Molecular dynamics simulations of thermal conductivity in 2D complex Yukawa liquids

Aamir Shahzad¹,², Mariam Sultana¹, Arffa Aslam¹ and Mao-Gang He²
¹Department of Physics, Government College University Faisalabad, Allama Iqbal Road, Faisalabad 38000, Pakistan
²Key Laboratory of Thermo-Fluid Science and Engineering of Ministry of Education (MOE), Xi’an Jiaotong University, Xi’an 710049, P. R. China
E-mail: aamirshahzad_8@hotmail.com, aamir.awan@gcuf.edu.pk

Abstract. The thermal conductivity in strongly coupled complex dusty plasma liquids (SCCDPLs) has been investigated through an improved homogenous nonequilibrium molecular simulation (HNEMS) method, for the first time. The HNEMS method has been employed for two-dimensional (2D) Yukawa systems in a canonical ensemble. The thermal conductivities with suitable normalizations (plasma and Einstein frequencies), in the value of low force field strength, have been computed for a wide range of plasma state points of Coulomb coupling (Γ) and screening strength (κ). The new simulation results are found to obey the simple analytical temperature scaling law. The present HNEMS results are in generally with parts of earlier HNEMS, equilibrium molecular dynamics (EMD) and experimental data in the literature for the 2D and there-dimensional (3D) SCCDPLs. It is shown that the HNEMS method can be used to estimate the thermal conductivity very effectively and to understand the fundamental behaviours in 2D Yukawa systems.

1. Introduction
In recent applications, the transport problems in non-ideal systems of interacting particles are of significant interest in various fields of science and engineering (such are plasma physics, physics of polymers, medical, semiconductor and chemical industries, environmental safety and space plasmas, etc.) [1]. In practical applications, including those intended at developing novel thermal interface materials, micro and nano-level heat transport processes, and nano-particulate systems have been proposed to improve the efficient behaviour of the systems. Nanotechnology development in the latest decades revealed new outcomes in semiconductor nanowires (NWs) investigate and their interaction with fluids and transport properties of NWs, including the thermal conductivities are extensively amended from the macroscopic property [2].

The development features of heat transfer in materials at micro- and nano-levels have moved into the areas of technology issues, however, there are some areas, such as phonon thermal transports in semiconductor superlattices have much attention for researchers. Different practical novel applications and technologies such as thermoelectronic and photoelectronic devices, solar cells, and NWs-based thermoelectric systems have been proposed. Nano-particles themselves have low conductivity, however, their interactions along with larger particles are considered to increase the percolation threshold leading to better materials overall [3-5].
In addition to fundamental features, the study of thermal properties of complex (non-ideal) systems is of practical interest for the developments of micro- and nano-systems. A four components plasma (nonideal complex dusty plasma system) plays extremely significant part in a number of new technological advances (such as heat technology tools for process/chemical industries, plasma processing for semiconductor industries, medical tool treatments and surface cleaning, and future energy production and storage devices, etc) and this strongly coupled complex dusty plasma (SCCDP) is containing grains of dust particles (solid matter) which found everywhere in nature [6-8]. These systems require a deep understanding of the interaction of complex (nonideal) systems with nano- and microstructuring of surfaces and of the behaviour of particles (micro and nano-levels) and chemically active particulates. One important challenge in using micro and nanotechnologies is the lack of knowledge regarding their thermal conductivity. A novel homogenous nonequilibrium molecular simulation (HNEMS) approach is to be needed to compute the thermal conductivity of complex (nonideal) systems of much of the thermophysical property research in the fields of science and technology [9-11].

The purpose of the current study is to investigate all possible dependences of the heat conductivity ($\lambda$) on the plasma parameters ($\kappa$, $\Gamma$) using the nonequilibrium molecular dynamics (HNEMD) technique as reported in Shahzad and He [12], for the first time in two-dimensional (2D) SCCDP liquids (SCCDPLs). In addition, the effects of the screening length ($\kappa$) on the dust particle interaction for $\lambda$ with different system sizes and temperatures are also computed by using extensive computer simulations for 2D SCCDPLs. The design of this paper is as follows: in Section 2, the improved form of mathematical model for the $\lambda$ coefficient for 2D Yukawa liquids (SCCDPLs) using HNEMS algorithm is given, and this section also presents the molecular mechanics dynamics (MMD) simulation method. In Section 3, the HNEMS results are illustrated and discussed with previous reported experimental and computer simulation data by other author’s. Finally, in Section 4, the work is summarized.

2. Theory and Nonequilibrium MMD Algorithm

Classical mechanics (CM) provide a fundamental description of any system (simple, dense and complex). In theory, CM calculations depend on parameters used and it is desirable to use the most sophisticated approach to CM for any calculation.

Currently, a well known model in laboratory plasma of gas discharge is Yukawa interaction model (screened Coulomb interaction), which is used for the account of the interactions between dust particles (Yukawa particulates) computationally for our case and this model has been used in may physical and chemical systems (for instances, ionic systems, medicine and biological sciences, physics of polymers, environment, etc.)

$$\phi(|r|) = \frac{Q^2}{4\pi\varepsilon_0} \frac{e^{-\lambda r}}{|r|}, \quad (1)$$

where $\lambda_0$ is the screening strength (Debye length), $Q$ is the charge on a dust particles and $r$ is the interparticle distance.

The general microscopic expression for thermal conductivity computationally is regarded as Green-Kubo relation (GKR) for thermal coefficients of uncharged particles [13]. This relation has been employed for one component Coulomb plasmas (OCCPs) [14] and SCCDPLs [2,5,9-11], using different numerical methods.

$$\lambda = \frac{1}{2k_BAT^2} \int_0^\infty \langle J_\phi(t)J_\phi(0) \rangle dt \quad (2)$$

where $T$ is system temperature, $k_B$ is Boltzmann’s constant and $V$ is volume of the system under HNEMS method. The heat energy flux vector $J_\phi$ in terms of microscopic form can be written as
\[ \mathbf{J}_\alpha A = \sum_{i=1}^{N} E_i \mathbf{p}_i m - \frac{1}{2} \sum_{i<j} r_{ij}(\mathbf{p}_i \cdot \mathbf{F}_j), \text{ where} \quad E_i = \frac{p_i^2}{2m} + \frac{1}{2} \sum_{j \neq i} \phi_{ij} \tag{3} \]

where energy \( E_i \) of particle \( i \) with \( \phi_{ij} \) is the Yukawa pair interaction between particle \( i \) and \( j \), and the position vector and force are \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \) and \( \mathbf{F}_{ij} \), respectively, on particle \( i \) due to \( j \) and \( \mathbf{p}_i \) is the momentum vector of the \( i \)th particle, and \( \mathbf{J}_\alpha A \). The computationally microscopic heat energy flux vector \( \mathbf{J}_\alpha \) of the Yukawa liquids is given in Refs. 2 and 5. The Evans [15] proposed the non-Hamiltonian linear response theory and has been used for a system moving representing equations of motion

\[ \mathbf{r}_i = \frac{\mathbf{p}_i}{m}, \tag{4} \]

\[ \mathbf{p}_i = \sum_{j \neq i} \mathbf{F}_j + \mathbf{D}_{ij} (\mathbf{r}_i, \mathbf{p}_i, t) - \alpha \mathbf{p}_i. \tag{5} \]

In Eq. (5), \( \mathbf{D}_i = \mathbf{D}(\mathbf{r}_i, \mathbf{p}_i) \) is the tensor phase variable that describes the coupling of Yukawa system to the external force field \( \mathbf{F}_e(t) \), the total interparticle force acting on particle \( i \) is \( \mathbf{F}_i = -(\partial \phi_i / \partial r_i) \), and \( \alpha \) is the Gaussian thermostat multiplier. The linear response theory can be used in a straightforward fashion to a Yukawa system [2,5]. A thermostat (\( \alpha \)) has been employed to retain constant temperature in order to remove heat problem due to work done and it is given as [5]

\[ \alpha = \frac{\sum_{i=1}^{N} \left[ \mathbf{F}_i + \mathbf{D}_i (\mathbf{r}_i, \mathbf{p}_i, t) \right] \mathbf{p}_i}{\sum_{i=1}^{N} \mathbf{p}_i^2 / m_j} \tag{6} \]

We can use external force field of \( \mathbf{F}_e(t) = (0, F_z), \) which is parallel to the z-axis, then the final expression for thermal conductivity is given as:

\[ \lambda = \frac{1}{2k_B A T^2} \int_0^\infty \left\langle \mathbf{J}_{\phi_z}(t) \mathbf{J}_{\phi_z}(0) \right\rangle dt = \lim_{F_z, \lim_{\lambda \to 0}} \lim_{F_z \to \infty} \frac{-\left\langle \mathbf{J}_{\phi_z}(t) \right\rangle}{TF_z} \tag{7} \]

where \( \mathbf{J}_{\phi_z} \) is the z-component of the heat energy flux vector for SCCDPLs. The thermal conductivity is normalized by plasma frequency \( \lambda_0 = \lambda / n m o \sigma a^2 \). All time series data are recorded during HNEMS method by using Eq. (7) to compute \( \lambda_0 \).

2.1. HNEMD Simulation Method

In our simulation, three normalized parameters (in reduced units) are used for complete characterizing of the Yukawa model, given in Eq. (1), for interaction between particles [2,5,12-15]: the external force field strength \( F^2 = F_z; a_{ws} \), the plasma coupling (Coulomb) parameter \( \Gamma = (Q^2/4\pi\epsilon_0)(1/a_{ws}k_B T) \), and the screening strength parameter \( \kappa \equiv a_{ws}/\lambda_B \). It is mentioned that the \( \lambda_B \) is Boltzmann’s constant, \( T \) is system temperature and \( a_{ws} = (n\pi)^{-1/2} \) is the Wigner-Seitz radius [2,16] with \( n \) is the equilibrium particle number density. Time scales of interest are taken as inverse of the plasma frequency \( \omega_p = (Q^2/2\pi\epsilon_0 ma^3)^{1/2} \), where \( m \) is the Yukawa dust particle mass. In order to implement our HNEMS method, a system of \( N = 1024-4096 \) particles is chosen and placed in a computational cell of Yukawa system with edge lengths of \( L_x/L_y = 24/3 \). For simulations of an infinite Yukawa system using HNEMS technique, we need to employ the periodic boundary conditions (PBCs) in all directions with the minimum image conventions of the dust particles. The Newton equations of motions are used for computer integration of number particles to obtain the particle trajectories, and in solving Eqs. (4) and (5) we use the predictor-corrector algorithm [17]. In the HNEMS method, the particle number \( N \) was taken large enough to confirm the system size effects with efficient accuracy. Therefore, in order to save simulation time and computational power the present particle number \( N \) is acceptable for numerical simulations. The interaction force acting on the
i\text{th} particle \( F_i = (-\frac{\partial \phi_{ij}}{\partial r_i}) \) is computed by the Yukawa pairwise potential between particle \( i \) (at \( r_i \)) and the particle \( j \) (at \( r_j \)) and with its periodic images conventions of the Yukawa particles. A canonical ensemble that the Gaussian thermostat method was used for our HNEMS computations in order to maintain the temperature of Yukawa systems [2,13].

For the Ewald summation method detail has been reported by Shahzad and He [5,16], for Yukawa pairwise \( \kappa \)-dependent cutoff radius. Our simulations are carried out between \( 3.0 \times 10^5/\omega_p \) and \( 1.5 \times 10^5/\omega_p \) time units in the series of data recording of \( \lambda_0 \). The HNEMD numerical time step \( dt = 0.001/\omega_p \) is chosen to allow calculating the heat transport important data [2,5]. In this paper, the calculations are accounted for thermal conductivity of 2D SCCDPLs over wide range of plasma parameters of \((10 \leq \Gamma \leq 100)\) and \((1 \leq \kappa \leq 3)\).

3. Simulation Results and Discussion

In this section, thermal conductivity measurements with appropriate normalizations, in the limit of low equilibrium external force field strengths \( F^* = (F_z a_w)/a_\kappa \), are presented over a wide range of plasma coupling (\( \Gamma \geq 10 \)) and screening (\( \kappa \geq 1 \)) parameters. A different sequence of the thermal conductivity corresponding to a higher and lower sequence of applied external field strength is calculated to determine the linear regime of the HNEMD Yukawa system. The HNEMS data from at a reduced force field strength of \( F^* = 0.2 \) have a usually good agreement with the previous equilibrium molecular dynamics (EMD) investigations in 2D dissipative Yukawa systems by Khrustalyov and Vaulina [1], nonequilibrium EMD (NEMD) simulations of Hou and Piel [11], and experimental results of Nosenko \textit{et al} [3], Nunomura \textit{et al} [4], and Fortov \textit{et al} [6]. A simple analytical temperature representation of Yukawa thermal conductivity with normalized Einstein frequency (\( \omega_E \)) has also been performed. The present calculations with appropriate normalizations show that the position of minimum of 2D thermal conductivity lies at higher \( \Gamma \) with increasing \( \kappa \) same as in 2D Yukawa systems [1,11], and earlier experimental data [3,4,6].

The chief results obtained from the HNEMD simulations are given in Figs. 1-3 for \( \kappa = 1, 2 \) and 3, respectively, for the whole range plasma of the 2D Yukawa systems. The Figs. 1-3 display the present results as well as compared the previous results obtained from the earlier three-dimensional (3D) HNEMD simulations of Shahzad and He [2,5], Green-Kubo EMD of Salin and Caillol [9], and theoretical predictions of Faussurier and Murillo [10], and in addition the calculations taken from 2D means of Green-Kubo EMD of dissipative Yukawa systems of Khrustalyov and Vaulina [1]. Moreover, we have been compared our simulation results with the earlier 2D NEMD results of Hou and Piel [11], and experimental data of Nosenko \textit{et al} [3], Nunomura \textit{et al} [4], and Fortov \textit{et al} [6], nearly at the same plasma state points.

**Figure 1.** Comparison of results of thermal conductivity as a function of plasma coupling \( \Gamma \) (system temperature) for Yukawa liquid, obtained from HNEMS defined in Eq. (7), at \( \kappa = 1 \). HNEMS of Shahzad and He: SH 2D HNEMS: present results (for \( N = 1024 \) particles), HNEMD of Shahzad and He [5]: SH 3D HNEMD, EMD computations results of Salin and Caillol [9]: SC 3D EMD, theoretical variational procedure calculations of Faussurier and Murillo [10]: FM 3D VP.
The present thermal conductivity obtained from HNEMD simulations is slightly higher than those previously 3D numerical simulation results \cite{2,5,9,10} and lie close to the earlier 2D simulation results obtained from different simulation methods \cite{1,11}. The minimum values of frequency decreases with increasing of $\kappa$. The thermal conductivity obtained from HNEMD simulations is found to be in very good agreement with that obtained through the previously known 2D numerical simulations and experimental results for 2D Yukawa liquids \cite{1,3,4,6,11}.

**Figure 4.** Variation of normalized thermal conductivity by Einstein frequency $\lambda^* (T^*)$ with normalized temperature $T^*$ for SCCDP Yukawa system at different $\kappa=1$, 2 and 3, where $T^* \equiv T/T_m = \Gamma_m/\Gamma$ and $\Gamma_m$ corresponding to temperature at melting temperature. The solid line is obtained by using linear fitting for the simple Scaling Law: $\lambda^* = A T^* + B / T^* + C$, showing the temperature scaling law for 2D SCCDPs.
normalized temperature in the 2D SCCDPLs, confirming earlier simulation and experimental data [3,4,6]. The simulation results obtained for $\lambda^*$ using HNEMS method provide the best fitting and excellent trend for all the plasma state points ($\kappa$, $\Gamma$). The solid line given in figure 4 is obtained using the simple linear fitting of form, $\lambda^* = AT^* + B/T^* + C$, with coefficients: $A = 0.06143$, $B = -0.8409$, and $C = 1.13778$, showing the confirmation of temperature scaling law behaviours same as in 3D SCCDPLs Refs. 2 and 5. This scaling law is found to reproduce appropriately the shape of $\lambda^*(T^*)$ curves at three $\kappa$ values and it gives suitable relationship between $\lambda^*$ and $T^*$ for the whole plasma state points of ($\kappa$, $\Gamma$), confirming the earlier numerical results [2,5].

4. Conclusions
HNE MD simulation method has been used to calculate the thermal conductivity of 2D SCCDPLs over a wide range of plasma parameters ($\kappa$, $\Gamma$). New HNEMD simulations give more consistent results for 2D Yukawa conductivity than previous known numerical and experimental results, over all plasma state points, and illustrate a fair agreement with earlier HNEMD, EMD simulations and experimental data. Our results show that the $\lambda_0$ dependent on the temperature (plasma coupling) in 2D Yukawa liquids. The present results obtained indicate that the value of $\lambda_0$ at intermediate and higher Coulomb coupling nearly the same as $\kappa$ parameter increases, confirming earlier experimental results. The new HNEMD algorithm has strong advantages that easy to code, fast computing on small system sizes and showing efficient computing. In future work, it will also be of highly interest for analysis to see how quantum effects influence $\lambda_0$ in 2D and 3D SCCDPLs and it is suggested a need for an experiment or different simulations.

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