

Shear modulus of two-dimensional Yukawa or dusty-plasma solids obtained from the viscoelasticity in the liquid state

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Langevin dynamical simulations of two-dimensional (2D) Yukawa liquids are performed to investigate the shear modulus of 2D solid dusty plasmas. Using the known transverse sound speeds, we obtain a theoretical expression of the shear modulus of 2D Yukawa crystals as a function of the screening parameter κ , which can be used as the candidate of their shear modulus. The shear relaxation modulus $G(t)$ of 2D Yukawa liquids is calculated from the shear stress autocorrelation function, consisting of the kinetic, potential, and cross portions. Due to their viscoelasticity, 2D Yukawa liquids exhibit the typical elastic property when the time duration is much less than the Maxwell relaxation time. As a result, the infinite frequency shear modulus G_∞ , i.e., the shear relaxation modulus $G(t)$ when $t = 0$, of a 2D Yukawa liquid should be related to the shear modulus of the corresponding quenched 2D Yukawa solid (with the same κ value), with all particles suddenly frozen at their locations of the liquid state. It is found that the potential portion of the infinite frequency shear modulus for 2D Yukawa liquids at any temperature well agrees with the shear modulus of 2D Yukawa crystals with the same κ obtained from the transverse sound speeds. Thus, we find that the shear modulus of 2D Yukawa solids can be obtained from the motion of individual particles of the corresponding Yukawa liquids using their viscoelastic property.

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I. INTRODUCTION

The shear modulus G , also called the modulus of rigidity, is the elastic property of a solid to respond to a shear. It is one of several important quantities to measure the stiffness of materials, like Young's modulus, Poisson's ratio, and the bulk modulus [1]. For typical materials, the shear modulus G can be determined by measuring the deformation of a solid by applying one force parallel to one surface, and the other opposite force on its opposite surface [1]. The equation of the shear modulus is defined as $G = \frac{\tau_{xy}}{\gamma_{xy}}$, where τ_{xy} and γ_{xy} are the shear stress and shear strain, respectively. Here, the shear stress $\tau_{xy} = F/A$, where A is the area on which the force F acts. Several methods have been used to calculate the shear modulus in different physical systems. In colloidal crystals, their shear elastic modulus is usually measured through torsional resonance spectroscopy in which standing waves are excited when rotary oscillations are imposed on the colloidal crystals [2]. The shear modulus can also be obtained from the sound speed of the shear waves [3]. Liu and Goree also calculated the shear modulus of two-dimensional (2D) dusty plasmas directly from its definition (the ratio of shear stress and shear strain) in a simulation [3].

Dusty plasmas, the four component mixture of highly charged micron-sized dust particles, electrons, ions, and neutral gas atoms [4–9], have been widely studied in experiments

and simulations in the past decades. In a plasma, the sheath above the lower electrode has electric fields which can levitate and confine highly charged dust particles, so that they can self-organize into a single-layer suspension, called 2D dusty plasma [10]. The Yukawa potential can be used to describe the interaction between dust particles within this 2D plane [11,12], and these dust particles are strongly coupled due to the large interparticle potential energy provided by the large particle charge. As a result, a collection of these strongly coupled dust particles would exhibit collective behaviors of liquids and solids [13–19]. Many physical procedures of solid dusty plasmas have been studied, like melting [20], crystallization [21], structure stability [22], solid superheating [23], as well as elastic and plastic deformations [24,25]. Although it has solidlike properties, strongly coupled dusty plasma is extremely soft, so that the shear modulus of solid dusty plasma is much smaller than those of typical solids, like metals, or even colloidal crystals [26].

For liquid dusty plasmas, viscoelasticity has been quantified using the transverse current autocorrelation function [10] and the frequency-dependent complex viscosity [27,28]. The frequency-dependent complex viscosity has the real and imaginary parts, corresponding to the viscous and elastic properties, respectively [27–29]. Shear waves can propagate in our liquid dusty plasmas with a cutoff wave number [30,31], due to the elastic property of a liquid at a smaller length scale. At a shorter time scale of $t \ll \tau_M$ (where τ_M is the Maxwell relaxation time [28]), a liquid would exhibit the typical elastic behaviors [27,28,31] also. In principle, we should be able to obtain the elastic property of a liquid, like the shear modulus,

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through the viscoelasticity at the specific spatial and temporal scales.

This paper is organized as follows. In Sec. II, we introduce our Langevin dynamical simulation method. In Sec. III, we first derive the shear modulus of 2D Yukawa crystals, obtained from the transverse sound speeds over a wide range of the screening parameter κ . Then, we present our finding to calculate the shear modulus of a 2D Yukawa solid, using the individual particle motion from the viscoelasticity of a Yukawa liquid with the same κ value, no matter what temperature. After verifying the reliability of our finding in the Yukawa or dusty-plasma system, we also provide our physics interpretation of this finding. Finally, we give a brief summary.

II. SIMULATION METHODS

We use Langevin dynamical simulations to mimic 2D dusty plasmas, with the equation of motion for dust particle i of

$$m\ddot{\mathbf{r}}_i = -\nabla\Sigma\phi_{ij} - \nu m\dot{\mathbf{r}}_i + \xi_i(t). \quad (1)$$

Here, the first term on the right-hand side, $-\nabla\Sigma\phi_{ij}$, is the binary interparticle interaction, which is the Yukawa potential of $\phi_{ij} = Q^2 \exp(-r_{ij}/\lambda_D)/4\pi\epsilon_0 r_{ij}$ (Q is the charge of each dust particle, λ_D is the screening length, and r_{ij} is the distance between dust particles i and j). The other two terms of $-\nu m\dot{\mathbf{r}}_i$ and $\xi_i(t)$ are the frictional drag and the Langevin random kicks, respectively.

We use two dimensionless parameters to characterize our simulated 2D dusty plasmas, the screening parameter κ and the coupling parameter Γ . Here, $\kappa = a/\lambda_D$, where $a = (\pi n)^{-1/2}$ is the Wigner-Seitz radius with n the areal number density. The other parameter Γ is defined as $\Gamma = Q^2/(4\pi\epsilon_0 a k_B T)$, the ratio of the potential energy between two neighboring particles and the averaged kinetic energy of a single particle, where T is the kinetic temperature of dust particles and k_B is the Boltzmann constant. We can use the inverse of the nominal 2D dusty plasma frequency, $\omega_{pd}^{-1} = (Q^2/2\pi\epsilon_0 m a^3)^{-1/2}$, to normalize the time scale, and use the Wigner-Seitz radius a or the lattice constant b to normalize the length scale. Note that, for 2D triangular crystals as for 2D dusty-plasma solids, $b \approx 1.9a$.

In our simulation, the total $N = 1024$ particles are constrained within a rectangular box with the dimensions $61.1a \times 52.9a$ in the xy plane using the periodic boundary conditions. For our simulation conditions, we vary κ from 0.5 to 3.0, and choose the value of Γ as either the constant of $\Gamma = 8, 20$, and 68 (the typical liquid regime) or the melting points [32] for the corresponding κ , while the gas damping rate is specified to $\nu = 0.027\omega_{pd}$, a typical experimental value. The time step is chosen between $0.0093\omega_{pd}^{-1}$ and $0.037\omega_{pd}^{-1}$ depending on the Γ value, as justified in [33]. For each simulation run, we begin with a random configuration of dust particles and integrate more than 3×10^5 time steps at a desired temperature to achieve the final steady state. Then, we record the positions and velocities of all dust particles in the next 10^6 steps for the later data analysis. Other simulation details are the same as [34].

III. RESULTS AND DISCUSSION

A. Shear modulus of Yukawa crystals obtained from transverse sound speeds

For a 2D crystal or solid, the relationship between the shear modulus (G) and the transverse sound speed (C_t) is expressed as [1,35]

$$G = \rho C_t^2, \quad (2)$$

where ρ is the mass density and C_t is the transverse sound speed. For our 2D dusty plasmas, $\rho = \frac{m}{\pi a^2}$, where m is the mass of one dust particle. The longitudinal and transverse sound speeds of 2D dusty-plasma crystals for different κ values have already been theoretically obtained, as shown in Fig. 12 of [36]. It is possible to use an analytical expression to phenomenologically fit these transverse sound speed data as a function of κ in [36]. We find that an expression of $C_t/(\sqrt{Q^2/4\pi\epsilon_0 m a}) = (0.374 - 0.0690\kappa^{1.11})$ can work as the phenomenological fitting of the transverse sound speed [36] of a Yukawa crystal very well.

Our obtained result of the shear modulus G of 2D dusty-plasma crystals is

$$G(\kappa)/(Q^2/4\pi\epsilon_0 a^3) = (0.211 - 0.0389\kappa^{1.11})^2, \quad (3)$$

which is derived from the combination of Eq. (2) and the fitting expression of the transverse sound speed above. As in [36], Eq. (3) should be reliable when the screening parameter κ varies from 0.0 to 3.5.

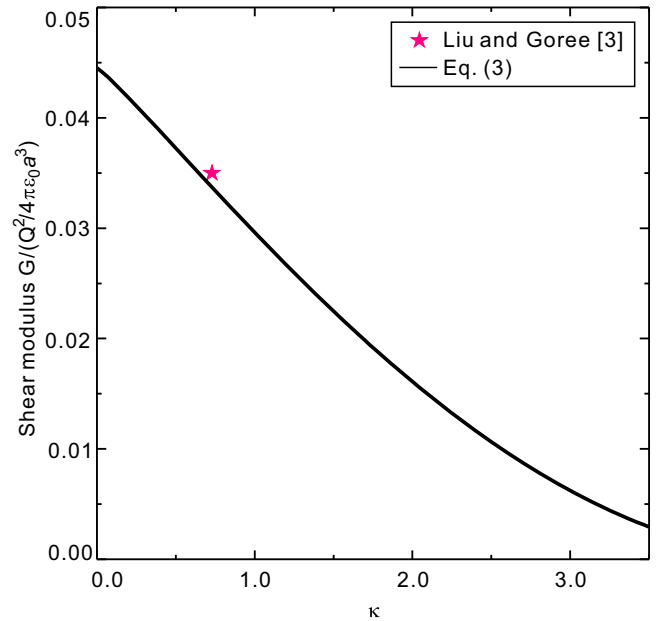


FIG. 1. The shear modulus of Yukawa crystals as a function of the screening parameter κ , Eq. (3), derived from the transverse sound speeds in [36]. The star indicates the shear modulus reported in [3], obtained from the definition of the shear modulus when $\kappa = 0.73$. The reported shear modulus in [3] agrees well with our obtained shear modulus results of Eq. (3). Later, this shear modulus expression of Eq. (3) can be used as the candidate of the shear modulus of 2D Yukawa crystals.

Figure 1 presents our obtained shear modulus of 2D Yukawa crystals of Eq. (3). Clearly, the shear modulus decays monotonically and substantially, as the screening parameter κ increases from 0.0 to 3.5. This is reasonable since, as the screening parameter κ increases, the shielding effect increases and the correlation between dust particles is weaker, so that the collection of dust particles is softer, similar to the bulk modulus [37]. We also plot the shear modulus data of 2D dusty plasmas, calculated from the definition of the shear modulus by manipulating a pair of laser beams in a simulation [3], marked as the star in Fig. 1. We can clearly see that the star nearly falls on the theoretical curve of Eq. (3). The shear modulus values obtained from these two different approaches are nearly the same, indicating that our obtained expression of the shear modulus of Eq. (3) should be reliable. In our literature search, we have not found any previous study of the shear modulus for 2D solid dusty plasmas over a wide range of κ values. We suggest that our obtained Eq. (3) above can work as a candidate of the shear modulus of 2D Yukawa crystals for future studies.

B. Shear relaxation modulus of 2D Yukawa liquids

The shear relaxation modulus is a typical property of a liquid, similar to viscoelasticity. We know that, while undergoing deformation, most materials would exhibit both viscous and elastic properties, which is called viscoelasticity [38]. The viscoelasticity of 2D liquid dusty plasma has been quantified using wave-number-dependent viscosity [10] and frequency-dependent viscosity [27,28]. Similarly, when undergoing time-dependent shear stress, these materials would exhibit time-dependent shear strain, indicating a time-dependent shear modulus, which is called the shear relaxation modulus [39]. For 2D systems, the shear relaxation modulus $G(t)$ can be written as

$$G(t) = \langle P_{xy}(t)P_{xy}(0) \rangle / Ak_B T, \quad (4)$$

where $P_{xy}(t)$ is defined as

$$P_{xy}(t) = \sum_{i=1}^N \left[mv_{ix}v_{iy} - \frac{1}{2} \sum_{j \neq i}^N \frac{x_{ij}y_{ij}}{r_{ij}} \frac{\partial \Phi(r_{ij})}{\partial r_{ij}} \right], \quad (5)$$

and A is the area of the studied system. The shear relaxation modulus of liquids, which is different from the shear modulus of solids, has been widely studied in polymers [40,41]. In polymer glasses [40], the correlation function may decay to a nonzero constant level of G_{eq} ; however, for typical liquids, this correlation function would decay to zero finally.

We calculate the shear relaxation modulus of 2D liquid dusty plasmas using our simulation data, as shown in Fig. 2. Here, we keep the temperature of liquid 2D dusty plasmas as a constant of $\Gamma = 68$, while changing the screening parameter κ from 0.5 to 3.0. From Fig. 2, we can find that, for 2D liquid dusty plasmas, the shear relaxation modulus $G(t)$ decays gradually to zero, not to a nonzero equilibrium value G_{eq} as in [40]. Note that, for a comparison, we use $Q^2/4\pi\epsilon_0 a^3$ to normalize the shear relaxation modulus, as for the theoretical expression of Eq. (3) in Fig. 1 above.

Viscoelastic materials would exhibit typical viscous or elastic properties at specific spatial and temporal scales.

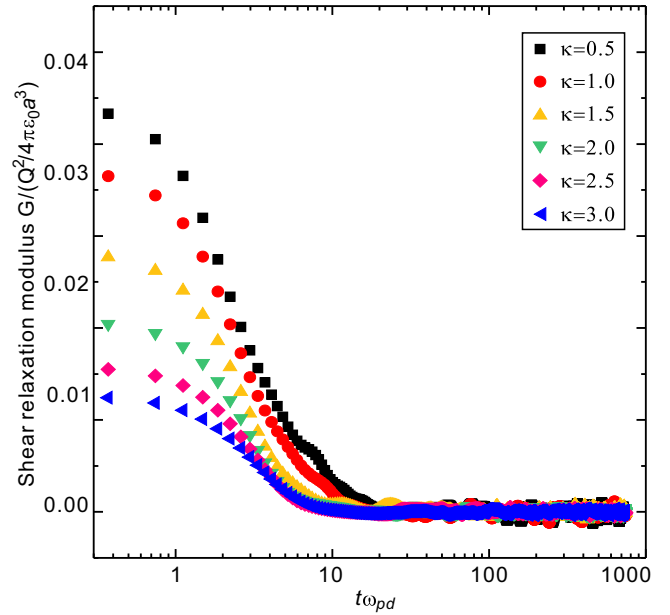


FIG. 2. Shear relaxation modulus $G(t)$ of 2D dusty plasmas with a constant liquid temperature of $\Gamma = 68$, while κ changes. Clearly, for 2D liquid dusty plasmas, the shear relaxation modulus $G(t)$ decays gradually to zero finally.

For example, transverse waves can still propagate with a cutoff wave number in our 2D liquid dusty plasmas [30,31]; that is to say, 2D liquid dusty plasmas exhibit the typical elastic property when the studied length scale is small enough. Also, when the time scale is small enough, much less than the Maxwell relaxation time τ_M , 2D liquid dusty plasmas would mainly exhibit the typical elastic property [28]. Following these results [28,30,31], we realize that 2D liquid dusty plasmas should exhibit the typical elastic property at smaller spatial and temporal scales.

Thus, we speculate that the shear relaxation modulus when $t\omega_{pd} = 0$, called the infinite frequency shear modulus G_∞ [or the instantaneous shear modulus $G(t=0)$] [42],

$$G_\infty = \langle (P_{xy}(0))^2 \rangle / Ak_B T, \quad (6)$$

of the liquid 2D dusty plasma should be related to the elastic property, such as the shear modulus of the solid dusty plasma. To compare the infinite frequency shear modulus G_∞ of Yukawa liquids with the obtained shear modulus of Eq. (3) for 2D Yukawa crystals above, we plot them together in Fig. 3. Clearly, they both nearly have the same trend, with nearly a constant difference, no matter how κ varies. We think probably this constant difference comes from the constant temperature of $\Gamma = 68$ in our simulations.

C. Our finding to determine shear modulus

To better understand the infinite frequency shear modulus G_∞ , we calculate its different contributions. The expression of the off-diagonal element of the shear stress $P_{xy}(t)$, Eq. (5), only has two parts, which are the kinetic part of $P_{xy}^{\text{kin}}(t) = \sum_{i=1}^N mv_{ix}v_{iy}$ and the potential part of $P_{xy}^{\text{pot}}(t) = -\frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \frac{x_{ij}y_{ij}}{r_{ij}} \frac{\partial \Phi(r_{ij})}{\partial r_{ij}}$ [42,43]. Thus, the shear relaxation

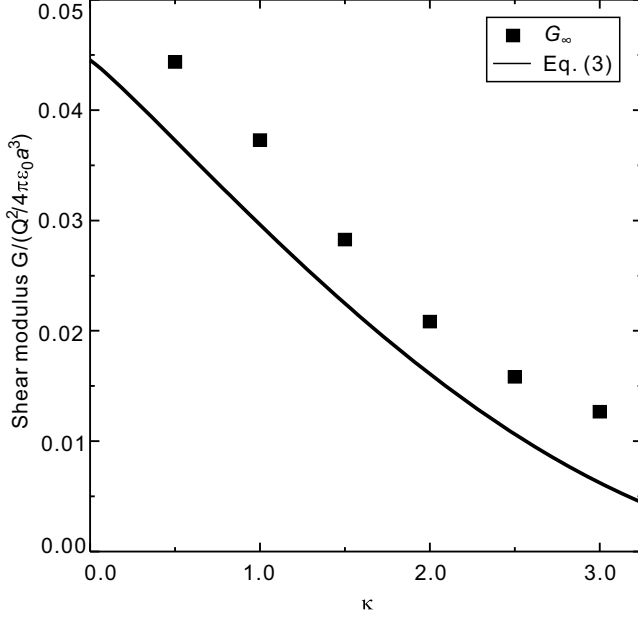


FIG. 3. A comparison of the infinite frequency shear modulus G_∞ from the simulation of 2D Yukawa liquids of $\Gamma = 68$ and the shear modulus of 2D Yukawa crystals of Eq. (3), for different κ values. They follow the same trend, but with nearly a constant difference, no matter how κ varies. This difference may come from the constant temperature of $\Gamma = 68$ in our simulations.

modulus $G(t)$ can be divided into three terms of the kinetic, potential, and cross portions. Thus, the three different components of the infinite frequency shear modulus G_∞ are

$$G_\infty^{kk} = \langle (P_{xy}^{\text{kin}}(0))^2 \rangle / Ak_B T, \quad (7)$$

$$G_\infty^{pp} = \langle (P_{xy}^{\text{pot}}(0))^2 \rangle / Ak_B T, \quad (8)$$

and

$$G_\infty^{kp} = \langle P_{xy}^{\text{kin}}(0)P_{xy}^{\text{pot}}(0) \rangle / Ak_B T, \quad (9)$$

corresponding to the kinetic, potential, and cross portions, respectively.

The three portions of the infinite frequency shear modulus of 2D liquid dusty plasmas, calculated from our simulation data, are compared in Fig. 4. Here, the candidate of the shear modulus of 2D Yukawa crystals of Eq. (3), obtained in Sec. III A, is also presented for the comparison. From Fig. 4, it is clear that the potential portion of the infinite frequency shear modulus, G_∞^{pp} , well agrees with Eq. (3) for 2D Yukawa crystals, while the kinetic portion G_∞^{kk} is almost constant for all conditions of various κ values and the cross portion G_∞^{kp} is almost zero. It seems that the comparison of the three portions in Fig. 4 would lead to a conclusion that probably the potential portion of the infinite frequency shear modulus, G_∞^{pp} , of 2D liquid dusty plasmas is equal to the shear modulus of the corresponding 2D solid dusty plasmas. This result verifies our previous speculation above (at the end of Sec. III B) that the difference between G_∞ and Eq. (3) in Fig. 3 comes from the constant temperature of $\Gamma = 68$ in our simulated liquid.

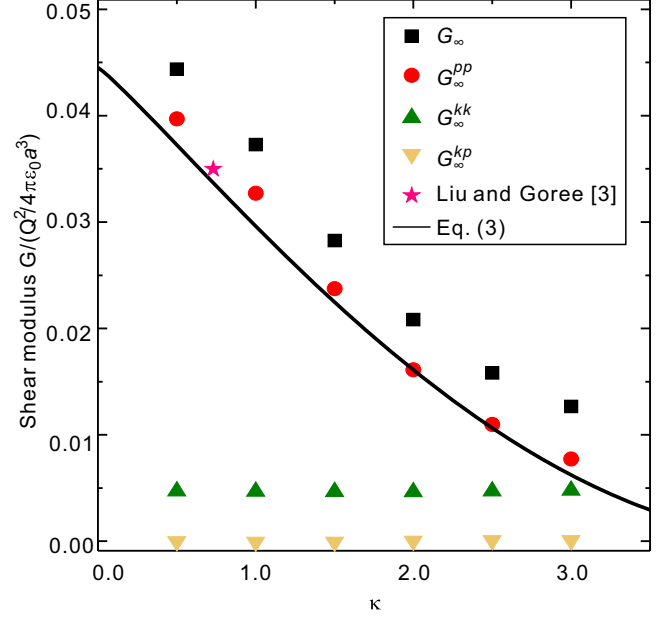


FIG. 4. Three components in the infinite frequency shear modulus, obtained from the simulation of 2D Yukawa liquids of $\Gamma = 68$ as presented in Fig. 3. These three components are the kinetic portion G_∞^{kk} , the potential portion G_∞^{pp} , and the cross portion G_∞^{kp} , respectively. Here, G_∞^{kp} is close to zero, which means that the correlation between the kinetic and the potential parts is negligible. Since in our simulation runs we specify a constant liquid temperature of $\Gamma = 68$, G_∞^{kk} is near unchanged for different κ values. The G_∞^{pp} almost fall on the obtained candidate of the shear modulus of 2D Yukawa crystals of Eq. (3). This result clearly suggests that the potential portion in the infinite frequency shear modulus G_∞^{pp} of a Yukawa liquid should be equivalent to the shear modulus of the corresponding quenched solid.

To further verify our conclusion that G_∞^{pp} in a 2D liquid dusty plasma can be used to calculate the shear modulus of the 2D solid dusty plasma, besides the coupling parameter of $\Gamma = 68$, we also perform studies with either higher temperatures, as shown in Figs. 5 and 6, or lower temperatures as in Fig. 6. Here, we perform Langevin simulations by specifying the temperatures as the higher temperatures (the lower Γ values) of $\Gamma = 20$ and 8, as in Figs. 5 and 6, and the lower temperatures of the corresponding melting points of Γ_m for various screening parameters κ from the phase transition diagram of 2D dusty plasmas [32]. In Fig. 5, we calculate the different components of the infinite frequency shear modulus of 2D liquid dusty plasmas as in Fig. 4, while at lower Γ values. Then we find that, at higher temperatures, the potential portion of the infinite frequency shear modulus of 2D liquid dusty plasmas, G_∞^{pp} , is not always larger than the kinetic portion G_∞^{kk} anymore. In Fig. 5(b), when $\Gamma = 8$, the kinetic portion always dominates, i.e., $G_\infty^{kk} > G_\infty^{pp}$ for our studied conditions. We can also clearly find that the symbols of the potential portion still fall around the solid curve, which is the obtained candidate of the shear modulus of 2D Yukawa crystals of Eq. (3), well consistent with our finding presented above. In Fig. 6, we plot the obtained potential portion of the infinite frequency shear modulus of 2D liquid dusty plasmas, G_∞^{pp} , at all studied temperatures presented above, as well as those at the melting points of Γ_m for different

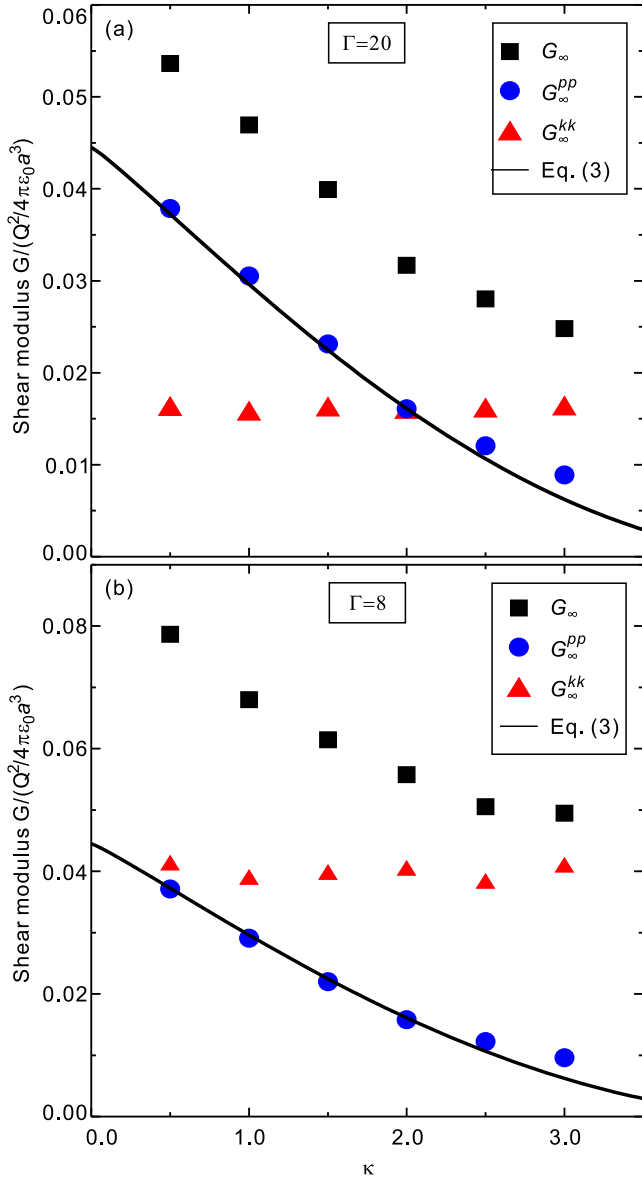


FIG. 5. The different components of the infinite frequency shear modulus for different higher temperatures of $\Gamma = 20$ (a) and $\Gamma = 8$ (b). At higher temperatures, the kinetic portion G_{∞}^{kk} becomes larger, even larger than the potential portion G_{∞}^{pp} for all data in (b). However, the results of the potential portion G_{∞}^{pp} still always fall around the solid curve, which is the obtained candidate of the shear modulus of the 2D Yukawa crystals of Eq. (3), well consistent with our finding of the shear modulus above.

screening parameters κ . Clearly, no matter what temperatures, at either the higher temperatures of $\Gamma = 8$ and 20, or the intermediate temperature $\Gamma = 68$, or even the lowest liquid temperature at the melting point Γ_m , the potential portion of the infinite frequency shear modulus, G_{∞}^{pp} , of 2D liquid dusty plasmas always well agrees with the the obtained candidate of the shear modulus of 2D Yukawa crystals of Eq. (3). Now, we are more confident to draw a conclusion that the shear modulus of 2D solid dusty plasmas can be calculated from the potential portion of the infinite frequency shear modulus G_{∞}^{pp} of 2D liquid dusty plasmas, no matter what temperature.

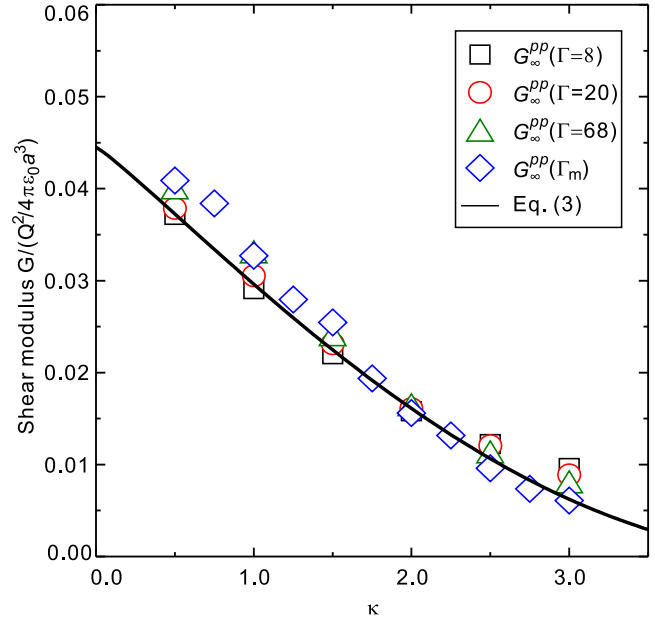


FIG. 6. The potential portion of the infinite frequency shear modulus G_{∞}^{pp} , obtained from the simulation of 2D Yukawa liquids at various conditions, i.e., different values for the coupling parameter of $\Gamma = 8$ (square), 20 (circle), and 68 (triangle) and the melting points Γ_m (diamond), while the screening parameter κ also changes. All these data well agree with the candidate of the shear modulus of 2D Yukawa crystals of Eq. (3). Thus, we can draw a conclusion that the shear modulus of 2D solid dusty plasmas can be obtained from the potential portion of the infinite frequency shear modulus G_{∞}^{pp} of 2D liquid dusty plasmas at any temperatures.

Probably this conclusion is valid not only for 2D Yukawa systems but also for other three-dimensional systems, such as soft condensed matter and colloidal systems.

Here, we provide our understanding of our finding using the potential portion of the infinite frequency shear modulus G_{∞}^{pp} of a liquid to determine the shear modulus of the corresponding solid here. The infinite frequency shear modulus of a liquid, G_{∞} , contains the potential, kinetic, and cross portions, where the cross portion is always negligible. If we only consider the potential portion of the infinite frequency shear modulus, G_{∞}^{pp} , that is to say, we remove the kinetic portion from G_{∞} , then it is equivalent to treat the liquid as the corresponding quenched solid, with all particles suddenly frozen at their locations in the liquid state. The infinite frequency means an extremely short time scale, which is just for the solid behaviors of the elasticity or shear modulus. Thus, the potential portion of the infinite frequency shear modulus, G_{∞}^{pp} , of this quenched solid would just reflect the shear modulus of this quenched solid. From all the above, it is reasonable that the potential portion of the infinite frequency shear modulus, G_{∞}^{pp} , of a liquid dusty plasma at any temperature can be used to determine the shear modulus of a solid dusty plasma at the same condition of the screening parameter of κ . We speculate that this conclusion, drawn from the 2D Yukawa system here, might be also valid for other systems, such as soft condensed matter and colloids, so that maybe further investigations in these systems could be performed in the future.

IV. SUMMARY

In summary, we performed Langevin dynamical simulations of 2D liquid dusty plasmas to study the shear modulus of 2D solid dusty plasmas. We presented our finding to determine the shear modulus of a solid dusty plasma from the potential portion of the infinite frequency shear modulus G_{∞}^{pp} of the liquid dusty plasma with the same screening parameter of κ , no matter what temperature. We also presented our understanding of the underlying physics of this finding: the G_{∞}^{pp} of the liquid dusty plasma is just equivalent to the shear modulus of the corresponding quenched solid dusty plasma. Besides this finding, using the previously obtained transverse sound speeds, we also obtained the shear modulus of 2D Yukawa crystals as a function of κ , Eq. (3), which might be a candidate of the shear modulus of 2D Yukawa

or dusty-plasma crystals. The results of the shear modulus of 2D solid dusty plasmas using different approaches agree with each other very well. We think probably our finding of using G_{∞}^{pp} to determine the shear modulus of a solid can also be applicable in other systems, so that further investigations in other physical systems are strongly suggested.

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