of "a free-moving particle" [3]. Second, according to Eq. (9), the shape of \( S(k, \omega) \) at a fixed \( k \) is determined by the bicubic polynomial in the variable \( \omega \). Analysis of (8) allows one to obtain the dispersion equation for the high-frequency quasi-acoustic mode

\[ s^3 + B(k)s^2 + \left[ \Delta_1(k) + \frac{8}{5} \Delta_2(k) \right] s + B(k)\Delta_1(k) = 0, \]  

(11)

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

\[ \omega_c(k) = \sqrt{3} \left( \sqrt[3]{Z(k) - q(k)} + \sqrt[3]{Z(k) + q(k)} \right), \]  

(12)

FIG. 2. Wavenumber dependence of the scaled frequency parameters \( \Delta_2(k)/\omega_0^2 \) (yellow diamonds), \( \Delta_3(k)/\omega_0^2 \) (green squares) and \( \Delta_4(k)/\omega_0^2 \) (dark blue circles) obtained by molecular dynamics simulations of the Yukawa-OCP for nine thermodynamic states and some combinations of \( \Gamma \) and \( \kappa \). Solid and dashed lines correspond to relations (6a) and (6b), respectively.

FIG. 3. Dynamic structure factor vs. the wavenumber \( ka \) and the frequency \( \omega/\omega_0 \) 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).
FIG. 4. Dynamic structure factor spectra, multiplied by the plasma frequency, for the thermodynamic states at various values of $\Gamma$ and $\kappa$ and at the various wavenumbers. 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.

The spectral density $C_L(k, \omega)$ and find the dispersion relation $\omega_L(k)$ for the longitudinal acoustic-like excitations:

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

with

$$C_{\pm}(k) = \sqrt{\frac{A_3(k)}{4} - \frac{A_1^2(k)}{216} \pm \sqrt{\frac{A_1^2(k)}{16} - \frac{A_5(k)A_3^2(k)}{432}}}.$$ 

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.

Now we check to which extend 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]. Accurate theoretical description has been provided earlier by the theory based on the method of frequency moments — 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 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 is 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 wavenumber $k_m = 4.3$ $a^{-1}$ [see Fig. 1 (a)]. The basic features of the microscopic collective dynamics appear at the wavenumbers $k \in (0; k_m)$. 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 function of the scaled wavenumber $ka$ and frequency $\omega/\omega_p$. The Brillouin doublet in $\omega_p S(k, \omega)/\rho$ is seen as symmetric maxima located at non-zero frequencies for the wavenumbers up to $k \approx 4.0$ $a^{-1}$.

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 wavenumbers, the self-consistent relaxation theory reproduces the MD simulation results quite accurately and describes all the spectral features. At small wavenumbers $k < k_m/2$ corresponding to an extended hydrodynamic range, the spectra of $S(k, \omega)$ contain just a high-frequency Brillouin component. With the wavenumber $k$ 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 Eq. (14) describe the MD simulations results for the dispersions characteristics $\omega_s(k)$ and $-\delta(k)$ as well. From the low-$k$ asymptotes $\omega_s(k \to 0) \approx v_s k$ and $\delta(k \to 0) \approx -\Gamma_s k^2$ it is possible to determine the sound velocity $v_s$ and the sound attenuation coefficient $\Gamma_s$. For the conditions pointed out in Fig. 5 (top panel), we found $v_s/\omega_p \approx 0.938$ and $\Gamma_s/\omega_p^2 \approx 0.078$ for $\Gamma = 50$, $\kappa = 1$, and $v_s/\omega_p \approx 0.39$ and $\Gamma_s/\omega_p^2 \approx 0.083$ 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 ($\Gamma, \kappa$) combinations are given. The proposed theoretical description with Eq. (16) properly reproduces the low-$k$ asymptotic forms and the roton minima located at $ka \approx 4.3$ 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 $\Gamma$ and with an increase in $\kappa$, so that the roton minimum is practically absent when $\Gamma = 20$ and $\kappa = 2$. The extremum condition for the...
dispersion $\omega_L(k)$ is
\[
\frac{\partial A_3}{\partial k} = \omega^2_L(k) \frac{\partial A_1}{\partial k}. \tag{17}
\]

Then, with the known static structure factor $S(k)$ for a specific combination $(\Gamma, \kappa)$, 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 $(\Gamma, \kappa)$ demonstrate correct asymptotic forms at large wavenumbers into the regime of a free-particle dynamics: $\omega_L(k) = \sqrt{2/(3\Gamma)}\omega_0ka$.

In conclusion, 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 non-perturbative, 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 quasi-localized charge approximation [49]. Conclusions with respect to the analyticity of the system direct dielectric function envisaged in [57] and elaborated in [58] are confirmed (details are provided in the Supplemental Material [25]).

This work was supported by the Russian Science Foundation (Project No. 19-12-00022). I.M.T. acknowledges the financial support provided by the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan (Project No. AP09260349). A.V.M. acknowledges the Foundation for the Advancement of Theoretical Physics and Mathematics “BASIS” for supporting the computational part of this work. The authors are grateful to R.M. Khusnutdinoff and B.N. Galimzyanov for discussion of the results of molecular dynamics simulations.

[1] L. D. Landau, E. M. Lifshitz, *Statistical Physics* (Oxford: Pergamon Press, 1980).
[2] I.Z. Fisher, *Statistical Theory of Liquids* (University of Chicago Press, 1964).
[3] J.-P. Hansen, I. R. McDonald, *Theory of Simple Liquids* (Academic Press, London, 2006).
[4] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (New York: Dover Publ., 1991).
[5] U. Balucani and M. Zoppi, *Dynamics of the Liquid State* (Clarendon Press, Oxford, 1994).
[6] W. Gütze, *Complex Dynamics of glass forming liquids. A mode-coupling theory* (Oxford: Oxford University Press, 2009).
[7] D. L. Price, M.-L. Saboungi, F. J. Bermejo, *Rep. Prog. Phys.* 66, 407 (2003).
[8] T. Scopigno, G. Ruocco, F. Sette, *Rev. Mod. Phys.* 77, 881 (2005).
[9] F. Leclercq-Hugeux, M.-V. Coulet, J.-P. Gaspard, S. Pouget, J.-M. Zanotti, *C. R. Physique* 8 (2007).
[10] Yu. V. Arkhipov, A. Askaruly, A. E. Davletov, D. Yu. Dubovtsvet, Z. Denkó, P. Hartmann, I. Korolov, L. Conde, I. M. Tkachenko, *Phys. Rev. Lett.* 119, 045001 (2017).
[11] Y. Choi, G. Dharuman, M. S. Murillo, *Phys. Rev. E* 100, 013206 (2019).
[12] H.M. Van Horn, *Phys. Lett. A* 28, 706 (1969).
[13] S. A. Khrapak, A. G. Khrapak, A. V. Iveliev, H. M. Thomas, *Phys. Plasmas* 21, 123705 (2014).
[14] S. A. Khrapak, I. L. Semenov, L. Couëdel, H. M. Thomas, *Phys. Plasmas* 22, 083706 (2015).
[15] A. A. Vedhorst, T. B. Schröder, J. C. Dyre, *Phys. Plasmas* 22, 073705 (2015).
[16] S. Ichimaru, *Rev. Mod. Phys.* 65, 255 (1993).
[17] J.-P. Hansen, H. Löwen, *Annu. Rev. Phys. Chem.* 51, 209 (2000).
[18] V. E. Fortov, A. V. Iveliev, S. A. Khrapak, A. G. Khrapak, G. E. Morfill, *Phys. Rep.* 421, 1 (2005).
[19] V. E. Fortov, A. G. Khrapak, S. A. Khrapak, V. I. Molotkov and O. F. Petrov, *Physics-Uspekhi* 47, 447 (2004).
[20] T.C. Killian, T. Pattard, T. Pohl, J.M. Rost, *Phys. Rep.* 449, 77 (2007).
[21] K. Kremer, M. O. Robbins, and G. S. Grest, *Phys. Rev. Lett.* 57, 2694 (1986).
[22] T. Ott and M. Bonitz, *Phys. Rev. Lett.* 103, 195001 (2009).
[23] M. Bonitz, Z. Donkó, T. Ott, H. Kähler, and P. Hartmann, *Phys. Rev. Lett.* 105, 055002 (2010).
[24] M. S. Murillo and D. O. Gericke, *Journal of Physics A: Mathematical and General* 36, 6273 (2003).
[25] See Supplemental Material for more details, which includes Refs. [5] [10] [25] [57] [58].
Problem and Extremal Problems, Translations of Mathematical Monographs (American Mathematical Society, Providence, 1977), Vol. 50.

[27] V. M. Adamyan, T. Meyer, and I. M. Tkachenko, *Fiz. Plazmy* 11, 826 (1985) [English translation: Sov. J. Plasma Phys. 11, 481 (1985)].

[28] I. M. Tkachenko, Yu. V. Arkhipov, A. Askaruly, *The Method of Moments and its Applications in Plasma Physics* (LAP Lambert Academic Publishing, Saarbrücken, 2012).

[29] Yu. V. Arkhipov, A. B. Ashikbayeva, A. Askaruly, A. E. Davletov, and I. M. Tkachenko, *Phys. Rev. E* 90, 053102 (2014).

[30] Y. V. Arkhipov, A. Ashikbayeva, A. Askaruly, A. E. Davletov, D. Y. Dubovtsev, K. S. Santybayev, S. A. Syzganbayeva, L. Conde, I. M. Tkachenko, *Phys. Rev. E* 102, 053215 (2020) and references therein.

[31] A.V. Mokshin and B.N. Galimzyanov, *J. Phys.: Condens. Matter* 30, 085102 (2018).

[32] O.V. Dolgov, D.A. Kirzhnits, E.G. Maksimov, *Rev. Mod. Phys.* 53, 81 (1981).

[33] R.M. Yulmetyev, A.V. Mokshin, P. Hänggi, V. Yu. Shurygin, *Phys. Rev. E* 64, 057101 (2001).

[34] A.V. Mokshin, R.M. Yulmetyev, T. Scopigno, P. Hänggi, *J. Phys.: Condens. Matter* 15, 2235 (2003).

[35] A. V. Mokshin, *Theor. Math. Phys.* 183, 449 (2015).

[36] A.V. Mokshin, R.M. Yulmetyev, P. Hänggi, *Journal of Chemical Physics* 121, 7341 (2004).

[37] W. Götze, *Z. Phys. B* 56, 139 (1984).

[38] K. Miyazaki, *J. Chem. Phys.* 121, 8120 (2004).

[39] S. Takeno, F. Yoshida, *Prog. Theor. Phys.* 62, 883 (1979).

[40] L.F. Elizondo-Aguilera and Th. Voigtmann, *Phys. Rev. E* 100, 042601 (2019).

[41] J. Florencio, O. F. de Alcantara Bonfim, *Front. Phys.* 8, 557277 (2020).

[42] J. P. Mithen, J. Daligault, G. Gregori, *Phys. Rev. E* 84, 056407 (2012).

[43] G. Szamel, *Progress of Theoretical and Experimental Physics* 2013, 012J01 (2013).

[44] A.V. Mokshin, R.M. Khusnutdinoff, Y.Z. Vilf et al., *Theor. Math. Phys.* 206, 216 (2021).

[45] R.M. Khusnutdinoff, C. Cockrell, O.A. Dicks, A.C.S. Jensen, M.D. Le, L. Wang, M.T. Dove, A.V. Mokshin, V.V. Brazhkin, K. Trachenko, *Phys. Rev. B* 101, 214312 (2020).

[46] J. Ortner, *Physica Scripta* T84, 69 (2000).

[47] J. P. Mithen, J. Daligault, B. J. B. Crowley, G. Gregori, *Phys. Rev. E* 84, 046401 (2011).

[48] J. P. Mithen, J. Daligault, G. Gregori, *Phys. Rev. E* 85, 056407 (2012).

[49] J. P. Hansen, I. R. McDonald, and E. L. Pollock, *Phys. Rev. A* 11, 1025 (1975).

[50] O.V. Dolgov, D.A. Kirzhnits, E.G. Maksimov, *Rev. Mod. Phys.* 53, 81 (1981).

[51] P. Magyar, G.J. Kalman, P. Hartmann, Z. Donkó, *Phys. Rev. E* 104, 015202 (2021).
SUPPLEMENTAL MATERIAL

I. Here we wish to clarify the interrelations between the self-consistent relaxation theory we apply in the main text and the self-consistent version of the moment approach called there the FM-theory.

Let us start with the fluctuation-dissipation theorem (FDT). If we denote the inverse dielectric function as \( \eta(q, \omega) \), then the FDT classical version can be written as (in this Supplemental Material we use the dimensionless wavenumber \( q = ka \), \( a \) being the Wigner-Seitz radius)

\[
\Im \eta(q, \omega) = -\pi \phi(q) \beta \omega S(q, \omega)
\]

where \( \phi(q) = 4\pi (ea)^2/q^2 \) and \( \beta \) is the inverse temperature in energy units. As in the main text, we employ the power frequency moments of the dynamic structure factor (DSF) \( S(q, \omega) \):

\[
S_l(q) = \frac{1}{\rho} \int_{-\infty}^{\infty} \omega^l S(q, \omega) \, d\omega.
\]

The FM-theory expression for the DSF [10, 26, 30]

\[
\pi S(q, \omega) = \frac{\omega_q^2 (\omega^2 - \omega_q^2)^2}{\omega^2 (\omega^2 - \omega_q^2)^2 + \hbar^2 (\omega^2 - \omega_q^2)^2}
\]

is a direct consequence of Nevanlinna's theorem as applied to the truncated Hamburger problem of five moments \( \{S_0, S_2, S_3, S_4, S_5\} \), which is the DSF for a classical system, to the Nevanlinna parameter function \( Q(q) \subset R_0 \) (this is a subclass of \( R \) with an additional condition on the limiting form of the function:

\[
\lim_{z \to \infty} Q(z; q)/z = 0
\]

to be valid in the upper half-plane of the complex frequency \( z = \omega + i\delta \), \( \delta > 0 \); this requirement guarantees the fulfillment of the moment conditions regardless of the specific form of \( Q(z; q) \). The coefficients of the fractional-linear transformation \([19]\), \( D_2(q) = (\omega^2 - \omega_q^2) \) and \( D_3(q) = \omega (\omega^2 - \omega_q^2) \) are orthogonal polynomials with the even weight \( \bar{S}(q, \omega)/\rho \):

\[
\frac{1}{\rho} \int_{-\infty}^{\infty} D_2(q) S(q, \omega) \, d\omega = 0,
\]

while the polynomials \( E_3(q; \omega) \) and \( E_2(q; \omega) \) are their conjugate ones:

\[
E_j(q; \omega) = \frac{1}{\rho} \int_{-\infty}^{\infty} \frac{D_2(q; \omega) - D_2(q; \omega)}{\omega^l - \omega} S(q, \omega) \, d\omega', \quad j = 1, 2,
\]

that is

\[
E_3(q; \omega) = S_0(q) (\omega_1^2 (q) - \omega_2^2 (q) + \omega^2)
\]

and

\[
E_2(q; \omega) = \omega S_0(q)
\]

It should be emphasized that the theorem [19] gives the most accurate expression for the DSF within the five-moment Hamburger problem: restore the DSF from the moments \( \{S_0, S_2, 0, S_4\} \), where \( S_0(q) = S(q) \) is the system static structure factor. The explicit expressions for the moments are well-known, in particular, it can be shown that the expression for the second-order relaxation parameter

\[
\Delta_2(q) = \Delta_1(q) [3S(q) - 1] + \omega_0^2 D(q)
\]

can be rewritten as

\[
\Delta_2(q) = \omega_0^2 \left[ \frac{q^2}{q^2 + \kappa_1^2} + \frac{q^2}{3TS(q)} + U(q) \right],
\]

where two equivalent forms of the interaction contribution \( U(q) \) can be employed [5]

\[
U(q) = \frac{1}{12\pi} \int_0^\infty \exp(-\kappa x) (g(x) - 1) f_1(q, x, \kappa) \, dx
\]

with

\[
f_1(q, x, \kappa) = \left( \frac{2 (\kappa x)^2 + 6 \kappa x + 6}{\kappa^2 (1 - j_0(qx))} \right)
\]

or [10]

\[
U(q) = \frac{1}{12\pi} \int_0^\infty [S(p) - 1] f_2(p, q, \kappa) \, dp
\]

with

\[
f_2(p, q, \kappa) = \frac{2 (3q^2 - \kappa^2 - p^2)}{q^2} \left( \frac{q^2 - \kappa^2 - p^2}{2q^2} \right) \times \ln \left( \frac{\kappa^2 + (q + p)^2}{\kappa^2 + (q - p)^2} \right) - \frac{8p^2}{3 (\kappa^2 + p^2)}
\]

Here \( h(x) = g(x) - 1, g(x) \) is the radial distribution function. The frequency relaxation parameters \( \Delta_1(q) \) and \( \Delta_2(q) \) are related to the characteristic frequencies \( \omega_1^2(k) \) and \( \omega_2^2(k) \) by the following relations:

\[
\omega_1^2(q) = \Delta_1(q),
\]

\[
\omega_2^2(q) = \Delta_1(q) + \Delta_2(q).
\]

The Kramers-Kronig relations for the inverse dielectric function \( \eta(q, \omega) = \epsilon^{-1}(q, \omega) \) and the FDT should be applied to make use of the exact mathematical result [19]:

\[
\eta(q, \omega + i0^+) = 1 + \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Im \eta(q, \omega') \, d\omega'}{\omega - \omega - i0^+} = 1 - \phi \beta \rho \left( S_0(q) - \frac{S(q, \omega') \, d\omega'}{\omega - \omega'} \right) = 1 + \frac{\phi \beta \rho S(q, \omega^2(q)) (\omega + Q(q)) (\omega^2 - \omega_1^2(q))}{\omega^2 - \omega_2^2(q)} + Q(q) (\omega^2 - \omega_1^2(q)).
\]
Thus,
\[
S(q, \omega) = \frac{\rho S(q)}{\pi \omega} \text{Im} \frac{-\omega_1^2 (\omega + Q(\omega; q))}{\omega (\omega^2 - \omega_2^2(q)) + Q(\omega^2 - \omega_1^2(q))}.
\]  
(25)

Notice that the latter expression can be rewritten as a truncated continuous fraction:
\[
\frac{\pi S(q, \omega)}{\rho S(q)} = \frac{1}{\omega} \text{Im} \left( 1 - \frac{\omega}{\omega - \frac{\omega_1^2}{\omega - \omega_2^2}} \right). \tag{26}
\]

In [10] [27][30] the Nevanlinna parameter function \(Q(z; q)\) was approximated by its static value \(Q(0^+; q) = i h(q)\). In this case
\[
\frac{\pi S(q, \omega)}{\rho S(q)} = -\frac{\omega_1^2}{\omega} \text{Im} \left( \omega (\omega^2 - \omega_2^2(q)) + i h(\omega^2 - \omega_1^2(q)) \right) = \frac{\omega_1^2 h (\omega^2 - \omega_1^2)}{\omega^2 (\omega^2 - \omega_2^2)^2 + h^2 (\omega^2 - \omega_1^2)^2}. \tag{27}
\]

In [10] on the basis of some physical considerations the positive static parameter function \(h(q)\) was related to the characteristic frequencies \(\omega_1(q, \kappa)\) and \(\omega_2(q, \kappa)\), which permitted to express the dynamic properties of one-component classical plasmas to their static characteristics, i.e., the static structure factor.

In the present work the function \(Q(z; q)\) is obtained within the Zwanzig-Mori formalism as [31]
\[
\tilde{Q}(z; q) = -\frac{\Delta_3(q)}{2\Delta_4(q)} \left( z - \sqrt{z^2 - 4\Delta_4(q)} \right). \tag{28}
\]

This model Nevanlinna function satisfies the asymptotic requirement [20], but it is obviously not analytical in the upper half-plane of the variable \(z\), i.e., \(\tilde{Q}(z; q) \notin R\). Nevertheless, if we substitute into
\[
\tilde{Q}(\omega; q) = -\frac{\Delta_4(q)}{2\Delta_4(q)} (\omega - i \sqrt{4\Delta_4(q) - \omega^2}), \tag{29}
\]
for the frequencies such that \(\omega^2 \ll \Delta_4(q)\), it stems from [26] and [29] that
\[
\frac{\pi S(q, \omega)}{\rho S(q)} = \frac{\Delta_1(q)\Delta_2(q) \Delta_3(q) \sqrt{\Delta_4(q)} / \Delta_4(q) - \Delta_3(q))}{\omega^6 + A_1(q)\omega^4 + A_2(q)\omega^2 + A_3(q)}, \tag{30}
\]
with
\[
A_1(q) = \frac{\Delta_3^2(q) - \Delta_2(q) \Delta_3^2(q)}{\Delta_4(q) - \Delta_3(q)} - 2\Delta_4(q),
\]
\[
A_2(q) = \frac{\Delta_3^2(q)\Delta_4(q) - 2\Delta_1(q)\Delta_3^2(q)}{\Delta_4(q) - \Delta_3(q)} + \Delta_1^2(q) + \frac{\Delta_1(q)\Delta_2(q) \Delta_3^2(q)}{\Delta_4(q) - \Delta_3(q)},
\]
\[
A_3(q) = \frac{\Delta_1^2(q) - \Delta_3^2(q)}{\Delta_4(q) - \Delta_3(q)}.
\]

Observe that the coefficients \(A_j(q)\) coincide with the coefficients \(A_j(q), j = 1, 2, 3\) introduced in the main text. Notice also that when the conditions
\[
\omega^2 \ll \Delta_4(q)
\]
and
\[
[\Delta_1(q) + \Delta_2(q)]^2 \Delta_4(q) = 2\Delta_1(q) \Delta_3^2(q)
\]
are satisfied, expressions for the DSF, [30] and [27] coincide and when \(\Delta_3(q) = 0\), they possess joint poles
\[
z_\pm = \pm \omega_2(q) = \pm \sqrt{\Delta_1(q) + \Delta_2(q)}.
\]

It is also very important that the asymptotic forms of the inverse dielectric function related to these two expressions for the DSF also coincide, i.e. they satisfy the involved sum rules automatically, independently of the chosen model expression for the Nevanlinna function.

The overall quality of both outlined approaches is corroborated by the comparison with the simulation data carried out in the main text.

II. The self-consistent relaxation theory allows one to obtain the dispersion equation in the analytical form (see equation (11) in the main text). Then it turns out to be appropriate to discuss the issue of analyticity of the direct dielectric function like it was done in the works [57] and [58]. If we make the substitution \(s = -iz\), equation (11) in the main text takes the following form:
\[
z \left( z^2 - \Delta_1(q) - \frac{8}{5} \Delta_2(q) \right) + i B(q) (z^2 - \Delta_1(q)) = 0, \tag{31}
\]
whose roots \(z = \pm \omega_c - i \delta\) are the poles of the inverse dielectric function of the system, \(\eta(q, z)\) [30]. The location of these poles in the lower half-plane of the complex frequency implies that the sound attenuation coefficient in the system under investigation is positive and thus it is stable [57]. The last condition is fulfilled for all thermodynamic states considered in this work. If in the equation (31) we make the replacement \(\Delta_1(q) = \Delta_1(q) - \omega_p^2\), then roots with a positive imaginary part will appear in its solution, which corresponds to a negative sound attenuation coefficient and the system instability. This behavior of solutions to the equation (31) with this replacement means that the following inequality holds:
\[
\frac{\Delta_1(q)}{\omega_p^2} < 1. \tag{32}
\]

This condition is equivalent to the negativity of the direct static dielectric function \(\epsilon(q, z = 0)\) and means the fulfillment of the causality principle described in the work [57] and studied in detail for the Coulomb one-component plasma in [58].