Thermal Conductivity Analysis of two-dimensional Complex Plasma Liquids and Crystals

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Abstract: A novel homogenous perturbed nonequilibrium molecular dynamics (HPMD) scheme, proposed by Evan-Gillan, has been employed to calculate the thermal conductivity of two-dimensional (2D) complex plasma liquids and crystals (CPLCs). The thermal conductivity has been reported using an improved HPMD method under the influence of constant external perturbation with different system sizes (N) and combinations of plasma parameters (Γ, κ). The current HPMD scheme provides precise outcomes with fast convergence for small-to-large N effects over a complete range of (Γ, κ). Temperature scaling law is tested for 2D thermal conductivity with appropriate Einstein frequency and found excellent behaviors. New simulations show that the thermal conductivity of CPLCs depends on (Γ, κ) and N and a slightly decreasing behavior is noted for thermal conductivity with increasing Γ and N but overall thermal conductivity becomes constant at intermediate-to-large Γ. The reported thermal conductivity obtained from present HPMD method, in the limit of low equilibrium perturbation, is established a reasonable agreement with that obtained from earlier known 2D numerical and experimental data. It is demonstrated that the present HPMD method is an alternative efficient

tool to compute the thermal conductivity of 2D CPLCs and can be suitable method for complete trends of complex plasmas.

Keywords: Thermal conductivity, complex plasma, molecular dynamics simulations, Einstein frequency, plasma parameters

I. INTRODUCTION

The technology developments have guided the demand to transport of fluid materials (and or devices) at micro- to nano-levels. There have been ongoing attempts in manufacturing micro- to nano-mechanical systems working in high thermal conductivity, however, high thermal conductivity of low dimensions is beyond our current microscopic machine technology.[1] Complex liquids are broad class of materials and binary combinations that can be coexistence between two phases such as, solid-gas (smoke, dust or granular matter), solid-liquid (colloidal suspensions, polymeric melts or dense solutions), liquid-gas (fog or foams), and liquid-liquid (vinegar). These complex liquids show remarkable outcomes to applied force due to the structural limitations that the phase coexistence enforces. The dynamics of such complex liquids are highly nonlinear in nature. The transport processes include thermal transport between liquid-like and solid-like behavior as well as transitions. The associated transport properties may be recognized as characteristics such as thermal response, thermal conductivity, order-disorder, thermal diffusivity, and clustering on various dimensions.[2] Currently, the dimensions of different devices (electronic and electro-mechanical) are reduced up to nanoscale dimensions where the thermal transport becomes relatively significant because thermoelectric, piezoelectric, photoelectric and thermogalvanic devices are demanded where considerable energy be wasted in a small region. On the other hand, for the thermal transport of complex liquid materials in real devices, the experimental observation of thermal transport becomes rather difficult and impossible for atomistic level devices.[3] Therefore; the development of reliable theoretical and computational techniques becomes current area of interest for predicting the thermal transport of microscopic to nanoscopic complex fluid materials and devices.

There are many two-dimensional (2D) physical systems, some of them at a microscopic scale that can be in ordered or disordered forms. These include a Wigner lattice of electron on the surface of liquid helium,[4] an array of vortices and dynamics of He mixed state of type-II superconductors,[5] colloidal suspensions,[6] ions confined magnetically in a penning trap,[7] dusty plasmas,[8, 9] Brownian's motion for 2D system of particles on water surface.[10] Determinatiuon of

thermal management of 2D CPLCs (having micron-size charged dust particles) is significant for numerical experiments and theories relevant to the fundamental study of physics and technology of plasmas, semiconductor and chemical industries, physics of polymers, nuclear energy generation, environmental/ space sciences, dense stars (dwarfs) and planetary interi ors (Jovian planets), highly ionized gases and even material processing through plasma.[11] However, the complex (dusty plasmas) liquids have obtained a remarkable interest as well the directions of engineering and science. Non-ideal complex systems (dusty plasmas) have opened up an entirely new line of research in the areas of applied plasma physics and technology development. In addition to ions, electrons, and neutrons in "ordinary" plasmas, dusty plasmas comprise of massive particles of nanometer to micrometer size. This extra heavy micron-size particle, having a wide range of values for the mass-to-charge ratio, is referred to as "dust" in the dusty plasma literature.[12] The existence of dust particle is predicted to result in novel effects in the thermal management of plasma with very weak external force and the dynamical behavior of dusty plasma is more complex than the dynamics of the gases and liquids.[13] Recently, different functional, statistical and mechanical approaches to the microscopic dynamical system theory of transport issues have been developed for simple and complex liquids.[14-16] In addition to fundamental properties, the investigations of microscopic information and estimations of transport processes of non-ideal complex physical systems are of particular interest for the development of micro- and nano technologies. The microscopic transport source of heat transfer processes, with and without an external force, is a basic problem in statistical mechanics with the derivation of improved equations of motion and fully homogenous physical systems as the alternative goal of many thermophysical researchers.[17]

Modern day high-performance computers are making available to scientist's solutions to transport problems of ever-increasing complexity. Computational methods are a fast-moving topic for resolving problems which only recent years ago were impossible, such as three-dimensional (3D) transient flows of polymeric liquids and thermal transport in low dimension devices. Non-isothermal non-Newtonian flows in 2D geometry of complex systems are now being tackled owing to the availability of parallel computers, adaptive methods and advances in constitutive modeling. Computational techniques trace the development of numerical methods for Newtonian and non-Newtonian flows. Moreover, with the help of these techniques, some important transport problems of academic and industrial interest are now treated in a detailed and

up-to-date exposition. Among all other numerous simulation techniques, molecular dynamic (MD) simulation is the best tool to investigate the transport properties of complex fluids (dusty plasmas). It provides the deep understanding of micro scale processes, especially for the thermal conductivity that is difficult property from the computational point of view because it is sensitive to internal energy of molecules.[18] Currently, it is a still challenging issue to extend the approach to the spatial and temporal scale of macroscopic heat transport phenomena. The two most frequently used approaches in molecular simulations are the "direct technique" and the Green–Kubo relations (GKRs). These simulation techniques are classified as non-equilibrium molecular dynamics (NEMD) and equilibrium molecular dynamics (EMD) simulations for the determination of transport properties of fluids. Practically, the heat transport is a non-equilibrium phenomenon and the direct simulation method (NEMD) of the heat transfer problem is much more preferred and faster.[19,20] Various earlier MD methods have been reported for the investigations of thermal conductivity and these are based on generally three NEMD techniques that use a temperature gradient,[21] a heat energy flux[22] and a homogeneous external force field technique.[23] The first two simulation methods have some disadvantages that are reported by Ciccotti *et al*.[24] In the last-mentioned technique, the impose perturbation is used in the equations of motion to generate required heat energy flow and the thermal conductivity is then obtained from the heat energy flux and external perturbation relationship.

This paper may be regarded as an update literature and unique method of thermal conductivity of the 2D complex plasmas (CPs) as compared to different molecular simulations and experimental techniques. One experimental group[25] with 2D crystalline complex plasmas investigated the heat transfer coefficients at kinetic level and standard parameters. Nosenko *et al*,[26] have been experimentally investigated the heat transport processes of the fluid dusty structures in 2D CPs (monolayer). Khrustalyov and Vaulina[27] numerically measured the heat transfer constants in 2D Yukawa systems with parameters close to conditions of dusty plasma laboratory experiments. A considerable amount of earlier theoretical studies and computer simulations have been done to understand the thermal conductivity in simple and molecular liquids (Refs.19-22,28, references therein). The homogenous NEMD (HNEMD) technique has long been employed and is well developed as an efficient tool in statistical mechanics and material sciences. Recently, Galamba and Nieto-de-Castro,[29] and Mandadapu *et al*,[30] extend the HNEMD method to calculate the thermal coefficients for ionic liquids and this method was

employed on a variety of issues such as for the estimation of rheological behaviors of fluids.[14,28] Wang *et al*,[31] and Mandadapu *et al*,[32] have developed a computer algorithm based on the HNEMD approach and compute the thermal conductivity of semiconductor materials with increasing external force field strengths. Moreover, in addition to theoretical and computational work for simple and ionic materials, a number of computer simulations have been reported to complement the experimental investigation of 2D and 3D strongly coupled CPs (SCCPs).[8,13,25,26] Pierleoni *et al*,[33] modified the HNEMD algorithm of the Evan-Gillan scheme and estimated the thermal conductivity of one component Coulomb plasma (OCCP). The thermal conductivity of 3D SCCPs was calculated by GKR-EMD simulation of Salin and Caillol,[34] variational procedure (VP) of Faussurier and Murillo,[35] and inhomogenous NEMD (InHNEMD) work of Donko and Hartmann,[36] Hou and Piel[37] performed NEMD simulation to investigate heat conduction in 2D SCCPs. Recently, Shahzad and He have employed the 2D and 3D HNEMD[1,11,16-18,38] and 3D homogenous perturbed MD (HPMD)[39] methods and computed the thermal conductivity of SCCPs. Very recently, dynamical structure factor of 3D SCCPs through HNEMD is reported by Shahzad and He.[40] Moreover, numerous calculations of the thermal properties have been studied for the behavior of 2D SCCPs in Refs.1,11,27,37,41, and transport properties have been considered for the behavior of 3D SCCPs.[34-40] A full understanding of 2D thermal conductivity and even of 3D strongly coupled dusty systems is still lacking. This shows the ongoing debate on the existence and nature of thermal coefficients of 2D SCCPs with alternative method through Yukawa interaction.

The main objective of present work is to calculate the normalized plasma thermal conductivity $\lambda_0(\Gamma, \kappa)$ in 2D complex plasma liquid and crystals (CPLCs) by using the unique technique,[39] under constant external perturbation, for various plasma state points (Γ, κ). This work provides more precise information's of 2D λ_0 through a novel HPMD method, with computational time cost-effective, in strongly-coupled (SC) CPLCs and can employ to other related physical systems. Very recently, we have been published some preliminary data for 2D SC-CPLCs,[42] where we have reported data with constant external perturbation and small N and small-intermediate range of ($\Gamma \equiv$ 1-100) for the λ_0. This paper also helps to review a current picture of $\lambda_0(\Gamma, \kappa)$ by varying the number of particles (N) from small-to-intermediate ($N \equiv$1024 to 14400) and large system sizes ($N \equiv$ 22500 to 64000), for the first time. It should be noted here that HPMD simulations take very long time and computational power for using such

intermediate-to-large system sizes. Moreover, this proposed HPMD method is used to study the performance of algorithm and compared the outcomes obtained to those obtained through 2D GK-EMD, NEMD, HNMED simulations and experimental results for the 2D SCCPs.

II. COMPUTATIONAL SCHEME

A. HPMD algorithm and thermal conductivity

In this subsection, we describe HPMD algorithm for calculating the thermal transport coefficient and it shows little close relation to experiment. This algorithm is found to be grossly efficient with results (for calculated thermal conductivity) and can also adapt different system size very efficiently. To simulate the behavior of dust particles in dusty plasma, the determination of a suitable interaction potential is critical. The best-known interaction model is the Yukawa interaction (screened Coulomb) potential for the description of pair interaction of repelling dust particles. In addition, Yukawa potential served as the interaction model to describe the pair wise interaction between dust particles and this interaction model is also used to describe the interactions that are present in many physical systems of interest, including biomedicine, astrophysics, chemical and biological systems, physics of polymers, hydrodynamics, and aerodynamics, materials for energy generation, colloidal suspensions, etc. The Yukawa interaction potential, a screened Columbic potential, is the most common model that is currently employed for investigating the interaction between charged dust grains (particles) *i* and *j* in dusty plasma system.[1,9,11,33-42]

$$\phi_{ij}(|\mathbf{r}|) = \frac{Q^2}{4\pi\varepsilon_0}\frac{e^{-|\mathbf{r}|/\lambda_D}}{|\mathbf{r}|}, \tag{1}$$

where λ_D represents the Debye screening length, r stands for the inter-particle spacing (of the dust particles), ε_0 denotes the permittivity of free space and Q is the charge on the dust particle. In present case, the Ewald Summations is considered in order to account for the pairwise interactions between dust particles and additional information is reported in our earlier work of Refs. 38, 39.

Thermal transport coefficient is obtained from well known GKRs of uncharged particles[14,15,19-24] and the corresponding transport relations with screened interaction model that may minimize the complexities usually faced when employing MD simulation to examine transport processes in complex dusty plasma systems. Well established GKRs of a simple fluid have been used to

compute the thermal conductivity of 2D and 3D SC-CPLCs and weekly coupled complex plasmas:[1,9,27,33-39]

$$\lambda = \frac{1}{2k_{\mathrm{B}}AT^2}\int_0^{\infty}\left\langle \mathbf{J}_Q(t).\mathbf{J}_Q(0)\right\rangle dt, \tag{2}$$

here, T is the system temperature, A is area of the system and k_{B} is the Boltzmann's constant. It is noted that the angular brackets <….> compute the average value (ensemble average) of all dust particles in the whole HPMD simulation run. In Eq. (2), $\mathbf{J}_Q$ is the microscopic form of heat energy vector and it is measured as

$$\mathbf{J}_Q A = \sum_{i=1}^{N}\left[E_i - \frac{1}{2}\sum_{i\neq j}(\mathbf{r}_i - \mathbf{r}_j).\mathbf{F}_{ij}\right].\frac{\mathbf{p}_i}{m}, \tag{3}$$

where the interparticle position vector is $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, total interparticle force is $\mathbf{F}_{ij}$ on particle i due to j, at time t, and momentum vector of the ith particle is $\mathbf{p}_i$. Here in Eq. (3), the total energy E_i of particle i (for $i \neq j$) is the sum of kinetic Energy ($p_i^2/2m$) and potential energy ($1/2\Sigma\ \phi_{ij}|\mathbf{r}|$), where $\phi_{ij}|\mathbf{r}|$ is the Yukawa pair potential between particles i and j, given in Eq. (1), and E_i is expressed as

$$E_i = \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\phi_{ij}\left|\mathbf{r}\right|. \tag{4}$$

According to the linear response theory the perturbed equations of motion, proposed by Evans-Gillan reported in Refs. 14, 20, 22, when perturbed by external filed $\mathbf{F}_{\mathrm{e}}(t)$, are expressed as

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m}, \tag{5}$$

and

$$\dot{\mathbf{P}}_i = \sum_{j=1}^{N}\mathbf{F}_i + \mathbf{D}_i(\mathbf{r}_i,\mathbf{p}_i).\mathbf{F}_e(t), \tag{6}$$

where, the total interparticle force acting on the particle i is $\sum_{j=1}^{N}\mathbf{F}_i = -\frac{\partial\phi_{ij}\left|\mathbf{r}\right|}{\partial r_i}$ and the tensorial phase space distribution function is $\mathbf{D}_i$ $\{(\mathbf{r}_i, \mathbf{p}_i), i = 1,2….,N\}$ with $\mathbf{r}_i$ and $\mathbf{p}_i$ are the position and momentum vectors of the i^{th} particle in an N-particle system. This function explains the coupling of the system to the external perturbation $\mathbf{F}_e(t)$.[14] Very recently, we have stated a detailed study

on the thermal conductivity expression for Yukawa system and the Ewald-Yukawa sums is discussed for the tensor element $\mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i)$ in the case of microscopic heat energy vector $\mathbf{J}_Q(t)$ of 2D and 3D Yukawa systems.[1,39-40,42] In order to established an equilibrium in the system, a thermostat is applied in the dynamics by included a term $\alpha\mathbf{p}_i$ to the right side of Eq. (6), here α is the Gaussian thermostat multiplier and can be obtained from Eq. (10) of our earlier work in Ref. 39. Thermal conductivity is obtained by choosing a external force parallel to the z-axis $\mathbf{F}_e(t) = \boldsymbol{\delta}(0, P_z)$, here, P_z is the external perturbation strength and $\boldsymbol{\delta}$ is Dirac delta function,

$$\lambda = \frac{1}{ATP_Z}\int_0^\infty \left\langle \mathbf{J}_{QZ}(t).\mathbf{J}_{QZ}(0)\right\rangle dt, \tag{7}$$

where, $\mathbf{J}_{Qz}$ is the z-component of heat flux vector, T is the system temperature and P_z is the external perturbation. The above mentioned Eq. (7) is the basic relation for computation of autocorrelation function (ACF) of heat energy current ($\mathbf{J}_{Qz}$) by applying an external perturbation P_z. The thermal conductivity parameter (λ) is obtained by measuring the thermal response of the Yukawa system under a suitable week external perturbation where signal-to-noise ratio is acceptable for all plasma parameters (Γ, κ). It is mentioned here that the perturbation is Dirac delta function, consequently, the heat flux vector response is proportional to ACF rather than time integral of function.[42] Very recently, Shahzad and He have given a comprehensive discussion on performance of thermal conductivity through thermal response of heat energy with week-to-moderate P_z and Ewald-Yukawa sums for microscopic heat energy vector[39]

B. Technique and parameters

This section presents the execution steps of the HPMD algorithm, Eq. (7), for calculating the thermal conductivity of SC-CPLCs that is described by employing Yukawa model to account for pair wise dust interactions. Three scaled parameters that can completely describe the SC-CPLCs:[1,20,38,39] first is plasma coupling (also known as Coulomb coupling), $\Gamma = (Q^2/4\pi\varepsilon_o)(1/ak_BT)$ parameter, here T denotes the system temperature and, $a = (n\pi)^{-1/2}$ represents the Wigner-Seitz (WS) radius[33-37] with n provides the number density ($n = N/A$) of dust particle, second scaled parameter is the screening (Debye screening) length, $\kappa = a/\lambda_D$, and the third additional scaled parameter is external perturbation strength for HPMD $F_e(t) = P_z a$. This additional parameter has normalized value $P^* = P_z a/J_{QZ}$, where J_{QZ} gives the thermal heat energy

along z-axis.[1] Moreover, the plasma dust frequency $\omega_p = (Q^2/2\pi\varepsilon_o ma^3)^{1/2}$ describes the time scale for SC-CPLCs, here m indicates the mass of dust particle.

The HPMD simulations are executed in the canonical ensemble (*NVT*) for small-moderate to large number of particles. In present case, it is chosen N = 1024-4096-14400-22500-32400 and 64000 using periodic boundary conditions (PBCs) and the minimum image convention of the dust particles. It is to be mentioned here that a sufficient time step is chosen in present HPMD simulations in order to conserve system thermal energy and an adequate simulation box size that allows computing meaningful quantity of measured thermal conductivity at long times. The different numbers of particles (small-intermediate-large) are enclosed in a computational cell of CPLCs with edge length L_y / L_z, and these particle numbers are sufficient to test a system size effects. The dimension of square simulation cell is $L_y\, a \times L_z\, a$. A Gaussian thermostat is used to maintain the system at constant temperature. It is tested here that the Gaussian thermostat performs more accurately than other thermostat (like Nose-Hoover) as for small-intermediate Yukawa systems.[1,38-40] The basic scheme for HPMD is to dynamically simulate equations of motion of the N-Yukawa dust particles with pair-wise interaction through screened Coulomb (Yukawa) potential given in Eq. (1). This includes producing the dust particles trajectories containing the SC-CPSLs system that is obtain by finding positions and momenta of dust particles *w.r.t* time step of $dt = 0.001/\omega_p$. The algorithm scheme used in MD computations is explained here. In the first step, input parameters are decided to explain the model. The appropriate Ewald-Yukawa sums, system temperature (inverse of plasma coupling), screening length, perturbation strength, number of particles, simulation time steps, total simulation run, etc are selected to meet the provisions of the 2D plasma thermal conductivity. In the second step, the force on an individual dust particle is computed from the interatomic potential by determining the negative derivative of the Yukawa interaction energy, i.e., $\mathbf{F}_i = -\frac{\partial \emptyset|\mathbf{r}|}{\partial r_i}$ (total force). The third step provides the information's of acceleration ($\mathbf{a}_i = \mathbf{F}_i / m_i$) of each dust particle by integrating Newton's equation of motions, using above calculated forces ($\mathbf{F}_i$). The velocities and displacements of each dust particles are calculated by subsequent integrations. Here, in our case, a well known predictor-corrector method is used for integrations.[9,11] The displacements yielded the new positions and this sequence is repeated over the specified time which outcomes in computing the trajectory of the SC-CPLCs. The most computational time-

consuming measurement of the interatomic interactions is minimized with an increase of P^* (external perturbation). Without using the subtraction method, the employed scheme is implemented through an appropriate value of external perturbation. The present HPMD simulations are performed between 3.5 x $10^5/\ \omega_p$ and 2.5 x $10^5/\ \omega_p$ time units (total simulation time) in the sequence of results recording for most of $\lambda_0(\Gamma, \kappa, N)$ on production stages. It should be noted here that our simulations are also carried out between 4.5 x $10^5/\ \omega_p$ and 1.5 x $10^5/\ \omega_p$ time units at specified $\lambda_0(\Gamma, \kappa)$ and small-intermediate N, in order to test the performance and consistency of employed method. It is observed that real space sum part alone computes results of $\lambda_0(\Gamma, \kappa, N)$ with enough efficiency and acceptable accuracy. In this article, the HPMD scheme is used for the plasma $\lambda_0(\Gamma, \kappa)$ of 2D SC-CPLCs for a whole range of plasma coupling ($1 \leq \Gamma \leq 300$), screening length ($1 \leq \kappa \leq 4$) and small-intermediate to large system sizes ($1024 \leq N \leq 64000$) that earlier employed for strongly coupled 2D complex plasmas.

III. SIMULATION RESULTS AND DISCUSSION

This section focused on the plasma coupling (temperature ≡ 1/ Γ), screening length (density) and particle number (N) dependence of thermal conductivity with suitable normalizations (ω_p and ω_E) for 2D CPLCs. Thermal conductivity of CPLCs with $\kappa \geq 1$ is studied at the plasma coupling range from $\Gamma \geq 10$. It should be mentioned here that the thermal conductivity normalized by plasma ($\lambda_0 = \lambda/nm\omega_p a^2$) and Einstein ($\lambda^* = \lambda/nm\omega_E a^2$) frequencies has already been used for the calculations of OCCPs[33] and SCCPs.[1,9,11,16-18,34-42] The reported plasma thermal conductivities are measured in the limit of suitable low value of normalized external perturbations ($P^* = P_z a/J_{QZ}$). Different sequences of HPMD are employed with an increasing and decreasing pattern of P^* in order to trace a more satisfactory low value of P^*, where signal to noise ratios are allowable over a whole range of plasma parameters (Γ, κ). In our case, the traceable normalized value of P^* (= 0.02) provides the steady state (near-equilibrium) values of plasma λ_0 within statistical limits, confirming the earlier numerical and experimental results.[1,8,11,25-27,37,41,42] However, it is noted that the HPMD algorithm gives noisy measurements mainly for $\Gamma < 10$ (κ = 1, 2, 3 and 4) at normalized $P^* = 0.02$, these noisy results may be improved at some other more suitable P^* values. Moreover, it is mentioned that the λ_0 increases with an increase of κ at $\Gamma = 10$ for small N (= 1024 and 4096). It is remarkable that we have extend the limits of N (≡ 22500-64000) and the

obtained results are well matched with earlier known 2D numerical and experimental data at nearly same set of plasma states in the nonideal gas-like, liquid-like and crystal-like phases.

The main outcomes are shown in Figs. 1-4, where we compute the $\lambda_0(\Gamma, \kappa)$ through HPMD technique of a typical Yukawa systems in a 2D strongly coupled domain of different plasma couplings ($\Gamma \equiv$ 10, 20, 50, 100, 200 and 300) and N ($\equiv$ 1024, 4096, 14400, 22500, 32000 and 64000) for each four screening lengths κ ($\equiv$ 1, 2, 3 and 4) at constant normalized P^* ($\equiv$ 0.02). These figures also display the previous 2D numerical results calculated from NEMD (Brownian dynamics) estimations of Hou and Piel,[37] HNEMD simulations of Shahzad and He with different N (1024, 4096 and 14400)[11] and GKR-EMD of dissipative Yukawa systems of Khrustalyov and Vaulins with three scaling factors ($\zeta \equiv$ 0, 1 and ∞).[27] Moreover, our HPMD computations of $\lambda_0(\Gamma, \kappa)$ are also compared and discussed with those computed in 2D experimental obviations of Nunomura *et al*.,[25] Nosenko *et al*.,[26] and 3D experimental measurements of Fortov *et al*.[8] In addition, the reported outcomes are also discussed with measurements of SCCPs taken from the 3D InHEMD investigations of Donko and Hartmann,[36] GKRs-EMD estimations of Salin and Caillol,[34] HNEMD simulations of Shahzad and He,[38] theoretical calculations of Faussurier and Murillo.[35]

Plots 1 and 2 show the $\lambda_0(\Gamma, \kappa)$ as a function of plasma (Coulomb) coupling at different values of N ($\equiv$ 1024, 4096, 14400, 22500 and 64000), respectively, for the cases of κ =1 and 2. We have performed eighteen (κ =1) and thirty (κ =2) different HPMD simulations at constant external perturbation of P^* ($\equiv$ 0.02) and particle number extended up to N = 14400 (κ =1) and N = 14400-22500-64000 (κ =2) particles. The reported HPMD data are normally in good agreement for the complete range of plasma parameters covering from nonideal gaseous state (Γ= 10) to strongly coupled state ($\Gamma \geq$ 180 for κ =1 and Γ = 300 for κ =2), for both cases. It is observed that the present data points of $\lambda_0(\Gamma, \kappa)$ are definitely higher at Γ= 10 (for N= 1024 and 4096) but the $\lambda_0(\Gamma, \kappa)$ lies more close to prior data sets of 2D GKR-EMD (dissipative Yukawa systems) estimations of Khrustalyov and Vaulina, NEMD calculations of Hou and Piel and HNEMD results of Shahzad and He (for different N) at intermediate to large Γ ($\equiv$ 20, 180) for κ =1 and Γ ($\equiv$ 20, 300) for κ =2. Further, it is can be seen from plots that new simulations of $\lambda_0(\Gamma, \kappa)$ are slightly lower at intermediate to large Γ ($\equiv$ 20, 300), for κ =1 (N = 14400) and κ =2 (N = 64000), as compared to prior known simulation data.[27,37] It can be seen from both figures that a

constant of $\lambda_0(\Gamma, \kappa)$ is observed at large Γ, for constant normalized P^* ($\equiv 0.02$), confirming the earlier numerical results reported in Refs. 27,37. However, at large N ($\equiv$ 14400, 22500 and 64000), instead, a constant fashion of $\lambda_0(\Gamma, \kappa)$ is noted that is very slightly decreasing with increasing Γ but unlike to earlier estimations stated in Ref. 11, where a slightly growing trend is noted with Γ. It is further examined that a steady $\lambda_0(\Gamma, \kappa)$ is started at large Γ for small range of N ($\equiv$ 1024 and 4096) and midway to large Γ for big N ($\equiv$ 14400, 22500 and 64000), verifying the previous numerical investigations.[11,27,37] Moreover, at small to intermediate Γ, the outcomes of plasma $\lambda_0(\Gamma, \kappa)$ are well matched with earlier recognized numerical and experimental investigations[11,27,37,25,26] and showing the existence of λ_0 but contrary to the data of Donko *et al*.,[41] where the presence of λ_0 was not found at small value of Γ. It is remarkable to mention here that the presence of plasma $\lambda_0(\Gamma, \kappa)$ remains for all values of Γ with increasing N and κ within satisfactory limited statistical uncertainty, validating the numerical data.[11,27,37] It is noted that the proposed Even-Gillan model provides more reliable outcomes of $\lambda_0(\Gamma, \kappa)$ as compare to earlier numerical approach of Shahzad and He,[11] where the existence of λ_0 shifts toward large Γ with an increase of N and κ. It can be observed that the reported 2D plasma $\lambda_0(\Gamma, \kappa)$ behavior is comparable to the previous 3D numerical investigations[33-36] in the region of small to intermediate Γ but unlike a nearly constant trend at larger Γ. Furthermore, HPMD outcomes for Γ ($\equiv$ 20) lie between HNEMD results of Ref. 11 and NEMD investigations of Ref. 37, however, for the region of Γ ($\equiv$ 50, 180) present results are definitely lower than earlier data,[11] at N = 1024 (κ = 1) and 4096 (κ = 1 and 2).

Two sets of plots are drawn to display the trends of measured plasma $\lambda_0(\Gamma, \kappa)$ of the 2D CPLCs at high values of κ = 3 and 4. Executing calculations with various system sizes (small-intermediate-large N) at varying Γ ($\equiv$ 10, 20, 50, 100, 200 and 300) and we analyzed the accuracy and consistency of the HPMD method for steady state values of plasma $\lambda_0(\Gamma, \kappa)$ at constant perturbation of P^* ($\equiv$ 0.02). Plots 3 and 4 (log- linear scale) demonstrate the plasma $\lambda_0(\Gamma, \kappa)$ simulated through an improved HPMD algorithm with varying $N \equiv$ 1024, 4096 and 14400 for both κ = 3 and 4 and particles number are extended up to $N \equiv$ 22500 and 32400 for κ = 3. For both cases, six different series of HPMD simulations are implemented with varying system sizes N (a total simulations of thirty and eighteen, respectively, for κ = 3 and 4). For both cases of κ = 3 and 4, plots show that the plasma $\lambda_0(\Gamma, \kappa)$ is significantly higher than prior investigations at Γ= 10 (for $N \equiv$ 1024, 4096, 22500 and 32400) and Γ= 20 (for $N \equiv$ 1024).

Moreover, for the Coulomb coupling range Γ (≡ 50, 300) and κ = 3 and 4, the present outcomes of $\lambda_0(\Gamma, \kappa)$ become nearly constant, however, a minor decreasing behavior is found with an increase of Γ at all N (≡ 1024-32400). It can be seen from both plots that at intermediate Γ (≡ 20) the HPMD outcomes lie between Khrustalyov and Vaulina GKR-EMD investigations of Ref. 27 and Hou and Piel NEMD simulations of Ref. 37, Shahzad and He calculations of Ref. 11 for N = 4096 (κ = 3 and 4) and 32400 (κ = 3). However, the HPMD simulations are definitely lower than earlier numerical investigations of GKR-EMD and HNEMD but slightly lower than NEMD results of Hou and Piel at Γ (≡ 20) for N = 14400 (κ = 3 and 4). Further, it is observed that the current data of $\lambda_0(\Gamma, \kappa)$ are lower as compared to earlier numerical data[37] for the coupling regions of Γ (≡ 50, 300) for N = 1024, 4096 (κ = 3 and 4) and N = 32400 (κ = 3), and Γ (≡ 20, 300) for N = 14400 (κ = 3 and 4) and N = 22500 (κ = 3).

Experimental comparison of thermal diffusivity $D_T(\Gamma)$ is made with present measured HPMD outcome of $\lambda_0(\Gamma, \kappa)$ and it is considered parameters of the mentioned experiments with liquid dusty plasmas for our computed $D_T(\Gamma)$. Analytically, thermal diffusivity relation can be written in the form $D_T(\Gamma) = \lambda_0/nc_p$; here, n is the density, c_p is the specific heat at constant pressure.[25] The normalized values of thermal diffusivity are used in the analysis and comparison of our present results with the existing numerical and experimental data. For whole range of plasma states (Γ, κ=1), the $D_T(\Gamma)$ is computed by taking referenced parameters that are employed in earlier known experiments.[25,26] Here, in our case of Coulomb coupling range of Γ (≡ 20, 180) and κ = 1, the computed $D_T(\Gamma)$ lies between ≈63.0 to 1.2 mm^2 s^{-1}, ≈26.0 to 0.3 mm^2 s^{-1} and ≈6.0 to 0.3 mm^2 s^{-1}, respectively, for N= 1024, 4096 and 14400. In case of taking reference parameters used by Nunomura *et al*.,[25] and for κ = 1, on the same coupling range from the previous discussion, the thermal diffusivity values are in between ≈95.0 to 1.7 mm^2 s^{-1} (N= 1024), ≈40.0 to 0.5 mm^2 s^{-1} (N= 4096) and ≈9.0 to 0.5 mm^2 s^{-1} (N= 14400), respectively. It has demonstrated that the experimental results for $D_T(\Gamma)$ are between ≈9.0 mm^{2}s^{-1} of Nosenko *et al*., for 2D the solid-liquid mixture state[26] and ≈30 mm^{2}s^{-1} of Nunomura *et al*., for 2D crystalline state,[25] and experimental values are 1.0 mm^{2}s^{-1} of Fortov et al., for 3D nonideal dissipative.[8] Further, it is observed that our 2D $D_T(\Gamma)$ values have range from ≈4.0 and ≈35 mm^{2}s^{-1} at most of plasma states, which are in satisfactory agreement with experimental data where the values of ≈9.0 to 30 mm^{2}s^{-1} were reported. It is remarkable mentioned here that our outcomes of $D_T(\Gamma)$ remain within range of ≈35.0 (24.0) to 2.0 (1.2) mm^2 s^{-1} for small to intermediate range of Γ (≡ 10, 50) at large

N = 14400 with mentioned reference experimental parameters of Nunomura *et al*. (Nosenko *et al*.). Moreover, it is mentioned here that the $D_T(\Gamma)$ remains between ≈40.0 to 2.0 mm^2 s^{-1} for intermediate to large range of Γ (≡ 20, 100) at intermediate N = 4096, ≈16.0 to 2.0 mm^2 s^{-1} for large Γ (≡ 50, 180) at small N = 1024. It is observed that the previously discussed $D_T(\Gamma)$ values are close to each other for approximately small to intermediate values of Γ. These results are valuable for the diagnostics of laboratory dusty plasmas. Further, it is examined that $D_T(\Gamma)$ remains close to the experimental results of thermal diffusivity of fluids for different κ corresponding to each Γ. These comparisons give an overall better comparison of our simulation results at this normalized constant P^* (= 0.02) at varying N.

It should be mentioned here that we have calculated the plasma λ_0 for the temperature (universal) scaling law at normalized P^* (≡ 0.02) and varying N (≡ 1024, 4096, 14400). The simple scaling expression that shows plasma λ^* (≡ $nm\omega_E a^2$) as a function of scaled system temperature T^* =T/ T_m (≡ Γ_m / Γ), where T_m and Γ_m are the melting points and associated detail is reported in earlier Refs. 1, 11, 35, 36, 38, 39, 42 and given as:

$$\lambda^* = K_1 T^* + \frac{K_2}{T^*} + K_3, \tag{8}$$

where K_1, K_2 and K_3 are unknown constants that can be obtained by curve fitting to calculated data for plasma $\lambda^*(T^*, \kappa)$, normalized by Einstein frequency (ω_E), and four values of κ (≡ 1, 2, 3 and 4). Here in our case, a temperature (quasi-universal) scaling law is also tested to the 2D plasma $\lambda^*(T^*, \kappa)$, proposed by Donko and Hartmann,[36] and this quasi-universal law with extra dependent term of κ and mentioned constant values is expressed as:[35]

$$\lambda^* = 0.018T^* + \frac{1.05}{T^*} + 0.115 + 0.127\kappa, \tag{9}$$

Universal and quasi-universal temperature scaling laws demonstrate that the plasma $\lambda^*(T^*, \kappa)$ is taken along vertical axis and scaled T^* (ratio of the Yukawa system and melting temperatures) is considered along horizontal axis and are revealed in plots 5 and 6. For universal temperature scaling law case, the plasma $\lambda^*(T^*, \kappa)$ is calculated with setting N = 1024 and 4096 for κ (≡ 1, 4). The particles number is extended up to N =14400 for $\lambda^*(T^*, \kappa)$ and the both universal and quasi-universal temperature scaling laws are tested at four values of κ. In order to confirm the

accurateness and reliability of plasma $\lambda^*(T^*, \kappa)$ we have performed calculations with different system sizes at constant P^* ($\equiv$ 0.02). For both plots of 5 and 6, we compute the twenty three, twenty two (see both panels of plot 5) and forty four (see both panels of plot 6) different data sets of $\lambda^*(T^*, \kappa)$ corresponding to each N (1024, 4096 and 14400) for four κ and varying T^*, covering from almost nonideal state (Γ = 10) to strongly coupled states (Γ = 180) and (Γ = 300), depending on κ. The dark lines are the curve fitting of the functional form of Eq. (8) with unknown constants: K_1 = 0.21251, K_2 = 1.15258 and K_3 = -1.38381 for N = 1024 and K_1 = 0.12827, K_2 = 1.122933 and K_3 = -1.34248 for N = 4096. Moreover, the fitting constants that are obtained after curve fitting of the functional form of Eq. (8): K_1 = 0.03228, K_2 = 0.37242 and K_3 = -0.39291 for N = 14400 and dark line is shown in plot 6 (a), confirming prior numerical trends.[1,11,42] Quasi-universal functional form, Eq. (9), is also tested for N = 14400 and it is found that the thick line is excellent fit as depicted in plot 6 (b). It is to be mentioned here that the fitting constants (K_1, K_2 and K_3) for scaled $\lambda^*(T^*, \kappa)$ are computed from present simulation outcomes (λ_0) revealed in plots 1-4. It can be suggested from both plots (5 and 6) that the scaled $\lambda^*(T^*, \kappa)$ is independent of N at small T^* ($\Gamma\equiv$ 10-20) and nearly less dependent of N at large T^* (intermediate to large, $\Gamma\equiv$ 50-300), contradicting earlier numerical results.[11] It is observed that the scattering of scaled $\lambda^*(T^*, \kappa)$ at large T^* and well aligned along dark line at small T^*. One possible case of scattering of these present data around dark line at large T^* is that this may come about due to positive value of "K_2" and high negative value of "K_3" in the universal functional fit of Eq. (8) but like to previous numerical data.[11] It is stated here that the calculated scaled $\lambda^*(T^*, \kappa)$ explains that the universal and quasi-universal functional forms of Eqs. (8) and (9) provide a satisfactory fits, confirming earlier 3D and 2D CPLCs results.

IV. CONCLUSIONS

Using homogenous perturbed MD simulations, the thermal conductivity $\lambda_0(\Gamma, \kappa, N)$ of 2D complex plasma is computed as a function of plasma coupling Γ (inverse of temperature), screening length κ and system size N at constant external perturbation (P^* = 0.02). It has been demonstrated that the normalized thermal conductivity $\lambda^*(T^*, \kappa, N)$ follows universal and quasi-universal scaling laws. It has been shown that the present HPMD scheme and previous 2D simulation methods have analogous performance and this proposed scheme is relatively perfect and efficient than the earlier NEMD, GKR-EMD and HNEMD methods. New simulations provide more consistent data of λ_0 in liquid-like and crystal-like regimes and the $\lambda_0(\Gamma, \kappa, N)$ are

in reasonable agreement with the reliable experimental and numerical data. The different systems sizes of CPLCs make experimental investigations rather challenging, however, the proposed HPMD method outlines a practical approach to employing classical measurements to explore thermal conductivity of complex dusty plasma systems. For future work, the HPMD scheme used here can be extended to the dusty plasma systems with an addition of polarization effects[43,44] and varying external perturbation effects can be investigated on $\lambda_0(\Gamma, \kappa, N)$ for 2D and 3D dusty plasma systems. The easy to code and straightforwardness of the present scheme shows this model can be modeled to other systems having screening Coulomb interactions and component complex systems.

ACKNOWLEDGMENTS

The authors thank Z. Donko (Hungarian academy of sciences) for facilitating us with his thermal conductivity data of Yukawa Liquids for the judgements of our simulation results. We are very obliged to the National Advanced Computing Centre of National Centre for Physics (NCP), Pakistan and National High-Performance Computing Center (NHPCC) of Xian Jiaotong University, P R China for allocating computer time to test and run our MD code.

Data Availability Statements:

Data available on request from the authors: The data that support the findings of this study are available from the corresponding author upon reasonable request.

References

[1]A. Shahzad and M.-G. He, Int. J. Thermophys. **36**, 2565–2576 (2015)

[2]M. E. Rosti and F. Picano, L. Brandt, *Numerical Approaches to Complex Fluids, Chp. 1* (Springer, Cham, 2019)

[3] P. Stachowiak, V. V. Sumarokov, J. Mucha, and A. Jezowski, Phys. Rev. B **58**, 2380 (1998).

[4]C. C. Grimes, G. Adams, Phys. Rev. Lett. **42**, 795 (1979).

[5]P. L. Gammel, D. J. Bishop, G. J. Dolan, J. R. Kwo, C. A. Murray, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. Lett. **59**, 2592 (1987).

[6]C. A. Murray, W. O. Sprenger, and R. A. Wenk, Phys. Rev. B **42**, 688 (1990).

[7]T. B. Mitchell, J. J. Bollinger, X.-P. Huang, W. M. Itano, and D. H. E. Dubin, Phys. Plasmas **6**, 1751 (1999).

[8]V. E. Fortov, V. E. Fortov, O. S. Vaulina, O. F. Petrov, M. N. Vasiliev, A. V. Gavrikov, I. A. Shakova, N. A. Vorona, Yu. V. Khrustalyov, A. A. Manohin, and A. V. Chernyshev, Phys. Rev. E 75, 026403 (2007).

[9]A. Shahzad and M.-G. He, Phys. Scr. **86**, 015502 (2012).

[10]K. Dietrich, D. Renggli, M. Zanini, G. Volpe, I. Buttinoni, and L. Isa, New J. Phys. **19**, 065008 (2017).

[11]A. Shahzad and M.-G. He, Phys. Plasmas **22**, 123707 (2015).

[12]A. Melzer and J. Goree, *Fundamentals of Dusty Plasmas, Chp. 6* (Weinheim: Wiley, 2008)

[13]A. Shahzad, M. Kashif, T. Munir, M. A. Shakoori, M.-G. He, S. Bashir, and Q. Ul Islam, online first in forthcoming issue, HT-HP, (2020).

[14]D. J. Evans and G. P. Morriss, *Statistical Mechanics of Non-Equilibrium Liquids* (Academic: London, 1990).

[15]J.-P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Academic: London, 1986).

[16]A. Shahzad and M.-G. He, Phys. Plasmas **23**, 093708 (2016).

[17]A. Shahzad, *Impact of Thermal Conductivity on Energy Technologies* (Intech: London, 2018)

[18]A. Shahzad, M.-G. He, S. I. Haider, and Y. Feng, Phys. Plasmas **24**, 093701 (2017).

[19]G. Ciccotti, G. Jacucci, and I. R. McDonald, J. Phys. C **11**, L509 (1978).

[20]D. J. Evans, Phys. Rev. A **23**, 1988 (1981).

[21]W. G. Hoover and W. T. Ashurst, Theor. Chem. Adv. Perspectives **1**, 2 (1975).

[22]M. J. Gillan and M. Dixon, J. Phys. C: Solid State Phys. **16**, 869 (1983).

[23]D. J. Evans, J. Phys. Lett. A **91**, 457 (1982).

[24]G. Ciccotti, G. Jacucci, and I. R. McDonald, J. Stat. Phys. **21**, 1 (1979).

[25]S. Nunomura, D. Samsonov, S. Zhdanov, and G. Morfill, Phys. Rev. Lett. **95**, 025003 (2005).

[26]V Nosenko, S. Zhdanov, A. V. Ivlev, G. Morfill, J. Goree, and A. Piel, Phys. Rev. Lett. **100**, 025003 (2008).

[27]Yu. V. Khrustalyov and O. S. Vaulina, Phy. Rev. E **85**, 046405 (2012).

[28]B. D. Todd and P. J. Daivis, Mol. Simul. **33**, 189 (2007).

[29]N. Galamba and C. A. Nieto de Castro, J. Chem. Phys. **126**, 204511 (2007).

[30]K. K. Mandadapu, R. E. Jones, and P. Papadopoulos, J. Chem. Phys. **130**, 204106 (2009).

[31]Z. Wang, X. Zu, F. Gao, W. J. Weber, and J.-O. Crocombette, Appl. Phys. Lett. **90**, 161923 (2007).

[32]K. K. Mandadapu, R. E. Jones, and P. Papadopoulos, J. Chem. Phys. **133**, 034122 (2010).

[33]C. Pierleoni, G. Ciccotti, and B. Bernu, Europhys. Lett. **4**, 1115 (1987).

[34]G, Salin and J.-M. Caillol, Phys. Plasmas **10**, 1220 (2003).

[35]G. Faussurier and M. S. Murillo, Phys. Rev. E **67**, 046404 (2003).

[36]Z. Donko and P. Hartmann, Phys. Rev. E **69**, 016405 (2004).

[37]L. J. Hou and A. Piel, J. Phys. A: Math. Theor. **42**, 214025 (2009).

[38]A. Shahzad and M.-G. He, Contrib. Plasma Phys. **52**, 667 (2012).

[39]A. Shahzad and M.-G. He, Phys. Plasmas **19**, 083707 (2012).

[40]A. Shahzad and M.-G. He, *Phys. Plasmas* **26**, 023704 (2019).

[41] Z. Donko, J. Goree , andP. Hartmann, B. Liu, Phys. Rev. E **79**, 026401 (2009).

[42]A. Shahzad, S. I. Haider, M. Kashif, M. S. Shifa, T. Munir, and M-G He, Commun. Theor. Phys. **69**, 704 (2018).

[43]T. S. Ramazanov, A. Zh. Gabdulin, and Zh. A. Moldabekov, IEEE Transactions on Plasma Science **43**, 4187 – 4189 (2015).

[44]T. S. Ramazanov, Zh. A. Moldabekov, and M. T. Gabdullin, Phys. Rev. E **93,** 053204 (2016).

List of Figure Captions

FIG. 1. Variation of thermal conductivity $\lambda_0(\Gamma, \kappa, N)$ as a function of Coulomb (plasma) coupling along horizontal-axis of 2D SC-CPLCs for N = 1024, 4096 and 14400 particles at κ = 1. Present outcomes with different N and earlier numerical data for NEMD investigations of Hou and Piel,[37] HNEMD results of Shahzad and He with different N [11] and GKR-EMD simulations of Khrustalyov and Vaulina at different scaling factors.[27]

FIG. 2. Variation of thermal conductivity $\lambda_0(\Gamma, \kappa, N)$ as a function of Coulomb (plasma) coupling along horizontal-axis of 2D SC-CPLCs for N = 1024, 4096, 14400, 22500 and 64000 particles at κ = 2. For outcome comparison with earlier results, see the caption of Fig. 1**.**

FIG. 3. Variation of thermal conductivity $\lambda_0(\Gamma, \kappa, N)$ as a function of Coulomb (plasma) coupling along horizontal-axis of 2D SC-CPLCs for N = 1024, 4096, 14400, 22500 and 32400 particles at κ = 3. For outcome comparison with earlier results, see the caption of Fig. 1**.**

FIG. 4. Variation of thermal conductivity $\lambda_0(\Gamma, \kappa, N)$ as a function of Coulomb (plasma) coupling along horizontal-axis of 2D SC-CPLCs for N = 1024, 4096 and 14400 particles at κ = 4. For outcome comparison with earlier results, see the caption of Fig. 1.

FIG. 5. Thermal conductivity normalized by Einstein frequency (ω_E) $\lambda^*(T^*, \kappa, N)$ as a function of scaled temperature T^* for varying N at varying κ = 1, 2, 3, and 4. The dark line is sketched the simple scaling expression, Eq. (8), exhibiting the universal temperature law of 2D SC-CPLCs. The present curve fitting of 2D plasma system is well matched with earlier fitting of Ref. 11 (a) for N = 1024, (b) N = 4096 particles**.**

FIG. 6. Thermal conductivity normalized by Einstein frequency (ω_E) $\lambda^*(T^*, \kappa, N)$ as a function of scaled temperature T^* for constant N = 14400 at varying κ = 1, 2, 3, and 4. The solid line is sketched the simple scaling expression, Eq. (9), exhibiting the temperature scaling behaviors of 2D SC-CPLCs. The present curve fitting of 2D plasma system is well matched with earlier fitting of Ref. 11 (a) for universal temperature law, (b) for quasi-universal temperature law**.**