Origin of viscosity at individual particle level in Yukawa liquids

Dong Huang,[1] Shaoyu Lu,[1] Michael S. Murillo,[2] and Yan Feng[1,*]

[1]*Institute of Plasma Physics and Technology, School of Physical Science and Technology, Soochow University, Suzhou 215006, China*

[2]*Department of Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, Michigan 48824, USA*

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The transition of the viscosity η from a collisional gas through a minimum value to a correlated liquid is investigated using computer simulations with the Green-Kubo relation. It is discovered that, as the temperature varies, the transition of η is well described by the unity ratio of the instantaneous transverse sound speed C_T to the average particle speed $\bar{v}_p$. While $C_T/\bar{v}_p < 1$, η increases with the temperature, since in this regime the viscosity is dominated by the gaslike individual dynamics. However, when $C_T/\bar{v}_p > 1$ where the cooperative dynamics dominates, the fundamental origin of viscosity of liquids is found to be just losing or gaining neighbors for individual particles, so that the viscosity of a typical liquid reasonably decreases with the temperature. Our results reveal that the viscosity transition point of $C_T/\bar{v}_p = 1$ is just ≈20 times the corresponding melting point for both two-dimensional and three-dimensional Yukawa liquids with various screening parameters, which probably can be used as a new criterion to distinguish the strong and weak couplings in plasma physics.

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I. INTRODUCTION

The viscosity of a material, a measure of internal frictional forces [1–4], determines many of its properties, including rates of instability growth and sound attenuation. Interestingly, many fluids have a viscosity minimum [5–7], the value of which determines how "perfect" the fluid can be in the sense of behaving as a nondissipative fluid describable by the Euler hydrodynamics. The behavior of the viscosity around this minimum impacts a range of applications, ranging from the Earth's interior [8] to quark-gluon plasmas [9,10]. The viscosity is described through a transport coefficient that serves to incorporate microphysical processes into macroscopic equations [11]. In the past decades, numerous studies have attempted to address the origin of viscosity for liquids in various physical systems [12–23]. For example, the viscosity is determined by the change of the local topological structure of the atomic connectivity network in extremely high temperature metallic liquids [18–20]. However, despite the recent theoretical progress [12], details of the behavior of the viscosity around its minimum remains poorly understood [13–23]. Here, we examine this behavior in the context of dusty plasmas because of their nearly unique ability to allow experimental measurements of the individual particle motion.

As a model system, dusty plasma [24–32], or complex plasma, refers to the combination of micron-sized dust particles with plasma, which provides the individual particle tracking capability. In the typical laboratory conditions, these dusts are highly charged in plasma, interacting with each other through the Yukawa repulsion [33], which can form a single layer suspension, i.e., two-dimensional (2D) dusty plasma, due to the electric field in the sheath. When the potential energy between two nearest neighboring particles is higher than the average kinetic energy, as for most cases of laboratory dusty plasmas, it is defined as the strong coupling [34], while the reverse is the weak coupling. During experiments, the collection of tens of thousands of dust particles exhibits the typical collective solid- and liquidlike behaviors [24–32]; as a result, various physics procedures in liquids, like the momentum transport of viscosity, can be studied at the atomistic scale in dusty plasmas [35–41]. Due to easily adjusted parameters or conditions, computer simulations of Yukawa liquids and solids play an important role in the dusty plasma investigations.

II. SIMULATION METHODS

We perform equilibrium molecular dynamics (MD) simulations [42,43] of 2D Yukawa liquids to mimic 2D dusty plasmas as in [43], with the equation of motion for each particle as $m\ddot{\mathbf{r}}_i = -\nabla\Sigma\phi_{ij}$. As in 2D dusty plasmas, the interparticle interaction term is specified as the Yukawa repulsion [33] $\phi_{ij} = Q^2\exp(-r_{ij}/\lambda_D)/4\pi\epsilon_0 r_{ij}$, where λ_D is the Debye length and r_{ij} is the distance between the particles i and j. We simulate $N = 4096$ dust particles constrained within a rectangular box with the periodic boundary conditions. The simulation parameters are specified in the liquid state, i.e., with the coupling parameter Γ varying from 0.1 to about the corresponding melting point Γ_m [44] for each of the three values of $\kappa = 0.75$, 1, and 2. For each simulation run, first we run 2×10^6 steps using the Nosé-Hoover thermostat to reach the specified conditions of Γ and κ. Then, we turn off the

*fengyan@suda.edu.cn

thermostat to integrate the next 10^6 steps, with the obtained data used for the viscosity calculation presented here. Note, as in [45], our time step is chosen to be small enough, so that the fastest particle cannot move beyond the distance of $a/2000$ in one step, and the energy conservation is adequately obeyed for our simulation data. Other simulation details are the same as in [43].

Traditionally [27–32], we use the screening parameter $\kappa = a/\lambda_D$ and the coupling parameter $\Gamma = Q^2/(4\pi\epsilon_0 a k_B T)$ to characterize 2D Yukawa liquids, where $a = (n\pi)^{-1/2}$ is the Wigner-Seitz radius for the areal number density of n. In our simulations, the specified conditions are always in the typical liquid state, i.e., the chosen Γ values are always $<\Gamma_m$, where Γ_m is the melting point for the corresponding κ value [44].

III. RESULTS AND DISCUSSIONS

A. Universal scaling laws of viscosity and speed ratio

Viscosity of 2D dusty plasmas has been quantified in various experiments [35–41] and simulations [41,45–55]. The random thermal motion of individual particles in liquids is often used to quantify the viscosity from the Green-Kubo relation [46–53] of $\eta_{GK} = (\int_0^\infty \langle P_{xy}(t)P_{xy}(0)\rangle dt)/(Ak_BT)$, where P_{xy} is the off-diagonal element of the stress tensor [4], and A is the studied area. In experiments [35–39], viscosity is determined from either the velocity profile fitting [35–37] or its definition directly [38,39]. In simulations [48], viscosity is also quantified from the SLLOD [56] and the introducing momentum methods. These obtained viscosity values from 2D dusty plasma experiments and 2D Yukawa simulations [35–41,45–55] using various methods are well consistent with each other.

The previous viscosity investigations [21,23,35,46–48,55] indicate that, as the temperature varies, the viscosity of 2D or 3D Yukawa liquids always exhibits a minimum at an intermediate temperature. In [21,23,46,47], this crossover of the viscosity variation is attributed to the temperature dependence of the kinetic and potential contributions in the Green-Kubo relation. However, a quantitative physics picture of this variation, or the viscosity transition, is still unclear. Furthermore, the microscopic atomic origin of viscosity in the typical liquid state of any physical system is also unknown. In this paper, we focus on the physical mechanism of the viscosity transition in Yukawa liquids, to reveal the fundamental origin of the liquid viscosity.

Our shear viscosity results, obtained from the Green-Kubo relation with our 2D Yukawa liquid simulations, exhibit a universal scaling law for various κ values, as shown in Fig. 1. Here, our choice of the normalization for viscosity η_{GK}, $m\bar{v}_p n^{1/2}$, is suggested by the elementary kinetic theory for the dense medium of particles [57–60]. We normalize Γ using the melting point Γ_m as in [48].

From Fig. 1, the dimensionless viscosity $\eta_{GK}/(m\bar{v}_p n^{1/2})$ reaches its transition of minimum when $\Gamma/\Gamma_m = 0.05$. While $\Gamma/\Gamma_m > 0.05$, the viscosity increases monotonically with Γ; however, this variation trend is reversed when $\Gamma/\Gamma_m < 0.05$. Note, a scaling law of viscosity is also demonstrated in [48] using a different normalization for viscosity, with the data well agreeing with our current results, as presented next. We obtain

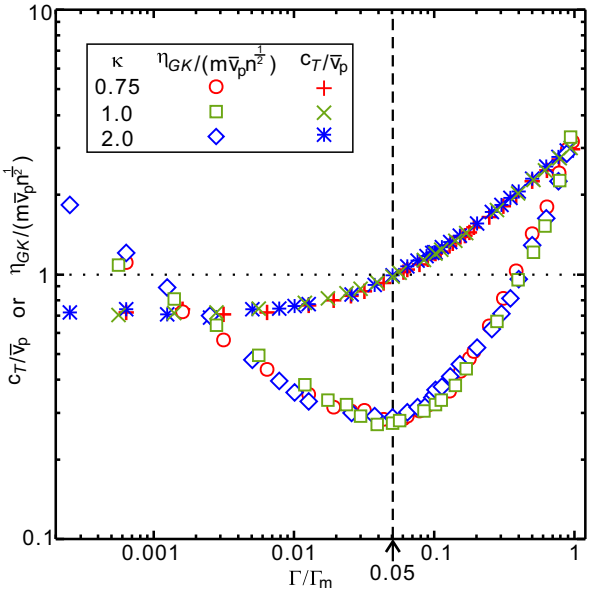

FIG. 1. Obtained shear viscosity $\eta_{GK}/(m\bar{v}_p n^{1/2})$ of 2D Yukawa liquids, as well as the ratio of the instantaneous transverse sound speed to the average particle speed $C_T/\bar{v}_p$, while the coupling parameter Γ and the screening parameter κ vary. A universal scaling law is well demonstrated in the viscosity data by normalizing η_{GK} and Γ using $m\bar{v}_p n^{1/2}$ and Γ_m, respectively, where Γ_m is the corresponding melting point. The ratio of $C_T/\bar{v}_p$ also exhibits a universal law here. For 2D Yukawa liquids with various κ values, we discover that the minimum of $\eta_{GK}/(m\bar{v}_p n^{1/2})$ always occurs at $\Gamma/\Gamma_m = 0.05$, when the ratio of $C_T/\bar{v}_p$ is just unity. We attribute $C_T/\bar{v}_p = 1$ to the transition between the individual and cooperative dynamics. When $C_T/\bar{v}_p > 1$, the viscosity is determined by the cooperative dynamics of particles. Thus, as Γ increases, the interparticle interaction is enhanced, so that the momentum transport of the cooperative dynamics is more substantial, leading to the increase of viscosity. However, while $C_T/\bar{v}_p < 1$, the viscosity is dominated by the gaslike dynamics of individual particles; as a result, the momentum transport by individual dynamics is more substantially when Γ decreases, leading to the reasonable increase of viscosity then.

the viscosity data from [48] by capturing the data points in Fig. 3(a) of [48]. In Fig. 2, we plot the viscosity data for 2D dusty plasma liquids reported in [48] normalized by $m\bar{v}_p n^{1/2}$ with our results reported in Fig. 1. From Fig. 2, our results reported in Fig. 1 and the data points in [48] overlap with each other, clearly indicating that our obtained viscosity data well agree with the previous investigations of 2D Yukawa liquids [48].

To understand the mechanism of the viscosity transition with varying Γ values, we also present $C_T/\bar{v}_p$, i.e., the ratio of the instantaneous transverse sound speed $C_T = (G_\infty/\rho)^{1/2}$ [4] to the the average particle speed $\bar{v}_p$ [61] in Fig. 1. Here, $G_\infty = \langle (P_{xy}(0))^2\rangle/(Ak_BT)$ is the infinite frequency shear modulus [4], and $\rho = m/(\pi a^2)$ is the mass density. This ratio of $C_T/\bar{v}_p$ measures the relationship between cooperative and individual dynamics. Clearly, our $C_T/\bar{v}_p$ results for 2D Yukawa liquids also exhibit a universal law, which is surprisingly well obeyed by 3D Yukawa liquids too, as demonstrated next. This mysterious universal scaling law of $C_T/\bar{v}_p$ that we find

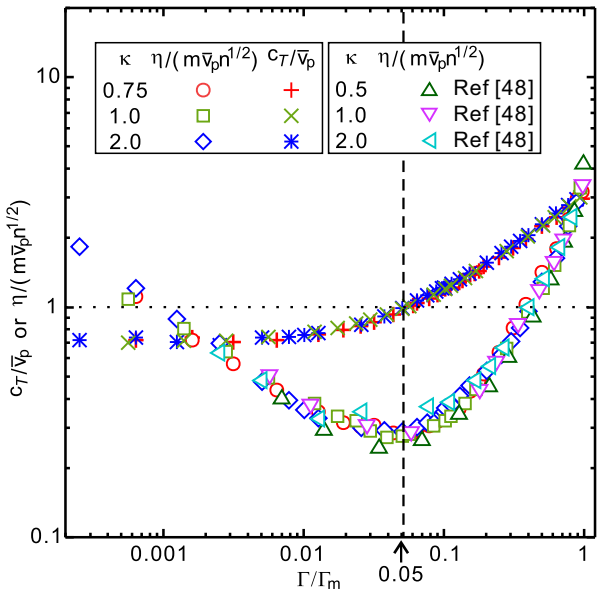

FIG. 2. Same data as in Fig. 1, combined with the viscosity values for 2D Yukawa liquids reported in [48]. Clearly, our obtained viscosity data for 2D Yukawa liquids well agree with the previous investigations of 2D Yukawa liquids [48].

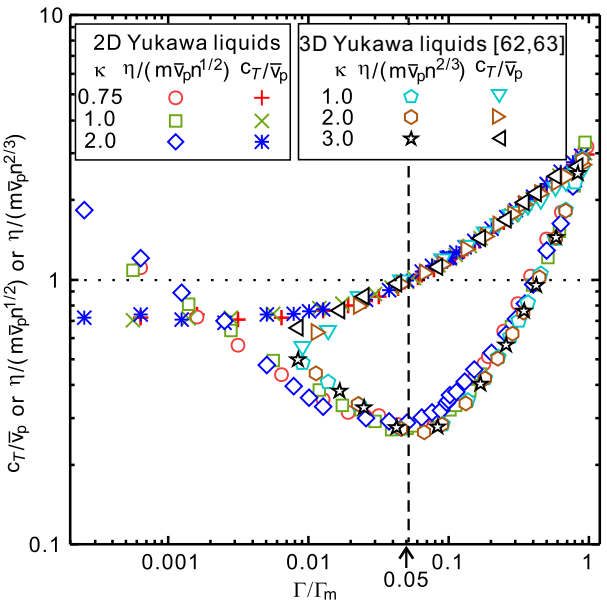

FIG. 3. Comparison of our obtained dimensionless viscosity and the ratio of $C_T/\bar{v}_p$ for 2D Yukawa liquids with those for 3D Yukawa liquids from [62,63]. While $\Gamma/\Gamma_m > 0.05$, all data points of the dimensionless viscosity for both 2D and 3D Yukawa liquids overlap with each other, which is also the same for the ratio of $C_T/\bar{v}_p$. These results clearly indicate that, when $\Gamma/\Gamma_m > 0.05$, the two physical quantities of the dimensionless viscosity and $C_T/\bar{v}_p$ both exhibit the universal scaling laws for 2D and 3D Yukawa liquids. These discovered dimensionality-independent scaling laws probably suggest that, while $\Gamma/\Gamma_m > 0.05$, the origin of the viscosity for 3D Yukawa liquids is the same as that for 2D Yukawa liquids. However, while $\Gamma/\Gamma_m < 0.05$, the results of the dimensionless viscosity and $C_T/\bar{v}_p$ for 3D and 2D Yukawa liquids seem to deviate a little bit, especially for $C_T/\bar{v}_p$. Note, to obtain the dimensionless viscosity for the comparison, the normalizations for 3D and 2D Yukawa liquids are slightly different as in [58–60].

here probably governs the fundamental dynamics of Yukawa liquids.

We compare our results of the dimensionless viscosity $\eta/(m\bar{v}_p n^{1/2})$ and $C_T/\bar{v}_p$ for 2D Yukawa liquids with those for 3D Yukawa liquids reported in [62,63]. We obtain the viscosity data for 3D Yukawa liquids by capturing the data points in Figs. 3(a), 4(a) and 5(a) of [62]. By capturing the data points in Fig. 5(a) of [63], we obtain the Maxwell relaxation time τ_M for 3D Yukawa liquids, so that we calculate the corresponding instantaneous transverse sound speed C_T using $C_T = [\eta/(\rho\tau_M)]^{1/2}$, since $\tau_M = \eta/G_\infty$ and $C_T = (G_\infty/\rho)^{1/2}$ from [4]. Thus, we achieve all data of the dimensionless viscosity and $C_T/\bar{v}_p$ for 3D Yukawa liquids from [62,63]. Note, as in [58–60], to obtain dimensionless viscosity, the normalizations of viscosity η_{GK} for 3D systems is $m\bar{v}_p n^{2/3}$, which is slightly different from $m\bar{v}_p n^{1/2}$ for 2D systems.

In Fig. 3, we plot the achieved dimensionless viscosity $\eta/(m\bar{v}_p n^{2/3})$ and the ratio of $C_T/\bar{v}_p$ for 3D Yukawa liquids from [62,63] with our results for 2D Yukawa liquids reported in Fig. 1. From Fig. 3, when $\Gamma/\Gamma_m > 0.05$, all data points of the dimensionless viscosity for both 2D and 3D Yukawa liquids overlap with each other. Similarly, in this cooperative regime, all data points of the ratio of $C_T/\bar{v}_p$ for both 2D and 3D Yukawa liquids also overlap with each other. That is to say, in this cooperative regime of $\Gamma/\Gamma_m > 0.05$, we discover the universal scaling laws of the dimensionless viscosity and the ratio of $C_T/\bar{v}_p$ for Yukawa liquids, valid both for 2D and 3D systems. These discovered dimensionality-independent scaling laws probably suggest that, when $\Gamma/\Gamma_m > 0.05$, the origin of the viscosity for 3D Yukawa liquids is the same as that for 2D systems. However, while $\Gamma/\Gamma_m < 0.05$, the results of the dimensionless viscosity and $C_T/\bar{v}_p$ for 3D and 2D Yukawa liquids seem to deviate a little bit, especially for $C_T/\bar{v}_p$. Since there are not enough data within $\Gamma/\Gamma_m < 0.05$ for 3D Yukawa liquids in [62,63], and the individual dynamics regime is beyond the scope of this paper, we do not draw any conclusions in the regime of individual dynamics for 3D Yukawa liquids either.

As the major result of this paper, we discover that the dimensionless viscosity $\eta_{GK}/(m\bar{v}_p n^{1/2})$ for 2D Yukawa liquids reaches its transition of minimum when $C_T/\bar{v}_p = 1$, as shown in Fig. 1. In fact, the condition of $C_T/\bar{v}_p = 1$ just corresponds to the transition between the cooperative and individual dynamics. When $C_T/\bar{v}_p > 1$, i.e., the instantaneous transverse sound speed is higher than the average particle speed, the momentum transport through transverse phonons plays the crucial role, so that the viscosity is dominated by the cooperative dynamics of particles. Thus, as Γ increases, the interparticle interaction becomes stronger, so that the momentum transport from the cooperative dynamics is more substantial, leading to the increase of viscosity, as the right branch of $\eta_{GK}/(m\bar{v}_p n^{1/2})$ shown in Fig. 1. However, while $C_T/\bar{v}_p < 1$, i.e., the average particle speed exceeds the instantaneous transverse sound speed, the momentum transport mainly relies on the gaslike dynamics of individual particles, leading to the reasonable increase of viscosity while

Γ decreases, as the left branch of $\eta_{GK}/(m\bar{v}_p n^{1/2})$ in Fig. 1 shows. Another striking point is that our discovered viscosity transition at $C_T/\bar{v}_p = 1$ in 2D Yukawa liquids is also valid for 3D Yukawa liquids, as presented above, further suggesting that this viscosity transition at $C_T/\bar{v}_p = 1$ has the fundamental physics significance.

B. Lifetime of local atomic connectivity

To study the mechanism of viscosity at the atomic/molecular scale, we calculate the lifetime of the local atomic connectivity τ_{LC}. As in [18,64], τ_{LC} describes the time for the atomic topological structure change, or the time for a particle to maintain its unchanged surrounding neighbors. We calculate τ_{LC} for our simulated 2D Yukawa liquids by tracking the neighbor list of each particle, where the neighbor is defined as the particle pair within the distance for the first minimum [18,64] of the radial distribution function $g(r)$ [1–4]. We assume that, in the initial configuration, there are $N(t_0)$ neighbors for the central particle, where t_0 is the initial reference time. As the time goes to $t_0 + t$, the neighbors of the central particle change, i.e., some of the initial neighbors are not its neighbors anymore, so that we can use $N(t_0 + t)$ to label the number of the initial neighbors which are still its neighbors at the time of $t_0 + t$. Thus, we define τ_{LC} as the time duration (relative to t_0) for the number of initial neighbors falls by 1 in the ensemble avarage, i.e., $\langle N(t_0)\rangle - \langle N(t_0 + t)\rangle = 1$ [18,64], for all central particles and the varying different initial time of t_0. Note, if one neighbor leaves the central particle for a while, and then comes back as a neighbor again, it is regarded as a new neighbor for the central particle. Thus, τ_{LC} can be regarded as the averaged time for the first of the initial neighbors of the central particle going beyond the distance of the first minimum of $g(r)$, or a reduction of the coordination number by one [64].

As shown in Fig. 4, our calculated τ_{LC} data for 2D Yukawa liquids, normalized by $a\bar{v}_p^{-1}$, also exhibit a universal scaling law. This scaling law of τ_{LC} is reasonable, since the normalization of $a\bar{v}_p^{-1}$ is just the timescale of the individual particle motion. The local atomic connectivity τ_{LC} is just the time for one particle to lose its original neighbors, which is reasonably caused by the individual particle motion. Note, our results of τ_{LC} here well agree with the data in [64].

The universal scaling law of $\tau_{LC}/(a\bar{v}_p^{-1})$ in Fig. 4 also contains a transition at $\Gamma/\Gamma_m = 0.05$, exactly the same condition of $C_T/\bar{v}_p = 1$ in Fig. 1. Clearly, $\tau_{LC}/(a\bar{v}_p^{-1})$ is a microscopic quantity; however, the dimensionless viscosity in Fig. 1 is the transport coefficient of fluids. The transitions of both the fluid coefficient and the microscopic topological structure at the same condition indicate that the fundamental mechanism of the viscosity probably can be interpreted from this atomistic diagnostic of τ_{LC}.

In Fig. 4, when $\Gamma/\Gamma_m < 0.05$, the value of $\tau_{LC}/(a\bar{v}_p^{-1})$ is nearly unchanged at $\approx$0.53. In fact, this value is just equivalent to the procedure of one particle, with the speed of $\bar{v}_p$, moving from the first maximum to the first minimum of $g(r)$ (just $\approx 0.53a$ for 2D Yukawa liquids), further confirming the individual dynamics dominates. Here, we provide our derivation of $\tau_{LC}/(a\bar{v}_p^{-1}) \approx 0.53$ when $\Gamma/\Gamma_m < 0.05$. From Fig. 5, for 2D Yukawa liquids with a constant κ, as the value

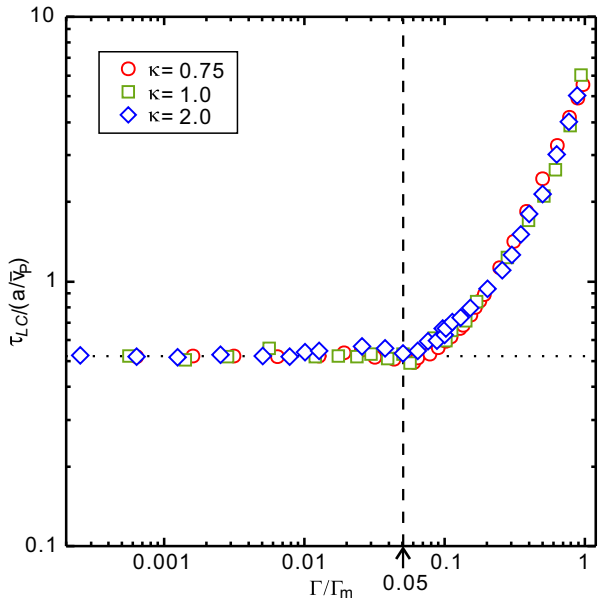

FIG. 4. Normalized lifetime of the local atomic connectivity $\tau_{LC}/(a\bar{v}_p^{-1})$ for 2D Yukawa liquids as Γ/Γ_m varies. For various κ values, our obtained data of $\tau_{LC}/(a\bar{v}_p^{-1})$ clearly exhibit a universal scaling law. Here, τ_{LC} is determined as the time for a particle to lose/gain one neighbor. When $\Gamma/\Gamma_m < 0.05$, the value of $\tau_{LC}/(a\bar{v}_p^{-1})$ is nearly unchanged, which just corresponds to the time for one particle moving from its location to the neighbor edge of the other particle, further verifying the individual dynamics dominates. When $\Gamma/\Gamma_m > 0.05$, the $\tau_{LC}/(a\bar{v}_p^{-1})$ increases monotonically with Γ. The transition of $\tau_{LC}/(a\bar{v}_p^{-1})$ at $\Gamma/\Gamma_m = 0.05$ just corresponds to $C_T/\bar{v}_p = 1$, i.e., the transition of viscosity in Fig. 1.

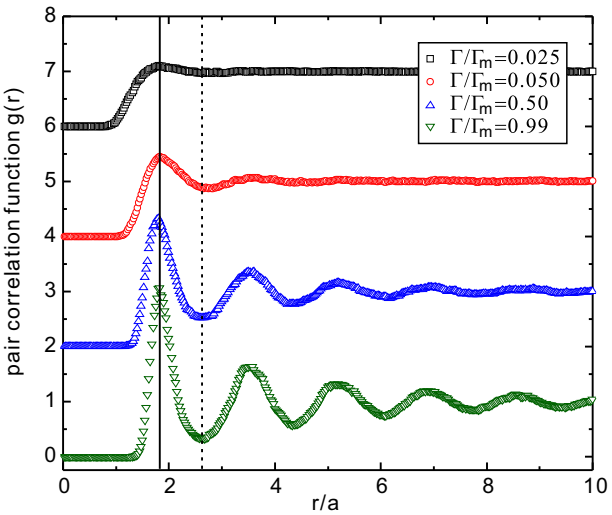

FIG. 5. Our calculated pair-correlation functions $g(r)$ of 2D Yukawa liquids for $\Gamma/\Gamma_m = 0.99$, 0.50, 0.050, and 0.025, respectively, while $\kappa = 2$. As the value of Γ decreases, or equivalently the temperature increases, the heights of peaks in $g(r)$ drop gradually. Except for $g(r)$ of the extremely low values of Γ whose maxima and minima are not very distinctive, the locations of the maxima and minima for $g(r)$ are nearly unchanged. For our calculated $g(r)$ of various Γ values, the locations of the first maximum and minimum are always at $r = 1.885a$ and $2.635a$, respectively, as the solid and dashed lines show.

of Γ decreases, the heights of peaks for the pair-correlation function $g(r)$ drop monotonically. However, the locations of the maxima (peaks) and minima of the pair-correlation function $g(r)$ are nearly unchanged, well agreeing with Fig. 1 of [65]. The locations of the first maximum and minimum of $g(r)$ are at $r = 1.885a$ and $2.635a$, respectively, so that the distance between them is just around $0.75a$. Thus, to calculate τ_{LC}, we define neighbors as the particle pair within the distance of $2.635a$, i.e., $r \leqslant 2.635a$. In the individual dynamics regime of $\Gamma/\Gamma_m < 0.05$, especially when Γ is very low, the pair-correlation function $g(r)$ has no distinctive maxima or minima anymore, just gradually increasing from 0 to the stable value of unity; however, our criterion of the particle pair of $r \leqslant 2.635a$ is still unchanged. Viewing from one central particle, in the range of $r \geqslant 1.885a$, other particles are nearly uniformly distributed with the number density of n. In addition, the particle velocity in one direction is just $\bar{v}_p/\sqrt{2}$ for our 2D systems. For a particle at the location r between $1.885a$ and $2.635a$, after it moves to the location of $2.635a$ in the radial direction with the speed of $\bar{v}_p/\sqrt{2}$, then it is not the neighbor of the central particle anymore. Thus, the lifetime of the local atomic connectivity τ_{LC} can be derived as the averaged time for all particles between $r = 1.885a$ and $2.635a$ to move outside of $r = 2.635a$ as

$$\tau_{LC} = \frac{1}{n(2.635a - 1.885a)} \int_{1.885a}^{2.635a} \frac{(2.635a - r)}{\bar{v}_p/\sqrt{2}} n\, dr$$
$$= \frac{\sqrt{2}}{0.75a\bar{v}_p} \int_{1.885a}^{2.635a} (2.635a - r) dr = 0.53\left(a\bar{v}_p^{-1}\right), \quad (1)$$

well agreeing with the obtained τ_{LC} in Fig. 4.

However, in Fig. 4, when $\Gamma/\Gamma_m > 0.05$, the value of $\tau_{LC}/(a\bar{v}_p^{-1})$ increases monotonically with Γ. To clarify this increase mechanism of $\tau_{LC}/(a\bar{v}_p^{-1})$, we also quantify the macroscopic viscoelasticity of liquids by calculating the Maxwell relaxation time [4] using $\tau_M = \eta/G_\infty$, as presented next.

C. Origin of viscosity

In Fig. 6, we find that our calculated τ_{LC}/τ_M for various 2D Yukawa liquids also exhibit a universal law as the values of Γ and κ vary. The ratio of τ_{LC}/τ_M connects the microscopic quantity τ_{LC} with the fluid quantity τ_M. An interesting feature here is that τ_{LC}/τ_M is just around unity when $\Gamma/\Gamma_m = 0.05$. That is to say, while $\Gamma/\Gamma_m < 0.05$, $\tau_{LC} < \tau_M$ corresponds to the individual dynamics regime; however, while $\Gamma/\Gamma_m > 0.05$, then $\tau_{LC} > \tau_M$ corresponds to the cooperative dynamics regime, as we interpret above. The same transition of τ_{LC}/τ_M here as that of $C_T/\bar{v}_p$ in Fig. 1 suggests the mechanism connection between τ_{LC}/τ_M and $C_T/\bar{v}_p$.

The most striking feature in Fig. 6 is that, when $\Gamma/\Gamma_m > 0.05$, all data points of τ_{LC}/τ_M and $(C_T/\bar{v}_p)^2$ overlap with each other. From this data overlapping, while $\Gamma/\Gamma_m > 0.05$, we are able to obtain $C_T^2\tau_M = \bar{v}_p^2\tau_{LC}$ for 2D Yukawa liquids, where $C_T^2\tau_M$ is just the kinematic viscosity η/ρ [35,41]. This expression clearly indicates that the momentum transport by transverse phonons is completed by the microscopic process of particles losing/gaining neighbors, at the atomistic level. However, while $\Gamma/\Gamma_m < 0.05$, the mechanism is not valid anymore, because the individual dynamics serve as the dominant momentum transport mechanism [21–23].

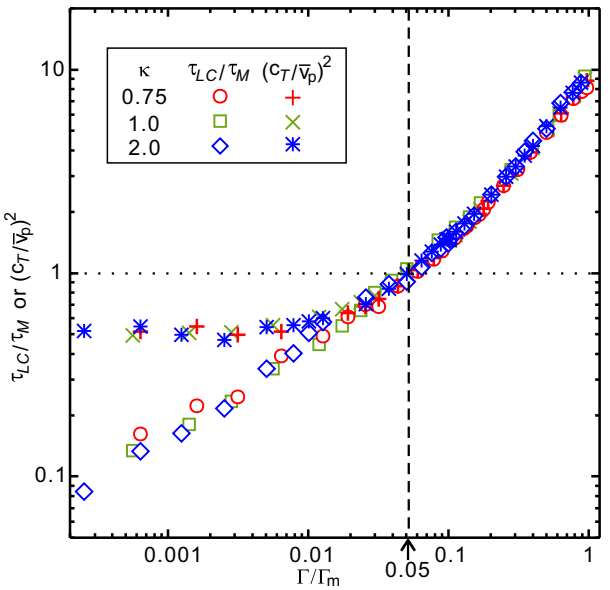

FIG. 6. Obtained ratio of the lifetime for local atomic connectivity τ_{LC} to the Maxwell relaxation time τ_M, and the square of the ratio $C_T/\bar{v}_p$, for various conditions of 2D Yukawa liquids. While $\Gamma/\Gamma_m > 0.05$, all data points of τ_{LC}/τ_M and $(C_T/\bar{v}_p)^2$ overlap with each other, indicating that $\tau_{LC}/\tau_M = (C_T/\bar{v}_p)^2$. This equation is equivalent to $C_T^2\tau_M = \bar{v}_p^2\tau_{LC}$, which suggests that the momentum transport by instantaneous transverse phonons in fluids (left-hand side) can be be expressed as the momentum transport by exchanging neighbors at the atomistic/kinetic level (right-hand side).

As the main conclusion of this paper, from our obtained $C_T^2\tau_M = \bar{v}_p^2\tau_{LC}$ in Fig. 6, we achieve the expression of viscosity for 2D Yukawa liquids at the atomistic/kinetic level as

$$\eta_{LC} = \rho\bar{v}_p^2\tau_{LC}. \quad (2)$$

Equation (2) provides the atomic origin of viscosity for 2D Yukawa liquids in the cooperative dynamics regime of $\Gamma/\Gamma_m > 0.05$. For metallic liquids at extremely high temperatures [18–20], the viscosity is found to be induced by the change of the local topological structure of the atomic connectivity network. Here, based on our obtained Eq. (2), it seems that this atomic picture of the local topological structure changing for viscosity is also applicable for our 2D Yukawa liquids at lower temperatures, or in the cooperative dynamics regime. From Eq. (2), the viscosity can be interpreted as the momentum transfer process of exchanging neighbors between particles, or gaining and losing neighbors for individual particles, i.e., while one particle loses a neighbor, another particle gains a new neighbor. In fact, from Eq. (2), we can also obtain the microscopic information of τ_{LC} directly from the fluid transport coefficient of viscosity. However, when $\Gamma/\Gamma_m < 0.05$, Eq. (2) is not applicable anymore, and the corresponding viscosity should be estimated using various theories related to the particle collisions as in [21–23].

As the minor conclusion from all figures above, we also obtain the transition point $\Gamma/\Gamma_m = 0.05$ between the cooperative and individual dynamics for 2D Yukawa liquids, no

matter how κ varies. This transition point is equivalent to $\approx$20 times of the corresponding melting point of the 2D Yukawa liquid, which can be clearly identified from the variation trends of both the viscosity η and the lifetime of the local atomic connectivity τ_{LC}. At this transition point, the ratio of $C_T/\bar{v}_p$ just equals unity, providing a clear physics picture that the contributions of the cooperative dynamics and individual dynamics are just comparable. Another interesting point is that, our obtained transition point of $\Gamma/\Gamma_m = 0.05$ for 2D Yukawa liquids is also surprisingly applicable to 3D Yukawa liquids, as presented above. We suggest that, instead of the traditional $\Gamma = 1$ [34], the condition of $\Gamma/\Gamma_m = 0.05$ could be considered as a new criterion to distinguish the strong- and weak-coupling regimes for Yukawa liquids, since it contains the fundamental physics significance. Note, besides this transition, the melting points of 2D and 3D Yukawa systems also surprisingly correspond to the same value of $C_T/\bar{v}_p = 3.1$ from Figs. 1 and 3.

IV. CONCLUSION

In conclusion, from our obtained universal scaling laws using MD simulations, we find that the variation transition of the dimensionless shear viscosity for Yukawa liquids always occurs at $C_T/\bar{v}_p = 1$, i.e., the instantaneous transverse sound speed C_T equals the average particle speed $\bar{v}_p$. When $C_T < \bar{v}_p$, the viscosity η_{GK} is mainly determined by the dynamics of individual particles. However, while $C_T > \bar{v}_p$, the cooperative dynamics become dominant. We discover that, for Yukawa liquids in the cooperative dynamics regime, the viscosity can be analytically expressed using the lifetime of the local atomic connectivity, i.e., Eq. (2), which provides the physics picture of viscosity at the atomistic scale. From this expression, the microscopic origin of the fluid/continuum transport coefficient of viscosity is just the momentum transfer process of losing/gaining neighbors for individual particles. We also suggest that the transition between the individual and cooperative dynamics of $C_T/\bar{v}_p = 1$, or equivalently $\Gamma/\Gamma_m = 0.05$, can be considered as a new criterion to distinguish the strong- and weak-coupling regimes for Yukawa liquids. Future investigations may be performed later to verify our analytical expression of viscosity, Eq. (2), and the scaling laws for other liquids with the different interparticle interactions.

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