Polarized Thermal Conductivity of Two-Dimensional Dusty Plasmas

Aamir Shahzad, Madiha Naheed, Aadil Mahboob, Muhammad Kashif, Alina Manzoor and H.E. Maogang

Abstract

The computation of thermal properties of dusty plasmas is a substantial task in the area of science and technology. The thermal conductivity ($\lambda$) has been computed by applying polarization effect through molecular dynamics (MD) simulations of two-dimensional (2D) strongly coupled complex dusty plasmas (SCCDPs). The effects of polarization on thermal conductivity have been measured for a wide range of Coulomb coupling ($\Gamma$) and Debye screening ($\kappa$) parameters using homogeneous non-equilibrium molecular dynamics (HNEMD) method for suitable system sizes. The HNEMD simulation method is employed at constant external force field strength ($F^*$) and varying polarization effects. The algorithm provides precise results with rapid convergence and minute dimension effects. The outcomes have been compared with earlier available simulation results of molecular dynamics, theoretical predictions and experimental results of complex dusty plasma liquids. The calculations show that the kinetic energy of SCCDPs depends upon the system temperature ($\equiv 1/\Gamma$) and it is independent of higher screening parameter. Furthermore, it has shown that the presented HNEMD method has more reliable results than those obtained through earlier known numerical methods.

Keywords: Plasma thermal conductivity, complex dusty plasma, Homogenous non-equilibrium molecular dynamics, force field strength, system size, plasma parameters etc.

1. Introduction

Recently, thermophysical properties of complex materials are a major concern in the field of science and engineering. The term thermophysical properties used to pass on both thermodynamic and transport properties. Experimental or theoretical methods to study properties of fluids depend on microscopic and macroscopic categories [1–4]. The conventional macroscopic measurements depend on the state of stress, temperature, and density. Thermodynamic properties are defined by the equilibrium conditions of the system which consist of temperature, heat capacity, entropy, pressure, internal energy, enthalpy, and density, whereas the transport properties comprise thermal conductivity, diffusion viscosity, and waves with their instabilities. For further explanation of the process in detail for these systems, data that is applicable to thermodynamics, transport, optics, transmission, light, and other features are required for non-ideal plasma [5–9]. In this regard, various opinions regarding computer research methods including theoretical and numerical
performance have greatly improved for non-ideal Plasma [10]. Determination for some reason, thermal conductivity is also a big problem for thermophysical researchers. Developmental aspects of heat transport in micron and nanoscale materials have shifted to the domain of technical issues as there are other areas, such as phonon heat transfer in semiconductor superlattices, which have received widespread attention from researchers. To study the internal energy of particles, their momentum, and heat transfer thus remains a crucial task. Therefore, thermal management, strategies sustainable high performance, reliability, and service life are main purposes. One such strategy is to develop new therapeutic materials based on dusty plasma that are more effective. Regulation with approval became a significant issue in modern technology [11]. Yet similar interests are present in plasma fusion, and it can be productive radiotoxic dust in plasma-wall reactions. In many ways, this chapter provides an update literature survey on thermal transport as well as heat flow strategies to determine thermal behaviors in two-dimensional (2D) complex liquids. The coefficients were computed through the Green Kubo (GK) equilibrium molecular dynamics (EMD) simulations by Salin and Caillol [12] and variance procedure (VP) estimation used by the Faussurier and Murillo [13]. Donkó and Hartmann employed the inhomogenous non equilibrium MD (InHNEMD) method to investigate the transport and thermal conductivity [14]. Very recently, a homogeneous NEMD (HNEMD) and homogenous perturbed MD (HPMD) schemes are introduced by Shahzad and He (current authors) for strongly coupled complex dusty plasmas (SCCDPs) to compute the thermal transport and behaviors of SCCDPs [15–17]. For the computation of transport properties, in particular, numerical models are proposed in interest to investigate thermal behavior over a suitable range of system temperature and density values ($\Gamma, \kappa$). Complex fluids (dusty plasma fluids) have been used for many purposes, like power generation, semiconductors industry, cosmetics, paper industry, etc. [18].

1.1 Plasma

As we all know that 99% of matter exist in space is plasma and it is called forth state of matter. Basically plasma occurs in electrified gas form, where atoms dissociated into electrons and positive ions. It is form of matter in different areas of physics such as technical plasma, terrestrial plasma and in astrophysics. Plasma is produced artificially in laboratory used in many technical purposes likely in fluorescent lights, display, fusion energy research and other more. Term “Plasma” first time used by Irving Langmuir [19], who is an American physicist and defined plasma as “plasma is quasi-neutral gas of charged particles which exhibit collective behavior”. Quasi-neutral means that gas becomes electrically neutral when number of ions equal to number of electrons ($ni \approx ne \approx n$). Where, $ni$ is ion density, $ne$ is electron density and $n$ is number density. Collective behavior means that charged particles collide with each other due to coulomb potential and electric field. Plasma is extensively used in the field of science and technology. It plays a very significant role in over daily life. Plasma is used in over daily life fields such as laser, sterilizing of medical instruments, lightening, intense power beams, water purification planet and many more.

In 1922, American scientist Irving Langmuir was the only one person who defined plasma for the first time. In 1930, the study of plasma physics was started by some scholars; they are inspired by some particle problems. In 1940, hydromagnetic waves were advanced by Hanes Alfven [19] and these waves are called Alfven waves. Furthermore, he described that these waves would be used for the study of astrophysical plasma. At the start of 1950, the research on magnetic fusion energy was started at the same time in Soviet, Britain and USA. In 1958, the research on
magnetic fusion energy was considered the branch of thermonuclear power. Primarily, this research was carried out as confidential but after the realization that controlled fusion research was not liked by military and therefore this research was publicized by above said three countries. Due to the reason, other countries may participate in fusion research based on plasma physics. At the end of 1960, plasma is created with different plasma parameters by Russian Tokomak configuration. In 1970 and 1980, various advanced tokomaks were built and approved the performance of tokomak. Moreover, fusion break almost achieved in tokomak and in 1990, the research on dusty plasma physics had begun. The dusty plasma is defined as “when charged particles absorbed in plasma, becomes four components plasma containing electrons, ions, neutral and dust particles” and dust particles alter the properties of plasma which is called “Dusty Plasma” [19].

1.2 Types of plasma

Plasma has complex characteristics and properties, characterized through temperature of electron and ion, density and degree of ionization. (i) Hot plasma: If plasma fulfills \( T_e \approx T_i \) this condition then plasma is considered as hot plasma because hot plasma has very high temperature and also thermal equilibrium obtains due to frequent interactions between particles. Hot plasma is also called thermal plasma. It approaches to local thermodynamics equilibrium (LTE) and is created with high gas pressure in discharge tube in the laboratory. Hot plasma is produced by sparks, flames and atmospheric arcs. (ii) Cold plasma: When plasma satisfies \( T_e > T_i > T_g \) this condition, plasma is called cold plasma. Where \( T_e, T_i, \) and \( T_g \) represent the temperature of electrons, ions and gas molecules. Cold plasma is created in laboratory with the positive column glow discharge tube. Motion of gas molecules is considered ignore because electron energy is very high as compared with gas molecules. Moreover, nonthermal equilibrium does not exist because collision between gas molecules and electrons is considers as low due to low gas pressure. On this regime, magnetic field is very weak and considered as ignore, only electric field is acted on charged particle. Application of cold plasma is self-decontaminating filter, food processing and sterilizing of tooth. (iii) Ultracold plasma: When the temperature of electrons and ions become low as 100mk and 10μk with density \( 2 \times 10^9 \) cm\(^{-3} \), then, plasma is called ultracold plasma. The behavior of ultracold plasma is obtained when Debye screening length becomes smaller than the sample size due to positive ions clouds trapped electrons. Ultracold plasma is considered as strongly coupled plasma because the coulomb interaction energy between the neighbor particles is more than thermal energy of charged particles. Such type of plasma is created in laboratory through pulsed laser and photoionizing laser cooled atoms [20].

1.3 Classification of dusty plasmas

Dusty plasma is characterized by an important parameter, coulomb coupling parameter \( \Gamma \). The Coulomb coupling parameter is explained as, consider there are two dust particles, having same charge and separated by distance ‘a’ from each other. The coulomb potential energy of dust particle is \( \varepsilon_c = \frac{q_d^2}{a} \exp \left( -\frac{a}{\lambda_d} \right) \), where, \( q_d \) is the charge on dust particle, \( a \) is the distance between dust particles and \( \lambda_d \) is Debye screening length of dust particle. The thermal energy of dust particle is \( K_B T_d \). Coulomb coupling parameter is defined as “ratio of coulomb potential energy to thermal energy”. On the basis of coulomb coupling parameter, the dusty plasma is classified in ideal plasma (weakly coupled dusty plasma) and non-ideal plasma.
(strongly coupled dusty plasma) and is represented as $\Gamma_c$. (i) **Ideal plasma**: Ideal plasma is defined by plasma parameter called coulomb coupling and denoted as $\Gamma = \frac{P}{E}$ and is defined as “when kinetic energy of plasma is much larger than potential energy at low temperature and low density”. Ideal plasma is also called weakly coupled dusty plasma and is known by $\Gamma > 1$ this condition. Ideal plasma does not have definite structure due to less collision between particles and low density. Moreover, weakly coupled plasma is defined by plasma parameter called coulomb coupling parameter $\Gamma$. When the value of coupling parameter becomes negligible then plasma is called weakly coupled plasma. Weakly coupled plasma is also called hot plasma. When the temperature of electron becomes equal to temperature of ion ($T_e \approx T_i$) then plasma is called hot plasma or ideal plasma. Hot plasma is generated in laboratory in the discharge tube with high gas pressure. Examples of hot plasma are flame, sparks and atmospheric arcs. Weakly coupled dusty plasma has not specific shape because at low density and high temperature and the interaction between interacting particles becomes very low. (ii) **Non-ideal plasma**: Dusty plasma will be strongly coupled when it satisfies this condition $\Gamma \geq 1$. Strongly coupled dusty plasma is also called nonideal plasma. Dust particle in several laboratory plasma systems is strongly coupled due to their small interparticle distance, low temperature and huge electric charge. Moreover, dusty plasma will be nonideal or strongly coupled, if average thermal energy of charged dust particle is much lesser than average potential energy. Examples of non-ideal plasma are laser generated plasma, brown dwarfs, exploding wires, high power electrical fuses, etc. Furthermore, the Yukawa potential or coulomb coupling potential $\Gamma$ is used to define strongly coupled plasma. The ratio of potential energy to kinetic energy is called coulomb coupling potential. When kinetic energy becomes lower than potential energy i.e., $\Gamma > 1$. Its mean strongly coupled dusty plasma is also called cold plasma because of inter-particle kinetic energy decreases from potential energy and particles in plasma turn into crystalline shape. Crystalline shapes of particles in plasma have examined in many laboratory experiments [1–10]. Food processing and sterilization of tooth are the application of cold plasma. In strongly coupled plasma charge particles are affected by electric field but magnetic field affect is neglected for such type of cold plasma.

### 1.4 Complex (dusty) plasma and applications

Dusty plasma is generally electron ion plasma containing additional charged particulates. This charged component is sometimes termed as dust particle with size of micron. The properties of dusty plasma become more complex when charged particle immerses in plasma. Due to this reason such plasma is called dusty plasma and dusty plasma is also called complex plasma. Dust particles may be made of ice particles or it may be metallic. Dust particles are heavier than ions and their size ranging from few millimeters to nanometer. When dust particle coexists with plasma (electron, ions, neutral and dust particle) it becomes dusty plasma. Dust particle exists in different shapes and size and it presents in entire universe and also in atmosphere. Usually it is solid form but also exists in liquid and gaseous form. Dust particle can be charge by the flow of electron and ions. Charged dust particle is affected by electric and magnetic field and their electric potential varies from 1 to 10 V. Dust particle can be grown in laboratory. Dusty plasma has attracted attention of many researchers Transport properties of dust plasma has played a very important role in the field of science and technology. Mostly the plasma exists in universe is dusty plasma. Dusty plasmas exist in atmosphere of stars, solar wind, sun, galaxies, planetary rings, cosmic radiation, magneto and ionosphere of earth.
Human life is influenced by plasma science. It plays a very significant role in laser developments of fusion energy, sterilizing of medical instruments, plasma processing, intense particle beam, high power energy sources, lightening, high power radiation sources and development of fusion energy controlling. Plasma governs diverse important devices and technological applications. Plasma processing technologies are one of the most important technologies. Plasma processing technologies are playing important role in advance modern technologies of superconductor film growth and diamond film. In addition, the practical application of plasma physics involves the treatment of materials by means plasma technologies. The ionization of system are used to produced particular physical characteristics of plasma, which involve three types of processes, Creation of new materials, Destruction of toxic materials and Superficial modification of existing materials. For industrial process, plasma technology uses two different types of plasma, the cold plasma and thermal plasma. The first type of plasma is cold plasma. Properties of cold plasma are described by electron temperature because electron temperature is greater than ion temperature. The surfaces modification is produced due to plasma particles interact with material, as a result different functional properties of materials are achieved. Cold plasma is produced in vacuum with microwave, dc source or low power rf. The second type of plasma is thermal plasma which is produced at high pressure by radio frequency, microwave source or direct or alternating current. Mostly, thermal plasma is used to devastate toxic materials. Furthermore, plasma has become one of the fast growing research fields which have attracted many researchers. Plasma has advanced applications in the field of industry, textile, plasma chemistry, fusion devices, environmental safety and printing technology and as well as in medical field. In the past decade, plasma physics has become fast developing research in medical field due to increase the atmospheric pressure of plasma sources. Plasma used in medicine has considered the latest developing novel research field with the connection of life science and plasma physics. Moreover, in past ten to fifteen years, World wild research group has set their attention on biological materials with cold atmospheric plasma interactions. Plasma used the field of life sciences in decontamination, in therapeutic medicine and in medical implant technology. The atmospheric pressure of plasma has used to reduce the efficiency of contaminations of food containers and food products. Feed gas humidity is used to adjust the level of contamination. Furthermore, plasma created in polymer tube, used in endoscopes [15–19]. Operating tools such as bone saw blade, neurosurgical and endoscope are sterilized before starting the surgery or dental treatments. Plasma plays a very dominant role in diagnostic system, treatments and in medical instruments. For decontamination of germs and sterilization operation tools, the non-equilibrium discharge plasma is used, is not dangerous for environment and patient as well [21].

2. Molecular dynamics simulations

MD simulation is a powerful technique that can be used to solve many physical problems in atomic material research. MD simulation is handled normally all microscopic information and molecular methods have proven to be the product of applied research. Plasmas and complex liquids have various uses, ranging from semiconductor chips, colloids, thin films, and electrochemistry to biochemical films and other important areas where structures play an important role. MD simulation plays an important role in all the advanced sectors, such as textile science, engineering, physics, plasma physics, astronomy, life sciences or organic sciences, and the chemical industry. Computer simulation has become increasingly important in...
detecting complex motion systems. Using faster and more sophisticated computer systems, it can be studied the habitat, composition, and behavior of large complex systems. In the 1950s, Alder [19], Wainwright and Rahman [19] used the first MD simulations for liquid argon [1–10], their references herein]. MD simulation has two basic kinds which rely on the properties so far which we can be going to calculate; one is EMD simulations (EMDS) and the other one is NEMD simulations (NEMDS). In the present work, NEMD is applied to investigate the thermal conductivity of complex plasma at different dusty plasma parameters.

2.1 Numerical model and algorithm

NEMD simulation is used to detect the dust trajectory of an interacting system using Yukawa forces between dust particles. In present case, the HNEMD simulation (HNEMDS) method is used to calculate the thermal flow of complex (dust) plasma formed using Yukawa interaction taking in to account the charged particles with polarization effects and it is given in the form [22]:

$$\phi_{ij}(r) = \frac{Q_i^2}{4\pi\varepsilon_0} \frac{e^{-|r|/\lambda_d}}{|r|} + \frac{d^2}{r^3} \left(1 + \frac{r}{\lambda_d}\right) e^{-|r|/\lambda_d},$$  \hspace{1cm} (1)

The first term in Eq. (1) provides the screened charge–charge interaction (form of Yukawa interaction) and the second term gives the screened dipole–dipole interaction. Yukawa potential model of dust particles interaction can be established to take into consideration the polarization effect, the temperature and the screening effects. Here $r'$ is the magnitude of interparticle distance, $Q$ is the charge of dust particles, and $\lambda_d$ is the Debye screening length. We have three normalized (dimensionless) parameters to characterize the Yukawa interaction model $\phi_Y(r)$, the Coulomb coupling parameter $\Gamma = \left(\frac{Q^2}{4\pi\varepsilon_0}\right)(1/a_{ws}k_B T)$, where $a_{ws}$ is Wigner Seitz radius and it is equal to $(n\pi)^{-1/2}$, here $n$ is the number of particles per unit area ($N/A$). The $k_B$ and $T$ are Boltzmann constant and absolute temperature of the system, and $A$ is the system area. The second is the screening strength (dimensionless inverse) $\kappa = a_{ws}/\lambda_d$, and additional normalized external force field strength, $F^* = (F_Z)/(a_{ws}/J_Q)$. GK relations (GKRS) for the hydrodynamic transport coefficients of uncharged particles of pure liquids have applied to calculate the thermal conductivity of 2D complex plasma. Here, $J_Q$ is the current heat vector at time $t$ of 2D case [1–4].

$$J_Q(t)A = \sum_{i=1}^{N} E_i F_i \frac{\dot{p}_i}{m} - \frac{1}{2} \sum_{i \neq j} (\hat{r}_i - \hat{r}_j) \cdot \left(\frac{\dot{p}_i}{m} F_{ij}\right)$$  \hspace{1cm} (2)

where $F_{ij}$ is the total interparticle force at time $t$, on particle $i$ due to $j$, $r_{ij} = r_i - r_j$ are the position vectors (interparticle separation), and $\dot{p}_i$ is the momentum vector of the $i$th particle. Where, $E_i$ is the total energy of particle $i$.

$$E_i = \frac{\dot{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \phi_{ij}$$  \hspace{1cm} (3)

$$\dot{r}_i = \frac{\dot{p}_i}{m}, \dot{p}_i = \sum_{j=1}^{N} F_i + D_i(r_i, \dot{p}_i) F_e(t) - \alpha \dot{p}_i.$$  \hspace{1cm} (4)

In Eq. (4), $F_i = -\frac{d\phi_Y(|r|)}{dr}$ is the Yukawa interaction force acting on particle $i$, where $\phi_Y(|r|$ is given from Eq. (1), and $D_i = D_i((r_i, \dot{p}_i), i = 1, 2, ..., N)$ is the phase
space distribution function with $\mathbf{r}_i$ and $\mathbf{p}_i$ being the coordinate and momentum vectors of the $i$th particle in an $N$-particle system. A Gaussian thermostat multiplier ($\alpha$) has been used to maintain the system temperature at equilibrium position and it is given as

$$\alpha = \frac{\sum_{i=1}^{N} \left[ \mathbf{F}_i + \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i).\mathbf{F}_i(t) \right].\mathbf{p}_i}{\sum_{i=1}^{N} \mathbf{p}_i^2/m_i} \quad (5)$$

When an external force field is selected parallel to the $z$-axis $\mathbf{F}_e(t) = (0, F_z)$, in the limit $t \to \infty$. Then the thermal conductivity is given as [8].

$$\lambda = \frac{1}{2k_B T^2} \int_0^\infty \left\langle J_{Q_z}(t)J_{Q_z}(0) \right\rangle dt = \lim_{F_z \to 0} \lim_{t \to \infty} \frac{-\left\langle J_{Q_z}(t) \right\rangle}{TF_z} \quad (6)$$

where $J_{Q_z}$ is the $z$-component of the heat flux vector (energy current). All time series data are recorded during HNEMD and used in Eq. (6) to calculate $\lambda$. The detail of present scheme with all parameters (Gaussian thermostat multiplier, external force, $\mathbf{D}_i, \mathbf{F}_i$, etc) for Yukawa interaction has been reported in our earlier works [8]. The most time consuming part of the algorithm is the calculation of particle interactions (energy and interaction forces). It has been shown in our previous work that the proposed method has the advantage of calculating Yukawa interaction and its associated energy with the appropriate computational power at the right time of the computer simulation. The actual HNEMD simulations are performed between $1.5 \times 10^5 / \omega_p$ and $3.0 \times 10^5 / \omega_p$ time units in the series of data recording of thermal conductivity ($\lambda$). Here, $\omega_p$ is the plasma frequency and it is defined as $\omega_p = (Q_d^2/2\pi\varepsilon_0 m_d a^3)^{1/2}$, where $m_d$ is the mass of a dust particle.

3. Simulation results and discussion

In this section, we have discussed the preliminary results obtained through HNEMED simulation for Coulomb coupling parameters of $\Gamma$ (= 10, 100), polarization values $\Gamma_d$ = (0, 1, 10, 20, 50 and 100) and Debye screening ($\kappa$ = 1.4, 2 and 3) at constant external force field ($F^* = 0.02$) of 2D strongly coupled dusty plasmas. We have chosen suitable number of particles ($N = 400$) in the simulation box with edge length ($L_x, L_y$). Periodic boundary conditions (PBCs) are applied along with minimum image convection in a simulation box of length $L$.

There are different conditions to improve the efficient results of thermal conductivity under polarization effects. These conditions include the system size ($N$), Coulomb coupling ($\Gamma$), Debye screening length ($\kappa$), system total length ($L$), simulation time step ($dt$), and external force field ($F^*$) strength and polarization values ($\Gamma_d$). We have chosen suitable parameters for precise results of thermal conductivity with increasing $\Gamma_d$ and $\kappa$. The simulation data are for a suitable system size ($N = 400$) with different $\Gamma$, which covers the values of strongly coupled plasma states (nonideal gases-liquid to crystalline) at constant force field strength ($F^* = 0.02$) with varying polarization values $\Gamma_d$ (0 to 100).

The polarized thermal conductivity of SCCDPs stated here may be scaled as $\lambda_0 = \lambda n m a d^2$ (by the plasma frequency). It is demonstrated that the $\omega_E$ decreases with increasing $\kappa$, $\omega_E \to \omega_p/\sqrt{3}$ as $\kappa \to 0$, for the 3D case [1–10]. Furthermore, for
the assessment of appropriate equilibrium range (nearly-equilibrium of external field strength) of 2D HNEMD scheme, various sequences of the polarized thermal conductivity corresponding to an increasing order of an external force field \[ F_e(t) = (0, F_z) \] are planned to measure the nearly equilibrium values of the \( \lambda_0 \). This possible appropriate \( F^* \) value gives the steady state \( \lambda_0 \) investigations, which are appropriate for the whole range of plasma states of \( \Gamma \equiv (10, 100) \) and \( \kappa \equiv (1.4, 3) \).

Figures 1–3 illustrate the normalized polarized thermal conductivity (plasma frequency, \( \omega_p \)), as a function of Coulomb coupling (system temperature \( \equiv 1 / \Gamma \)) for the cases of \( \kappa = 1.4, 2 \) and 3, respectively, at constant force \( F^* \) with varying six values of polarizations \( \Gamma_d = (0, 1, 10, 20, 50 \text{ and } 100) \). For three cases, the simulations are performed with setting \( N = 400 \) for \( \kappa = 1.4, 2 \) and 3, respectively, at constant

Figure 1.
Variations of thermal conductivity as a function of Coulomb coupling of strongly coupled complex plasma at \( \kappa = 1.4 \) with \( N = 400 \) and (a) \( \Gamma_d = 0 \), (b) \( \Gamma_d = 10 \), (c) \( \Gamma_d = 20 \), (d) \( \Gamma_d = 50 \), (e) \( \Gamma_d = 50 \) and (f) \( \Gamma_d = 100 \).
Performing HENMD simulations with varying polarizations at constant $F^*$ we examined the efficiency and reliability of the polarized $\lambda_0$ measurements. For three cases, we evaluate the six various simulation data sets covering from nonideal state ($\Gamma = 10$) to a strongly coupled liquid regime ($\Gamma = 100$). Figures show that the effects of polarization on the thermal conductivity have no significant changes and it is seen that the thermal conductivity remains constant under varying polarizations. However, the present results of thermal conductivity under varying polarizations are satisfactory agreement with earlier known available numerical data for a complete range of plasma parameters.

Figure 4 shows comparisons with earlier available 2D and 3D numerical data of thermal conductivity with setting $N = 1024$ and $\Gamma_d = 1$. The current results are
generally excellent agreement for the whole Coulomb coupling range and plot show overall the same behaviors as in the earlier simulation method s of 2D plasma systems. Figure involve the earlier work of 3D HNEMD and HPMD by Shahzad and He [8, 16, 23], EMD investigations of Salin and Caillol [12] and 3D theoretical prediction of Faussurier and Murillo [13] as well as 2D GKR-EMD of Khrustalyov and Vaulina [24].

Figure 3. Variations of thermal conductivity as a function of Coulomb coupling of strongly coupled complex plasma at $\kappa = 3.0$ with $N = 400$ and (a) $\Gamma_d = 0$, (b) $\Gamma_d = 10$, (c) $\Gamma_d = 20$, (d) $\Gamma_d = 50$, (e) $\Gamma_d = 50$ and (f) $\Gamma_d = 100$. 

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4. Conclusions

The HNEMD scheme is used for the investigation of thermal conductivity under the influence of varying polarization values for various screening lengths $\kappa$ (= 1.4, 3) and Coulomb couplings $\Gamma$ (= 10, 100) but constant force field strength. It has been shown that the current HNEMD scheme with polarization and earlier HPMD and GKR-EMD techniques have comparable efficiency over the suitable range of plasma parameters, both generating reasonable data of polarized $\lambda_0$. New simulation results provide more reliable and ample results for the polarized thermal conductivity for a whole range of $(\Gamma, \kappa)$ than previous known simulation data. Thermal conductivity results estimated from this newly developed HNEMD scheme are in well matched with available numerical results generally underpredicting within $\pm 20\%$ - $35\%$. The current HNEMD data with less statistical noise and best efficiency have been computed by taking different parameters $(N, 1/\Gamma, \kappa$ and $\Gamma_d)$ for the current HNEMD scheme to measure the thermal conductivity of 2D DP systems, at constant $F^* = 0.02$. For future work, the HNEMD method introduced here may easily extend to other physical systems with varying force field with modifications.

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Abbreviations

| Abbreviation                                                                 | Description                                |
|-----------------------------------------------------------------------------|--------------------------------------------|
| Strongly coupled complex dusty plasmas                                       | (SCCDP)                                    |
| Homogeneous non-equilibrium molecular dynamics                              | (HNEMD)                                    |
| Coulomb coupling                                                            | \( (\Gamma) \)                             |
| Debye screening length                                                       | \( (\kappa) \)                             |
| External force field strength                                                | \( (F') \)                                 |
| Homogenous non-equilibrium molecular dynamics                               | (HNEMD)                                    |
| Non-equilibrium molecular dynamics                                          | NEMD                                       |
| Molecular dynamics                                                           | (MD)                                       |
| Inhomogenous non-equilibrium molecular dynamics                             | (In HNEMD)                                 |
| Strongly coupled plasma                                                     | (SCP)                                      |
| Equilibrium molecular dynamics                                              | (EMD)                                      |
| Thermal conductivity                                                        | \( (\lambda) \)                            |
| Normalized thermal conductivity                                             | \( (\lambda_0) \)                          |
| Number of Particles                                                         | \( (N) \)                                  |

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