

## Entropy of strongly coupled Yukawa fluids

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The entropy of strongly coupled Yukawa fluids is discussed from several perspectives. First, it is demonstrated that a vibrational paradigm of atomic dynamics in dense fluids can be used to obtain a simple and accurate estimate of the entropy without any adjustable parameters. Second, it is explained why a quasiuniversal value of the excess entropy of simple fluids at the freezing point should be expected, and it is demonstrated that a remaining very weak dependence of the freezing point entropy on the screening parameter in the Yukawa fluid can be described by a simple linear function. Third, a scaling of the excess entropy with the freezing temperature is examined, a modified form of the Rosenfeld-Tarazona scaling is put forward, and some consequences are briefly discussed. Fourth, the location of the Frenkel line on the phase diagram of Yukawa systems is discussed in terms of the excess entropy and compared with some predictions made in the literature. Fifth, the excess entropy scaling of the transport coefficients (self-diffusion, viscosity, and thermal conductivity) is reexamined using the contemporary datasets for the transport properties of Yukawa fluids. The results could be of particular interest in the context of complex (dusty) plasmas, colloidal suspensions, electrolytes, and other related systems with soft pairwise interactions.

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### I. INTRODUCTION

Entropy is a central concept in thermodynamics and statistical mechanics. In statistical physics it is defined as a measure of the number of possible microscopic states (microstates) of a system in thermodynamic equilibrium for given macroscopic thermodynamic properties [1,2]. This connection between macroscopic and microscopic behavior is vital for understanding the structural and dynamical properties of gases, liquids, and solids. While in gases and solids the entropy can be readily evaluated, that is not the case in liquids. An accurate equation of state is required to evaluate the entropy by conventional thermodynamic integration. An accurate equation of state is not always available, and other methods can sometimes be useful.

The main purpose of this paper is to apply a vibrational paradigm of atomic dynamics in dense liquids to the strongly coupled Yukawa fluid. The vibrational picture [3] has been rather successful in describing certain transport properties of various simple fluids, such as the Stokes-Einstein relation between the self-diffusion and viscosity coefficients [4–6], as well as the thermal conductivity coefficient [7–11]. Within this paradigm, the solid-like oscillations of atoms around their temporary equilibrium positions dominate the dynamical picture. The temporary equilibrium positions of atoms do not form any regular structure and are not fixed, unlike in solids. Instead, they are allowed to diffuse, and this is why liquids can flow. However, this diffusive motion is characterized by much longer timescales compared to the period of solid-like oscillations. These long timescales are irrelevant from the

point of view of the system entropy. Hence, the vibrational model has been demonstrated to describe relatively well the excess entropy of inverse-power-law fluids with  $\propto r^{-n}$  repulsive interactions, including the extremely soft Coulomb ( $n = 1$ ) case, intermediately soft  $n = 6$  and  $n = 12$  cases, and the opposite hard-sphere interaction limit ( $n = \infty$ ) [12]. It is reasonable to expect that the same method would work when applied to a Yukawa fluid, and we verify this conjecture below.

The vibrational model is applied to the Yukawa fluid using the dispersion relations of collective modes from the quasilo-calized charge approximation (QLCA) [13–15] combined with a simple model of the radial distribution function [16]. The results are compared with those from extensive molecular dynamics (MD) simulation in Refs. [17,18], and good agreement is documented. Application of the Rosenfeld-Tarazona scaling to estimate the excess entropy is discussed, and a modified expression is put forward. This modified expression is used to discuss the location of the Frenkel line on the phase diagram of Yukawa fluids in terms of the excess entropy. The excess entropy scaling of transport coefficients proposed by Rosenfeld [19] is a very important corresponding state principle for the transport properties of fluids [20]. We use this opportunity to demonstrate how it applies to Yukawa fluids using contemporary transport data from extensive numerical simulations. A complete and intrinsically consistent picture of how the phase state, dynamical, and transport properties of Yukawa fluids are interrelated via the excess entropy thus emerges.

### II. SCREENED COULOMB (YUKAWA) FLUID

The pairwise screened Coulomb repulsive potential (also referred to as the Debye-Hückel or Yukawa potential) is

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usually used as a first approximation to describe interactions between charged particles in neutralizing media, such as plasmas, complex (dusty) plasmas, electrolytes, and colloidal suspensions [21–27]. The potential is

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

where  $Q$  is the electrical charge and  $\lambda$  is the screening length. The properties of Yukawa systems are described by two dimensionless parameters. They are the Coulomb coupling parameter  $\Gamma = Q^2/aT$  and the screening parameter  $\kappa = a/\lambda$ , where  $T$  is the temperature in energy units,  $a = (4\pi\rho/3)^{-1/3}$  is the Wigner-Seitz radius, and  $\rho$  is the number density. The screening parameter  $\kappa$  determines the softness of the Yukawa potential. It varies from the extremely soft and long-range Coulomb potential  $\propto 1/r$  at  $\kappa \rightarrow 0$ , which corresponds to the one-component plasma limit, to the hard-sphere-like interaction limit at  $\kappa \rightarrow \infty$ . In the context of complex plasmas and colloidal suspensions the relatively “soft” regime,  $\kappa \sim O(1)$ , is of particular interest. Most of the attention in the literature has focused on this regime, and we follow that tradition here.

The properties of the phase diagram of Yukawa systems are relatively well understood. Since the Yukawa potential is purely repulsive, there are no gas-liquid phase transition, gas-liquid coexistence, or critical and gas-liquid-solid triple points. There is a fluid-solid phase transition at sufficiently strong coupling. The location of the freezing line  $\Gamma_{\text{fr}}(\kappa)$  for  $\kappa < 5$  was tabulated in Ref. [18], and simple practical fits are available [28,29]. There is also a crossover between gas-like and liquid-like dynamics, known as Frenkel line on the phase diagram [30–33]. The Frenkel line appears to be parallel to the freezing line and is located at  $\Gamma/\Gamma_{\text{fr}} \simeq 0.05$ , as identified recently [34,35]. We will elaborate on this topic below. At a very high coupling, the possibility of the glass transition has been predicted. The traditional mode coupling theory results from Refs. [36,37] show that the glass transition line is also parallel to the freezing line and is predicted at  $\Gamma/\Gamma_{\text{fr}} \simeq 2 - 3$ , depending on the chosen closure to the integral equation theory used to obtain the structural information.

The transport phenomena and thermodynamics of three-dimensional Yukawa fluids have been investigated in dozens of publications; see, e.g., Ref. [3] for a recent overview. The main reference sources for this paper are Refs. [17,18] with regard to the fluid-solid phase transition and thermodynamics of Yukawa fluids. Regarding the transport coefficients discussed later in the context of the excess entropy scaling, for the self-diffusion coefficient we use numerical data from Ref. [38], for the shear viscosity coefficient we use data from Refs. [39,40], and for the thermal conductivity coefficient we use data from Refs. [41,42]. Collective mode properties are derived from the quasicrystalline approximation [13], which is more well known as the QLCA in the plasma-related context [14,15,43].

Dealing with thermodynamic quantities, we work only with their “excess” components, which comprise the actual quantity minus the ideal gas contribution at the same temperature and density [44]. Additionally, we work with dimensionless units. In particular, the reduced energy is  $u = U/NT$ , the reduced entropy is  $s = S/Nk_B$ , and  $c_V = C_V/Nk_B$  is the specific heat at constant volume.

To conclude this section we briefly discuss another important aspect related to excess entropy and Yukawa fluids. Excess entropy plays a central role in the theory of “isomorphs” [45,46]. Isomorphs are defined as lines in a thermodynamic phase diagram along which structure and dynamics in properly reduced units are invariant to a good approximation [46]. Constancy of excess entropy often serves as an identification of isomorphs. It can be rigorously proven that systems that have strong correlations between the equilibrium virial and potential energy fluctuations exhibit good isomorphs in their phase diagrams [45–47]. Such systems are usually referred to as “Roskilde-simple” or just “R-simple” systems [47]. It has been demonstrated that the Yukawa system has rather strong correlations between the virial and potential energies and thus belongs to the class of R-simple systems [48,49]. Therefore, the excess entropy plays a particularly important role in Yukawa fluids.

### III. VIBRATIONAL MODEL OF THE EXCESS ENTROPY AT WORK

Within the vibrational model, the reduced excess entropy of a liquid is obtained as an appropriate averaging over the frequencies of normal modes [12]:

$$s_{\text{ex}} = \frac{3}{2} - \frac{3}{2} \left\langle \ln \frac{m\Delta^2\omega^2}{2\pi T} \right\rangle, \quad (2)$$

where  $m$  is the mass,  $\Delta = \rho^{-1/3}$  is the structure independent mean interparticle separation, and  $\omega$  is the vibrational frequency. Although this resembles an expression for the excess entropy of a crystalline solid, there is an important difference. The reduced liquid excess entropy contains an additional +1.0 term compared to the solid entropy, which is sometimes referred to as “communal entropy” [50]. In the vibrational model, this term naturally occurs from the assumption of single-cell occupancy; see Ref. [12] for further detail.

The second term in Eq. (2) can be rewritten as

$$\left\langle \ln \frac{m\Delta^2\omega^2}{2\pi T} \right\rangle = \left\langle \ln \frac{\omega^2}{\omega_p^2} \right\rangle + \ln \Gamma + \ln \frac{2}{(4\pi/3)^{1/3}}, \quad (3)$$

where  $\omega_p = \sqrt{4\pi Q^2 \rho/m}$  is the plasma frequency. Following the standard practice, we express averaging over frequencies as an integral over the wave numbers [1],

$$\left\langle \ln \frac{\omega^2}{\omega_p^2} \right\rangle = \frac{2}{9\pi} \int_0^{q_{\text{max}}} q^2 dq \left( \ln \frac{\omega_l^2}{\omega_p^2} + 2 \ln \frac{\omega_t^2}{\omega_p^2} \right). \quad (4)$$

Here  $q = ka$  is the reduced wave number, and  $\omega_{l,t}(q)$  are the dispersion relations of the longitudinal and transverse modes, respectively. It is assumed that dense liquids support one longitudinal (compressional) and two transverse (shear) modes. The cutoff wave number  $q_{\text{max}} = (9\pi/2)^{1/3} \simeq 2.418$  ensures that the identity  $\langle \mathcal{X} \rangle = \mathcal{X}$  is satisfied, where  $\mathcal{X}$  is any quantity that does not depend on the wave number.

We perform averaging using the dispersion relations derived within the framework of the QLCA model. Moreover, since the long-wavelength range of the dispersion relations is mostly involved (due to the cutoff), it is practical to employ the simplified version of the QLCA in which the radial

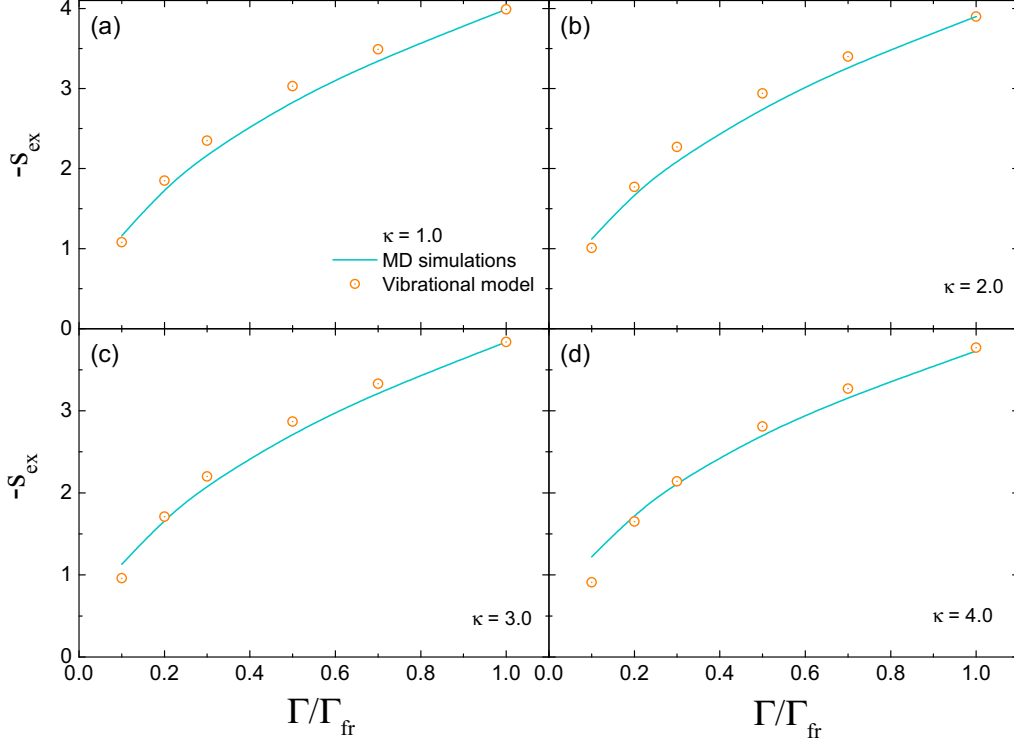


FIG. 1. Negative reduced excess entropy of the Yukawa fluid as a function of the reduced coupling parameter  $\Gamma/\Gamma_{fr}$ . The results for four screening parameters are presented: (a)  $\kappa = 1.0$ , (b)  $\kappa = 2.0$ , (c)  $\kappa = 3.0$ , and (d)  $\kappa = 4.0$ . The symbols correspond to the calculation using the vibrational model reported here. The solid curves are plotted using the results from MD simulations in Refs. [17,18] (see the Appendix for details).

distribution function (RDF) is modeled with a simple step function (excluded volume approximation). This results in simple analytical expressions which demonstrate high accuracy at long wavelengths [16,51,52]. These dispersion relations are

$$\frac{\omega_p^2}{\omega_s^2} = \frac{q^2}{\Gamma} + e^{-R\kappa} \left[ (1 + R\kappa) \left( \frac{1}{3} - \frac{2 \cos Rq}{R^2 q^2} + \frac{2 \sin Rq}{R^3 q^3} \right) - \frac{\kappa^2}{\kappa^2 + q^2} \left( \cos Rq + \frac{\kappa}{q} \sin Rq \right) \right], \quad (5)$$

$$\frac{\omega_t^2}{\omega_p^2} = \frac{q^2}{3\Gamma} + e^{-R\kappa} (1 + R\kappa) \left( \frac{1}{3} + \frac{\cos Rq}{R^2 q^2} - \frac{\sin Rq}{R^3 q^3} \right). \quad (6)$$

Here  $R$  is the excluded volume radius expressed in units of  $a$ . The excluded volume radius is chosen in such a way that the model RDF  $g(r) = \theta(r - aR)$  yields accurate results via energy or pressure equations [16]. The simple practical expression proposed in Ref. [51] is

$$R(\kappa) \simeq 1 + \frac{1}{\kappa} \ln \left[ \frac{3 \cosh(\kappa)}{\kappa^2} - \frac{3 \sinh(\kappa)}{\kappa^3} \right]. \quad (7)$$

Each of Eqs. (5) and (6) contains two terms. The first is the kinetic contribution. The second is the potential energy contribution, associated with the interaction between the particles. In the strongly coupled regime the potential contribution dominates, and kinetic terms are often omitted. We keep both contributions, which provides slightly better accuracy in estimating the excess entropy.

Substituting Eqs. (5) and (6) in formula (4) and performing a numerical integration, we obtain an estimation of the excess entropy within the vibrational model. The results of our theoretical calculation along with a comparison with numerical results is presented in Fig. 1. The agreement is remarkable, especially taking into account the simplicity of the model and the absence of any adjustable parameters.

It should be pointed out that the present approach neglects the so-called  $q$ -gap—the zero-frequency portion of the dispersion relation at low  $q$  also known as the propagation gap in the dispersion relation of the transverse collective mode [44,53–62]. Given the good agreement between the present theory and the actual results for the excess entropy, there does not seem to be a need to further complicate the model by taking the  $q$  gap into consideration. This is a major difference from the so-called phonon theory of liquid thermodynamics [58,63], where the  $q$  gap and the disappearance of the transverse modes when approaching the gaseous state play a major role. On the other hand, the vibrational model discussed here focuses on dense liquid states, in which the vibrational motion dominates, transverse modes are present, and the  $q$  gap is relatively narrow. The limits of the applicability of the vibrational model are discussed later in this paper.

Given the fundamental significance of the excess entropy in R-simple fluids such as Yukawa fluids, it will be very important in the future to obtain accurate MD or Monte Carlo (MC) simulation data for the excess entropy. The calculations based on the equation of state do not suffice, given the thermodynamic integration of the excess free energy that introduces

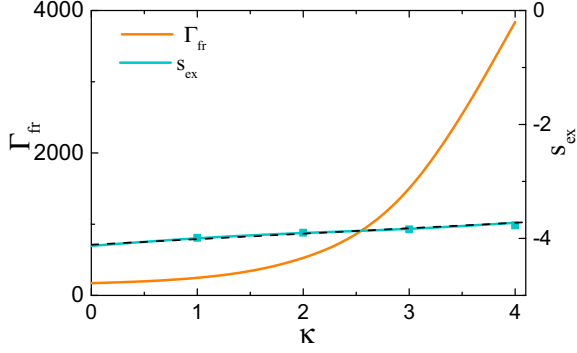


FIG. 2. The coupling parameter (left axis) and the excess entropy (right axis) at freezing of the Yukawa fluid as a function of the screening parameter  $\kappa$ . The solid curves are plotted using the MD results of Ref. [18]. The squares are excess entropies evaluated from the vibrational model. The dashed line is a linear fit of the data points from Ref. [18].

uncontrolled errors. Such indirect evaluation is possible based on the fundamental thermodynamic Euler equation combined with separate extractions of the excess internal energy, the excess pressure from the virial equation [64], and the excess chemical potential via the Widom insertion method [65,66]. Note that isomorph theory allows the exact tracking of isentropic lines via numerical simulations but does not allow the calculation of the excess entropy value along these lines. Nevertheless, it can be employed for rigorous cross-checking.

#### IV. EXCESS ENTROPY AT FREEZING

The excess entropy at freezing is a quasiuniversal quantity for many simple fluids such as the inverse-power-law fluid [67], Lennard-Jones fluid [68,69], and the Yukawa fluid considered here (see Fig. 1). In all cases  $s_{\text{ex}} \simeq -4$  applies (a somewhat smaller value for Yukawa fluids was reported in Ref. [70]; the reason for this deviation is unclear). Let us look in more detail at whether any systematic trend is present.

The coupling parameter and the excess entropy dependence on  $\kappa$  at freezing of the Yukawa fluid are shown in Fig. 2. Note that the excess entropy at freezing calculated with the help of the vibrational model is in excellent agreement with accurate results from numerical simulations [18]. While the freezing coupling parameter varies by more than 20 times as  $\kappa$  increases from 0 to 4, the excess entropy varies only very weakly, systematically increasing with  $\kappa$ . This increase can be very well described by the linear function

$$s_{\text{ex}}^{\text{fr}} \simeq -4.109 + 0.096\kappa, \quad (8)$$

which is shown in Fig. 2 by the dashed line. This fit applies for  $\kappa \leq 4$ .

There is a simple instructive explanation for why a quasiuniversal value  $s_{\text{ex}} \simeq -4$  should be expected at the freezing point. Consider Eq. (2) for the excess entropy within the vibrational model. Assuming for simplicity that all atoms vibrate with the same frequency (this is the Einstein approximation in solid state physics), we get

$$s_{\text{ex}} \simeq \frac{3}{2} - \frac{3}{2} \ln \frac{m\Delta^2\Omega_{\text{E}}^2}{2\pi T}, \quad (9)$$

where  $\Omega_{\text{E}}$  is the Einstein frequency. The average vibrational amplitude of an atom around its equilibrium position in a solid phase can be estimated within the framework of the Einstein model via

$$\frac{1}{2}m\Omega_{\text{E}}^2\langle\delta r^2\rangle = \frac{3}{2}T, \quad (10)$$

which just reflects the energy equipartition. The Einstein frequency in this harmonic approximation is thus related to the average vibrational amplitude as

$$\Omega_{\text{E}}^2 = \frac{3T}{m\langle\delta r^2\rangle}. \quad (11)$$

We can now estimate the Einstein frequency invoking Lindemann's melting criterion arguments. The famous Lindemann criterion [71] states that a three-dimensional (3D) solid melts when the square root of the particle mean-square displacement from the equilibrium position reaches a threshold value, which is roughly  $\sim 0.1$  of the interparticle distance. The Einstein frequency does not change much upon the fluid-solid phase transition. This is a quite general statement, but for Yukawa systems (dusty plasma) it has been carefully verified experimentally [72] and theoretically [73] [although those works refer to two-dimensional (2D) systems, the situation in 3D geometry is fully analogous]. Substituting the Einstein frequency into Eq. (9), we get

$$s_{\text{ex}} \simeq \frac{3}{2} - \frac{3}{2} \ln \left( \frac{3}{2\pi} \frac{\Delta^2}{\langle\delta r^2\rangle} \right) \simeq -4.3, \quad (12)$$

where it is assumed that  $\Delta^2/\langle\delta r^2\rangle \simeq 100$  at melting. This rough estimate is in very good agreement with the actual results presented in Fig. 2. Our simple arguments are not limited to the Yukawa fluid and apply equally well to other simple fluids [74], thus explaining quasiuniversal values of the excess entropy at freezing.

#### V. MODIFIED ROSENFELD-TARAZONA SCALING

Rosenfeld and Tarazona (RT) proposed a simple mathematical expression for the freezing temperature scaling of the thermal component of the excess internal energy of simple fluids [75]. Their derivation, based on the fundamental-measure free energy functional for hard spheres and thermodynamic perturbation theory, yields a quasiuniversal high density expansion, featuring a fluid Madelung energy with a thermal correction  $\propto T^{3/5}$ . In reduced units their result can be presented as

$$u_{\text{ex}} = u_{\text{st}} + u_{\text{th}} \simeq M_{\text{fl}}\Gamma + \delta \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{2/5}, \quad (13)$$

where  $u_{\text{st}}$  is the static component of the excess energy,  $u_{\text{th}}$  is the thermal component,  $M_{\text{fl}}$  is the analog of the Madelung energy for the fluid state, and  $\delta$  is a numerical coefficient. Rosenfeld further demonstrated that the numerical coefficient is also quasiuniversal for different simple fluids and that the thermal correction can be represented as [67]

$$u_{\text{th}} \simeq 3.0 \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{2/5}. \quad (14)$$

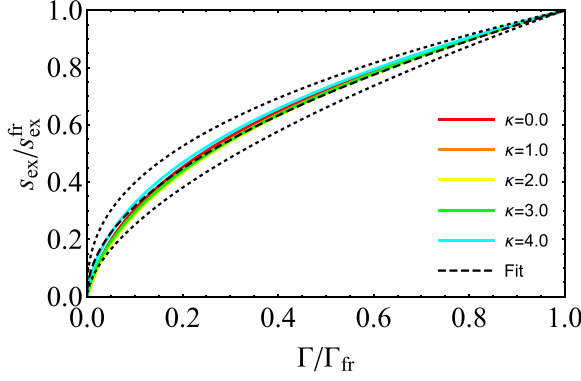


FIG. 3. The ratio  $s_{\text{ex}}/s_{\text{ex}}^{\text{fr}}$  as a function of the reduced coupling strength  $\Gamma/\Gamma_{\text{fr}}$ . The color curves correspond to the results of a MD simulation from Ref. [18]. The dashed curve is the fit using Eq. (18). The two dotted curves corresponding to the exponents 0.4 and 0.6 are plotted for comparison.

This RT scaling, sometimes with minor modifications, has been successfully used to develop simple practical methods to calculate thermodynamic functions of Yukawa fluids as well as some related properties [76–81]. The thermal component of the excess energy  $u_{\text{th}}$  gives direct access to the excess entropy by virtue of

$$\Gamma \frac{\partial s_{\text{ex}}}{\partial \Gamma} = -u_{\text{th}} + \Gamma \frac{\partial u_{\text{th}}}{\partial \Gamma}. \quad (15)$$

Combining Eq. (14) with (15) and integrating, Rosenfeld obtained [67]

$$s_{\text{ex}} \simeq s_{\text{ex}}^{\text{fr}} - \frac{9}{2} \left[ \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{2/5} - 1 \right], \quad (16)$$

where  $s_{\text{ex}}^{\text{fr}}$  is the excess entropy at the freezing point. Equation (16) delivers the correct value of  $s_{\text{ex}}$  at  $\Gamma = \Gamma_{\text{fr}}$  but does not generally reduce to  $s_{\text{ex}} = 0$  at  $\Gamma = 0$  as desired. As we discussed in relation to Fig. 2, the excess entropy at freezing of the Yukawa fluid is almost invariant,  $s_{\text{ex}}^{\text{fr}} \simeq -4$ . This means we will not make a big mistake by substituting the numerical coefficient  $-\frac{9}{2}$  by  $s_{\text{ex}}^{\text{fr}}$  in Eq. (16). This modification of Eq. (16) provides us with a reasonable interpolation between the weakly coupled and strongly coupled limits:

$$s_{\text{ex}} \simeq s_{\text{ex}}^{\text{fr}} \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{2/5}. \quad (17)$$

Our important observation is that Eq. (17) is *not the best option* to describe the actual dependence of the excess entropy on the reduced coupling strength. This is illustrated in Fig. 3. There the five colored curves correspond to the excess entropy calculated using the fits of excess energy provided in Ref. [18] for fluids with  $\kappa = 0$  (one-component plasma limit),  $\kappa = 1$ ,  $\kappa = 2$ ,  $\kappa = 3$ , and  $\kappa = 4$ . The first important observation is that the curves almost overlap with each other, thereby confirming the universal character of the dependence of  $s_{\text{ex}}/s_{\text{ex}}^{\text{fr}}$  on  $\Gamma/\Gamma_{\text{fr}}$ . The second observation is that a simple fit of the form

$$s_{\text{ex}} \simeq s_{\text{ex}}^{\text{fr}} \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{1/2} \quad (18)$$

excellently describes this universal dependence. We plot two additional dotted curves corresponding to the dependence  $s_{\text{ex}} = s_{\text{ex}}^{\text{fr}} (\Gamma/\Gamma_{\text{fr}})^\gamma$  for  $\gamma = 0.4$  (the original RT scaling) and  $\gamma = 0.6$ . They highlight the accuracy of the exponent 1/2 in Eq. (18).

What is essentially proposed is to use the scaling of  $s_{\text{ex}}$  with the freezing temperature instead of  $u_{\text{th}}$  in the original formulation of the RT scaling. This simplifies some thermodynamic derivations. For instance, for the excess specific heat at constant volume we get

$$c_V^{\text{ex}} = -\Gamma \frac{\partial s_{\text{ex}}}{\partial \Gamma} = -\frac{1}{2} s_{\text{ex}}^{\text{fr}} \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{1/2}. \quad (19)$$

For the thermal component of excess energy we get, in this approach,

$$u_{\text{th}} = (u_{\text{th}}^{\text{fr}} + s_{\text{ex}}^{\text{fr}}) \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right) - s_{\text{ex}}^{\text{fr}} \left( \frac{\Gamma}{\Gamma_{\text{fr}}} \right)^{1/2}. \quad (20)$$

This expression can be further simplified by taking into account  $s_{\text{ex}}^{\text{fr}} \simeq -4$  and  $u_{\text{th}}^{\text{fr}} \simeq 3$ .

## VI. FRENKEL LINE ON THE PHASE DIAGRAM

The existence and location of the Frenkel line, which marks the crossover between gas-like and liquid-like dynamics, are of considerable current interest (see, e.g., Refs. [3,30–33,82,83] and references therein). Various indicators of the crossover have been proposed over the years. Huang *et al.* performed extensive MD simulations of 3D and 2D Yukawa fluids and applied several diagnostics tools to locate the dynamical crossover [34]. They demonstrated that the specific heat at constant volume  $c_V$  reaches the threshold value, oscillations in the velocity autocorrelation function emerge, the local atomic connectivity and the shear relaxation times become equal to the inverse Einstein frequency, and the shear viscosity and the thermal conductivity coefficients have minima, all at the same relative coupling strength  $\Gamma/\Gamma_{\text{fr}} \simeq 0.05$ . They also found that at the crossover the transverse (shear) sound velocity reaches a quasiuniversal value of  $c_t \simeq \sqrt{2T/m}$ , which was then explained in Ref. [35].

We believe that one of the most convenient ways to distinguish between different dynamical regimes in simple fluids is by means of the excess entropy. A one-dimensional diagram of dynamical regimes sketched in Ref. [3] features three distinct regimes. For  $-1 \lesssim s_{\text{ex}} \lesssim 0$  the system is in a gas-like state, and the gas-like to liquid-like dynamical crossover occurs at around  $s_{\text{ex}} = -1$ . The region where  $-2 \lesssim s_{\text{ex}} \lesssim -1$  corresponds to the transitional regime where liquid-like properties start to prevail. For  $s_{\text{ex}} \lesssim -2$  the vibrational paradigm of atomic dynamics applies. This corresponds to the dense fluid regime, and this is where the vibrational model of transport coefficients and of excess entropy operates. The vibrational model is applicable up to the crystallization point, which roughly occurs at  $s_{\text{ex}} \simeq -4$ , as discussed above.

Adopting the value  $\Gamma/\Gamma_{\text{fr}} \simeq 0.05$  and using the scaling (18) with  $s_{\text{ex}}^{\text{fr}} \simeq -4$ , we get  $s_{\text{ex}} \simeq -0.89$  at the location of the gas-like to liquid-like dynamical crossover in the Yukawa fluid. This is remarkably close to the value  $s_{\text{ex}} \simeq -0.9 \pm 0.1$  derived from the careful analysis of the Stokes-Einstein

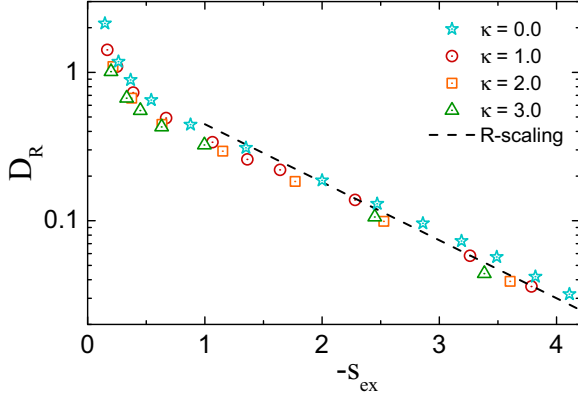


FIG. 4. Reduced self-diffusion coefficient of the Yukawa fluid as a function of the negative excess entropy. Symbols correspond to the numerical results from Ref. [38]. The dashed line is an exponential fit of Eq. (22).

relation in several simple fluids [4,33]. Using the scaling (19), we also estimate  $c_V^{\text{ex}} \simeq 0.45$  at the crossover, which is close to the threshold value  $c_V^{\text{ex}} \simeq 0.5$  [34].

## VII. EXCESS ENTROPY SCALING OF TRANSPORT COEFFICIENTS

In 1977 Rosenfeld proposed a relation between the transport coefficients and excess entropy of simple fluid systems [19]. In particular, he demonstrated that properly reduced diffusion and shear viscosity coefficients of several simple model fluids (hard-sphere, soft-sphere, one-component plasma, and Lennard-Jones fluids) are approximately exponential functions of the reduced excess entropy  $s_{\text{ex}}$ . A somewhat different variant of the entropy scaling of atomic diffusion in condensed matter was independently proposed by Dzугutov [84]. Later, Rosenfeld successfully applied his ideas of excess entropy scaling to the transport coefficients of Yukawa fluids [67,85]. At that time only a rather limited amount of transport data related to Yukawa fluids was available. Many more numerical datasets on transport properties have been published in recent years. Taking into account the important role the Rosenfeld's excess entropy scaling plays in condensed matter nowadays [20], it makes sense to revisit its application to strongly coupled Yukawa fluids using modern transport data.

The presented transport coefficients are normalized using the system-independent normalization adopted by Rosenfeld in his original work on the excess entropy scaling [19,86]:

$$D_R = D \frac{\rho^{1/3}}{v_T}, \quad \eta_R = \eta \frac{\rho^{-2/3}}{m v_T}, \quad \lambda_R = \lambda \frac{\rho^{-2/3}}{v_T}, \quad (21)$$

where  $v_T = \sqrt{T/m}$  is the thermal velocity.

Figure 4 presents results corresponding to the self-diffusion coefficient  $D_R$  of the Yukawa fluid. The symbols are the numerical simulation results from Ref. [38]. They nicely collapse to a quasiuniversal master curve. In the strongly coupled regime, the self-diffusion coefficient can be reasonably well described by the exponential function

$$D_R \simeq 1.1 \exp(0.9 s_{\text{ex}}). \quad (22)$$

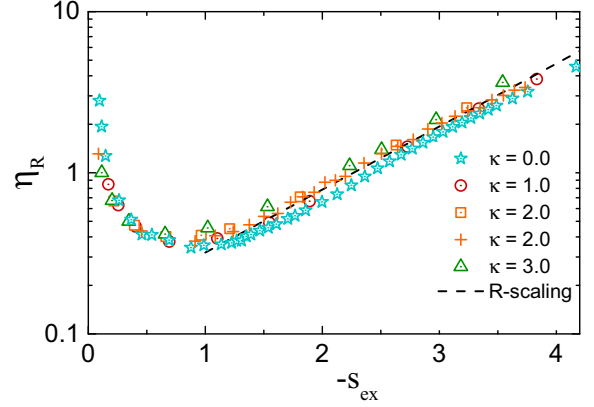


FIG. 5. Reduced shear viscosity coefficient of the Yukawa fluid as a function of the negative excess entropy. Symbols correspond to the numerical results from Refs. [39,40]. The dashed line is an exponential fit of Eq. (23).

Note that the onset of validity of this fit,  $s_{\text{ex}} \lesssim -1$ , corresponds to the crossover between the gas-like and liquid-like dynamics (Frenkel line).

The shear viscosity  $\eta_R$  data are summarized in Fig. 5. The symbols correspond to the numerical results from Refs. [39,40]. Similar to the case of self-diffusion, they nicely collapse to a quasiuniversal curve. In the strongly coupled regime, the reduced shear viscosity coefficient can be reasonably well fitted by the exponential function

$$\eta_R \simeq 0.13 \exp(-0.9 s_{\text{ex}}). \quad (23)$$

By construction, Eqs. (22) and (23) satisfy the Stokes-Einstein relation without the hydrodynamic diameter [87],

$$D_R \eta_R \simeq 0.14, \quad (24)$$

as they should [4,88]. The onset of this exponential dependence is again at the gas-like to liquid-like dynamical crossover, at  $s_{\text{ex}} \simeq -1$ . This is roughly where the minimum in  $\eta_R$  is reached [89].

Note that substituting an approximate scaling  $s_{\text{ex}} \simeq -4(\Gamma/\Gamma_{\text{fr}})^{1/2}$  into Eq. (23), we get  $\eta_R \simeq 0.13 \exp[3.6(\Gamma/\Gamma_{\text{fr}})^{1/2}]$ . This essentially coincides with an empirical fit for the reduced viscosity coefficient of the strongly coupled Yukawa fluid proposed in Ref. [90] based on the ideas from Ref. [91]. Now it becomes evident that this empirical fit is, in fact, consistent with Rosenfeld's version of excess entropy scaling.

The thermal conductivity  $\lambda_R$  data are summarized in Fig. 6. The symbols correspond to the numerical results from Refs. [41,42]. In this case the collapse of the data points is not as impressive as for the diffusion and viscosity coefficients. The reason is unclear at this point. In other fluids, such as Lennard-Jones fluids, the quality of the collapse is apparently better [92] (if near-critical effects are not considered). More data on the thermal conductivity coefficient of Yukawa fluids would be most welcome and would help us to understand the quality of the excess entropy scaling in this case. The dashed curve in Fig. 6 corresponds to the estimation using the vibrational model of heat transfer [9,10] assuming  $s_{\text{ex}} \simeq -4(\Gamma/\Gamma_{\text{fr}})^{1/2}$ . The agreement with the numerical results is

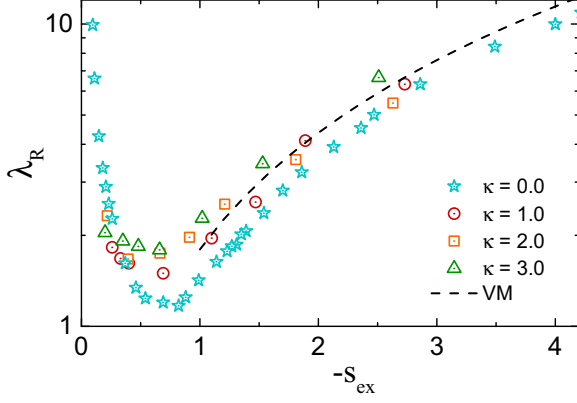


FIG. 6. Reduced thermal conductivity coefficient of the Yukawa fluid as a function of the negative excess entropy. Symbols correspond to the numerical results from Refs. [41,42]. The dashed line corresponds to the vibrational model of heat transfer, Eq. (13) from Ref. [10], under the assumption  $s_{\text{ex}} \simeq -4(\Gamma/\Gamma_{\text{fr}})^{1/2}$ .

fair. The minimum in  $\lambda_R$  is reached relatively close to  $s_{\text{ex}} \simeq -1$ , where the gas-like to liquid-like dynamical crossover takes place.

### VIII. CONCLUSION

The most important results of this study can be formulated as follows.

The vibrational model of atomic dynamics in dense fluids appears to be quite successful at describing the excess entropy of screened Coulomb (Yukawa) fluids. Without any adjustable parameters the model allows us to estimate the excess entropy with relatively high accuracy. The model provides a direct link between the collective properties and thermodynamics and as such contributes to better understanding of the liquid state.

The excess entropy at freezing of Yukawa fluids is almost constant,  $s_{\text{ex}} \simeq -4$ . This property apparently applies to many other simple fluids, and there is a solid explanation for why this should be approximately so. A weak dependence on the screening parameter is, nevertheless, still present and can be accounted for by a simple linear function.

A practical scaling of the excess entropy with the freezing temperature was put forward and can be considered a modification of the Rosenfeld-Tarazona scaling. It was observed that for Yukawa fluids, the excess entropy scales as  $s_{\text{ex}} \simeq s_{\text{ex}}^{\text{fr}}(\Gamma/\Gamma_{\text{fr}})^{1/2}$ , instead of the original RT exponent equal to  $2/5$ . The combination of the weak linear dependence of  $s_{\text{ex}}^{\text{fr}}$  on  $\kappa$  with the modified Rosenfeld-Tarazona scaling represents a simple practical tool to estimate the excess entropy across the entire phase diagram of Yukawa fluids.

The location of the gas-like to liquid-like dynamical crossover in Yukawa fluids was discussed. The excess entropy criterion  $s_{\text{ex}} \simeq -1$  agrees well with several other measures proposed in the literature.

Excess entropy scaling of transport coefficients works rather well for the self-diffusion and shear viscosity coefficients. Approximate formulas based on modern transport

datasets were suggested. The Stokes-Einstein relation without a hydrodynamic radius between the self-diffusion and shear viscosity coefficients is satisfied at strong coupling, as expected. The scaling of the thermal conductivity coefficient with excess entropy is not as impressive. More data are needed to resolve this issue, and this might be a reasonable suggestion for future simulations.

The ideas presented in this work can be straightforwardly extended to bi-Yukawa systems (relevant for complex plasmas) and to any multi-Yukawa system, at least when all interaction terms are purely repulsive. This is indicative of the generality of the results. In fact, the RT decomposition and scaling were already utilized for the construction of a very accurate bi-Yukawa equation of state for the excess internal energy [93].

Overall, the present results provide a systematic picture of the useful interrelations between the properties of collective modes, thermodynamics, and transport in simple fluids with soft pairwise repulsive interactions. They could be of particular interest in the context of complex (dusty) plasma, colloidal suspensions, electrolytes, and other related soft matter systems.

The data that support the findings of this study are available from the author upon a reasonable request.

The author has no conflicts of interest to disclose.

### APPENDIX: REFERENCE DATA FOR THE EXCESS ENTROPY

In Ref. [18] the excess entropy data are not directly available. What is presented is the equilibrium excess internal energy at  $\Gamma \geq 1$ , including the interaction with the neutralizing background, in the form of fitting expressions:

$$u_{\text{ex}}(\kappa, \Gamma) = a(\kappa)\Gamma + b(\kappa)\Gamma^{1/3} + c(\kappa) + d(\kappa)\Gamma^{-1/3}. \quad (\text{A1})$$

The coefficients  $a$ ,  $b$ ,  $c$ , and  $d$  are tabulated for several values of  $\kappa$  in the range  $1.2 \leq \kappa \leq 5$  in Table VIII of Ref. [18]. The regime  $\kappa \leq 1.0$  is treated separately in Ref. [17]. From the excess energy we can calculate the excess Helmholtz free energy by means of the integration

$$f_{\text{ex}}(\kappa, \Gamma) = \int_1^\Gamma u_{\text{ex}}(\kappa, \Gamma') \frac{d\Gamma'}{\Gamma'} + f_1(\kappa), \quad (\text{A2})$$

where

$$f_1(\kappa) = \int_0^1 u_{\text{ex}}(\kappa, \Gamma') \frac{d\Gamma'}{\Gamma'} \quad (\text{A3})$$

is obtained using the actual dependence of  $u_{\text{ex}}(\kappa, \Gamma)$  on  $\Gamma$  in the weakly coupled regime  $\Gamma \leq 1$ . The numerical values of  $f_1(\kappa)$  are listed in Table VII of Ref. [18] for  $0.0 \leq \kappa \leq 5.0$ . The reduced excess entropy is then obtained from

$$s_{\text{ex}}(\kappa, \Gamma) = u_{\text{ex}}(\kappa, \Gamma) - f_{\text{ex}}(\kappa, \Gamma). \quad (\text{A4})$$

- [1] L. D. Landau, E. M. Lifshic, and L. P. Pitaevskii, *Statistical Physics* (Butterworth-Heinemann, Oxford, 1980).
- [2] N. Sator, N. Pavloff, and L. Couedel, *Statistical Physics* (CRC Press, London, 2023).
- [3] S. A. Khrapak, Elementary vibrational model for transport properties of dense fluids, *Phys. Rep.* **1050**, 1 (2024).
- [4] S. A. Khrapak and A. G. Khrapak, Excess entropy and Stokes-Einstein relation in simple fluids, *Phys. Rev. E* **104**, 044110 (2021).
- [5] S. A. Khrapak, Self-diffusion in simple liquids as a random walk process, *Molecules* **26**, 7499 (2021).
- [6] S. A. Khrapak and A. G. Khrapak, Freezing density scaling of transport coefficients in the Weeks-Chandler-Andersen fluid, *J. Chem. Phys.* **160**, 134504 (2024).
- [7] S. A. Khrapak, Vibrational model of thermal conduction for fluids with soft interactions, *Phys. Rev. E* **103**, 013207 (2021).
- [8] S. A. Khrapak, Thermal conduction in two-dimensional complex plasma layers, *Phys. Plasmas* **28**, 010704 (2021).
- [9] S. A. Khrapak, Thermal conductivity of strongly coupled Yukawa fluids, *Phys. Plasmas* **28**, 084501 (2021).
- [10] S. A. Khrapak, Vibrational model of heat transfer in strongly coupled Yukawa fluids (dusty plasma liquids), *Plasma Phys. Rep.* **49**, 15 (2023).
- [11] S. A. Khrapak and A. G. Khrapak, Vibrational model for thermal conductivity of Lennard-Jones fluids: Applicability domain and accuracy level, *Phys. Rev. E* **108**, 064129 (2023).
- [12] S. A. Khrapak and S. O. Yurchenko, Entropy of simple fluids with repulsive interactions near freezing, *J. Chem. Phys.* **155**, 134501 (2021).
- [13] J. Hubbard and J. L. Beeby, Collective motion in liquids, *J. Phys. C* **2**, 556 (1969).
- [14] K. I. Golden and G. J. Kalman, Quasilocalized charge approximation in strongly coupled plasma physics, *Phys. Plasmas* **7**, 14 (2000).
- [15] Z. Donko, G. J. Kalman, and P. Hartmann, Dynamical correlations and collective excitations of Yukawa liquids, *J. Phys.: Condens. Matter* **20**, 413101 (2008).
- [16] S. A. Khrapak, B. Klumov, L. Couedel, and H. M. Thomas, On the long-waves dispersion in Yukawa systems, *Phys. Plasmas* **23**, 023702 (2016).
- [17] R. T. Farouki and S. Hamaguchi, Thermodynamics of strongly-coupled Yukawa systems near the one-component-plasma limit. II. Molecular dynamics simulations, *J. Chem. Phys.* **101**, 9885 (1994).
- [18] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, Triple point of Yukawa systems, *Phys. Rev. E* **56**, 4671 (1997).
- [19] Y. Rosenfeld, Relation between the transport coefficients and the internal entropy of simple systems, *Phys. Rev. A* **15**, 2545 (1977).
- [20] J. C. Dyre, Perspective: Excess-entropy scaling, *J. Chem. Phys.* **149**, 210901 (2018).
- [21] V. E. Fortov, A. G. Khrapak, S. A. Khrapak, V. I. Molotkov, and O. F. Petrov, Dusty plasmas, *Phys.-Usp.* **47**, 447 (2004).
- [22] V. E. Fortov, A. V. Ivlev, S. A. Khrapak, A. G. Khrapak, and G. E. Morfill, Complex (dusty) plasmas: Current status, open issues, perspectives, *Phys. Rep.* **421**, 1 (2005).
- [23] A. Ivlev, H. Löwen, G. Morfill, and C. P. Royall, *Complex Plasmas and Colloidal Dispersions: Particle-Resolved Studies of Classical Liquids and Solids* (World Scientific, Singapore, 2012).
- [24] S. Khrapak and G. Morfill, Basic processes in complex (dusty) plasmas: Charging, interactions, and ion drag force, *Contrib. Plasma Phys.* **49**, 148 (2009).
- [25] M. Chaudhuri, A. V. Ivlev, S. A. Khrapak, H. M. Thomas, and G. E. Morfill, Complex plasma—The plasma state of soft matter, *Soft Matter* **7**, 1287 (2011).
- [26] J. Beckers *et al.*, Physics and applications of dusty plasmas: The perspectives 2023, *Phys. Plasmas* **30**, 120601 (2023).
- [27] U. Konopka, G. E. Morfill, and L. Ratke, Measurement of the interaction potential of microspheres in the sheath of a rf discharge, *Phys. Rev. Lett.* **84**, 891 (2000).
- [28] O. S. Vaulina and S. A. Khrapak, Scaling law for the fluid-solid phase transition in Yukawa systems (dusty plasmas), *J. Exp. Theor. Phys.* **90**, 287 (2000).
- [29] O. Vaulina, S. Khrapak, and G. Morfill, Universal scaling in complex (dusty) plasmas, *Phys. Rev. E* **66**, 016404 (2002).
- [30] V. V. Brazhkin, Yu. D. Fomin, A. G. Lyapin, V. N. Ryzhov, and K. Trachenko, Two liquid states of matter: A dynamic line on a phase diagram, *Phys. Rev. E* **85**, 031203 (2012).
- [31] V. V. Brazhkin, Yu. D. Fomin, A. G. Lyapin, V. N. Ryzhov, E. N. Tsiok, and K. Trachenko, “Liquid-gas” transition in the supercritical region: Fundamental changes in the particle dynamics, *Phys. Rev. Lett.* **111**, 145901 (2013).
- [32] I. H. Bell, G. Galliero, S. Delage-Santacreu, and L. Costigliola, An entropy scaling demarcation of gas- and liquid-like fluid behaviors, *J. Chem. Phys.* **152**, 191102 (2020).
- [33] S. A. Khrapak, Gas-liquid crossover in the Lennard-Jones system, *J. Chem. Phys.* **156**, 116101 (2022).
- [34] D. Huang, M. Baggioli, Sh. Lu, Z. Ma, and Y. Feng, Revealing the supercritical dynamics of dusty plasmas and their liquid-like to gaslike dynamical crossover, *Phys. Rev. Res.* **5**, 013149 (2023).
- [35] N. Yu, D. Huang, S. Lu, S. Khrapak, and Y. Feng, Universal scaling of transverse sound speed and its isomorphic property in Yukawa fluids, *Phys. Rev. E* **109**, 035202 (2024).
- [36] A. Yazdi, A. Ivlev, S. Khrapak, H. Thomas, G. E. Morfill, H. Löwen, A. Wysocki, and M. Sperl, Glass-transition properties of Yukawa potentials: From charged point particles to hard spheres, *Phys. Rev. E* **89**, 063105 (2014).
- [37] F. L. Castello and P. Talias, Theoretical estimate of the glass transition line of Yukawa one-component plasmas, *Molecules* **26**, 669 (2021).
- [38] H. Ohta and S. Hamaguchi, Molecular dynamics evaluation of self-diffusion in Yukawa systems, *Phys. Plasmas* **7**, 4506 (2000).
- [39] Z. Donko and P. Hartmann, Shear viscosity of strongly coupled Yukawa liquids, *Phys. Rev. E* **78**, 026408 (2008).
- [40] J. Daligault, K. Ø. Rasmussen, and S. D. Baalrud, Determination of the shear viscosity of the one-component plasma, *Phys. Rev. E* **90**, 033105 (2014).
- [41] Z. Donkó and P. Hartmann, Thermal conductivity of strongly coupled Yukawa liquids, *Phys. Rev. E* **69**, 016405 (2004).
- [42] B. Scheiner and S. D. Baalrud, Testing thermal conductivity models with equilibrium molecular dynamics simulations of the one-component plasma, *Phys. Rev. E* **100**, 043206 (2019).
- [43] S. Khrapak, B. Klumov, and L. Couedel, Collective modes in simple melts: Transition from soft spheres to the hard sphere limit, *Sci. Rep.* **7**, 7985 (2017).
- [44] J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Elsevier, Amsterdam, 2006).



- [45] N. Gnan, T. B. Schroder, U. R. Pedersen, N. P. Bailey, and J. C. Dyre, Pressure-energy correlations in liquids. IV. Isomorphs in liquid phase diagrams, *J. Chem. Phys.* **131**, 234504 (2009).
- [46] J. C. Dyre, Hidden scale invariance in condensed matter, *J. Phys. Chem. B* **118**, 10007 (2014).
- [47] J. C. Dyre, Isomorphs, hidden scale invariance, and quasiuniversality, *Phys. Rev. E* **88**, 042139 (2013).
- [48] A. A. Veldhorst, T. B. Schroder, and J. C. Dyre, Invariants in the Yukawa system thermodynamic phase diagram, *Phys. Plasmas* **22**, 073705 (2015).
- [49] F. L. Castello, P. Talias, and J. C. Dyre, Testing the isomorph invariance of the bridge functions of Yukawa one-component plasmas, *J. Chem. Phys.* **154**, 034501 (2021).
- [50] J. Hirschfelder, D. Stevenson, and H. Eyring, A theory of liquid structure, *J. Chem. Phys.* **5**, 896 (1937).
- [51] S. A. Khrapak, Practical dispersion relations for strongly coupled plasma fluids, *AIP Adv.* **7**, 125026 (2017).
- [52] S. Khrapak and A. Khrapak, Simple dispersion relations for Coulomb and Yukawa fluids, *IEEE Trans. Plasma Sci.* **46**, 737 (2018).
- [53] H. Ohta and S. Hamaguchi, Wave dispersion relations in Yukawa fluids, *Phys. Rev. Lett.* **84**, 6026 (2000).
- [54] M. S. Murillo, Critical wave vectors for transverse modes in strongly coupled dusty plasmas, *Phys. Rev. Lett.* **85**, 2514 (2000).
- [55] J. Goree, Z. Donkó, and P. Hartmann, Cutoff wave number for shear waves and Maxwell relaxation time in Yukawa liquids, *Phys. Rev. E* **85**, 066401 (2012).
- [56] T. Bryk, F. Gorelli, G. Ruocco, M. Santoro, and T. Scopigno, Collective excitations in soft-sphere fluids, *Phys. Rev. E* **90**, 042301 (2014).
- [57] D. Bolmatov, M. Zhernenkov, D. Zav'yalov, S. Stoupin, Y. Q. Cai, and A. Cunsolo, Revealing the mechanism of the viscous-to-elastic crossover in liquids, *J. Phys. Chem. Lett.* **6**, 3048 (2015).
- [58] K. Trachenko and V. V. Brazhkin, Collective modes and thermodynamics of the liquid state, *Rep. Prog. Phys.* **79**, 016502 (2016).
- [59] C. Yang, M. T. Dove, V. V. Brazhkin, and K. Trachenko, Emergence and evolution of the  $k$  gap in spectra of liquid and supercritical states, *Phys. Rev. Lett.* **118**, 215502 (2017).
- [60] S. A. Khrapak, A. G. Khrapak, N. P. Kryuchkov, and S. O. Yurchenko, Onset of transverse (shear) waves in strongly-coupled Yukawa fluids, *J. Chem. Phys.* **150**, 104503 (2019).
- [61] N. P. Kryuchkov, L. A. Mistryukova, V. V. Brazhkin, and S. O. Yurchenko, Excitation spectra in fluids: How to analyze them properly, *Sci. Rep.* **9**, 10483 (2019).
- [62] N. P. Kryuchkov and S. O. Yurchenko, Collective excitations in active fluids: Microflows and breakdown in spectral equipartition of kinetic energy, *J. Chem. Phys.* **155**, 024902 (2021).
- [63] D. Bolmatov, V. V. Brazhkin, and K. Trachenko, The phonon theory of liquid thermodynamics, *Sci. Rep.* **2**, 421 (2012).
- [64] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon, Oxford, 1989).
- [65] B. Widom, Some topics in the theory of fluids, *J. Chem. Phys.* **39**, 2808 (1963).
- [66] B. Widom, Potential-distribution theory and the statistical mechanics of fluids, *J. Phys. Chem.* **86**, 869 (1982).
- [67] Y. Rosenfeld, Excess-entropy and freezing-temperature scalings for transport coefficients: Self-diffusion in Yukawa systems, *Phys. Rev. E* **62**, 7524 (2000).
- [68] S. A. Khrapak and A. G. Khrapak, Freezing temperature and density scaling of transport coefficients, *J. Phys. Chem. Lett.* **13**, 2674 (2022).
- [69] S. A. Khrapak and A. G. Khrapak, Freezing density scaling of fluid transport properties: Application to liquefied noble gases, *J. Chem. Phys.* **157**, 014501 (2022).
- [70] A. Joy, Universal scaling of pair-excess entropy and diffusion in Yukawa liquids, *Phys. Plasmas* **24**, 010702 (2017).
- [71] F. Lindemann, The calculation of molecular vibration frequencies, *Z. Phys.* **11**, 609 (1910).
- [72] C.-S. Wong, J. Goree, and Z. Haralson, Einstein frequency measurement for a strongly coupled dusty plasma, *IEEE Trans. Plasma Sci.* **46**, 763 (2018).
- [73] S. Khrapak and B. Klumov, High-frequency elastic moduli of two-dimensional Yukawa fluids and solids, *Phys. Plasmas* **25**, 033706 (2018).
- [74] S. A. Khrapak, Lindemann melting criterion in two dimensions, *Phys. Rev. Res.* **2**, 012040 (2020).
- [75] Y. Rosenfeld and P. Tarazona, Density functional theory and the asymptotic high density expansion of the free energy of classical solids and fluids, *Mol. Phys.* **95**, 141 (1998).
- [76] S. A. Khrapak and H. M. Thomas, Practical expressions for the internal energy and pressure of Yukawa fluids, *Phys. Rev. E* **91**, 023108 (2015).
- [77] S. A. Khrapak and H. M. Thomas, Fluid approach to evaluate sound velocity in Yukawa systems and complex plasmas, *Phys. Rev. E* **91**, 033110 (2015).
- [78] S. A. Khrapak, Thermodynamics of Yukawa systems and sound velocity in dusty plasmas, *Plasma Phys. Control. Fusion* **58**, 014022 (2016).
- [79] S. A. Khrapak, N. P. Kryuchkov, S. O. Yurchenko, and H. M. Thomas, Practical thermodynamics of Yukawa systems at strong coupling, *J. Chem. Phys.* **142**, 194903 (2015).
- [80] P. Talias, S. Ratynskaia, and U. de Angelis, Soft mean spherical approximation for dusty plasma liquids: Level of accuracy and analytic expressions, *Phys. Plasmas* **22**, 083703 (2015).
- [81] P. Talias and F. L. Castello, Isomorph-based empirically modified hypernetted-chain approach for strongly coupled Yukawa one-component plasmas, *Phys. Plasmas* **26**, 043703 (2019).
- [82] V. V. Brazhkin, A. G. Lyapin, V. N. Ryzhov, K. Trachenko, Y. D. Fomin, and E. N. Tsiok, Where is the supercritical fluid on the phase diagram? *Phys.-Usp.* **182**, 1137 (2012).
- [83] T. Bryk, F. A. Gorelli, I. Mryglod, G. Ruocco, M. Santoro, and T. Scopigno, Behavior of supercritical fluids across the Frenkel line, *J. Phys. Chem. Lett.* **8**, 4995 (2017).
- [84] M. Dzugutov, A universal scaling law for atomic diffusion in condensed matter, *Nature (London)* **381**, 137 (1996).
- [85] Y. Rosenfeld, Quasi-universal melting-temperature scaling of transport coefficients in Yukawa systems, *J. Phys.: Condens. Matter* **13**, L39 (2001).
- [86] Y. Rosenfeld, A quasi-universal scaling law for atomic transport in simple fluids, *J. Phys.: Condens. Matter* **11**, 5415 (1999).
- [87] L. Costigliola, D. M. Heyes, T. B. Schröder, and J. C. Dyre, Revisiting the Stokes-Einstein relation without a hydrodynamic diameter, *J. Chem. Phys.* **150**, 021101 (2019).

- [88] S. Khrapak, Stokes–Einstein relation in simple fluids revisited, *Mol. Phys.* **118**, e1643045 (2020).
- [89] S. A. Khrapak and A. G. Khrapak, Minima of shear viscosity and thermal conductivity coefficients of classical fluids, *Phys. Fluids* **34**, 027102 (2022).
- [90] S. Khrapak, Practical formula for the shear viscosity of Yukawa fluids, *AIP Adv.* **8**, 105226 (2018).
- [91] L. Costigliola, U. R. Pedersen, D. M. Heyes, T. B. Schröder, and J. C. Dyre, Communication: Simple liquids’ high-density viscosity, *J. Chem. Phys.* **148**, 081101 (2018).
- [92] I. H. Bell, R. Messerly, M. Thol, L. Costigliola, and J. C. Dyre, Modified entropy scaling of the transport properties of the Lennard-Jones fluid, *J. Phys. Chem. B* **123**, 6345 (2019).
- [93] F. L. Castello, P. Talias, J. S. Hansen, and J. C. Dyre, Isomorph invariance and thermodynamics of repulsive dense bi-Yukawa one-component plasmas, *Phys. Plasmas* **26**, 053705 (2019).