I. INTRODUCTION

In recent years, the interest in the transport knowledge of complex nonideal fluids has grown notably because of its applications in science and engineering. The study of natural phenomena and flow of non-Newtonian liquids is under rapid development in the nonlinear science and dynamical systems theory. This is mostly due to their numerous applications in the paper industry, manufacturing and processing of semiconductors, petroleum industry, and many other industrial applications, for example chromatography, packed bed reactors, biomechanics, filtration processes, insulation systems, enhanced oil recovery, ceramic processing, and many others. The dynamical properties in complex nonideal systems of interacting particles are of practical importance in various fields of science and technology. Thermal conductivity is important for the application of heat process and equipment design involving mass transport processes. Many investigation techniques for thermal transport have been derived. Partly motivated by the study of Non-Newtonian fluids, recent experimental work\cite{1} revealed that the complex plasma fluid has the signature of non-Newtonian property similar to other non-Newtonian fluids. Many researchers have documented the fact that non-Newtonian flow and natural phenomena are basically temporal, spatio-temporal, and or force-temporal processes.\cite{2} The derivation of new concepts from the dynamical systems theory shed light on the dynamics of many-body systems which has been examined in nonequilibrium statistical mechanics and thermodynamics for the last two decades. The issues of dynamics of non-Newtonian complex liquids present diverse challenges to applied physicists, mathematicians, numerical analysts, and modelers in developing appropriate numerical algorithms for calculating the transport behaviors.

Nonideal complex (dusty plasmas) systems 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.\cite{3} In industrial plasma processes, dust particles are produced from molecules in ionized gases to nanometer size particles.\cite{4} The existence of this new dust particle is predicted to result in novel effects in the collective-mode behavior in the plasma\cite{5} and the dynamical behavior of dusty plasma is more complex than the dynamics of the gases and liquids. Moreover, it is interesting to study that the number of forces applied on the multispecies charged fluid (dusty plasmas) is usually insignificant in typical plasmas. There are different ways for employing these forces and dust particles may be confined in various configurations which allow the study of equilibrium and dynamics in nonideal dusty plasmas in different geometries. Currently, various functional statistical mechanical
approaches to the microscopic dynamical system theory of transport problems have been developed for simple and complex fluids. In complex physical systems, for instance complex fluids (dusty plasma), different physical transport processes exist and interact simultaneously. 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 nano- and micro- technological processes. 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 final goal of many thermophysical researchers.

From different literature studies, the non-Newtonian fluids are mainly characterized on the basis of their dynamics in external force or shear rate. A fluid with a linear relationship between the heat flux and the external force, giving rise to a constant thermal conductivity, may be described as a Newtonian fluid. The Navier–Stokes equations are used for the description of flows of Newtonian fluid and precise solutions for Navier–Stokes equation are exceptional. For deep understanding of microscale processes, the molecular dynamics (MD) computer simulation methods have long been used and are well developed as a tool in statistical mechanics and chemistry. Currently, it is a still challenging issue to extend the approach to the spatial and temporal scale of macroscopic heat transport phenomena. In the semiconductor industry, thin film technology development demands the estimation of heat transport processes of nanometer level materials. The most powerful tool for the examination of the microscopic phenomena in heat transport is the MD simulation technique. The two most frequently used approaches in molecular simulations are the “direct technique” and the Green–Kubo relation (GKR). These computer simulation techniques are classified as nonequilibrium molecular dynamics (NEMD) simulations and equilibrium molecular dynamics (EMD) simulations for the determination of transport properties of fluids. Practically, the heat transport is a nonequilibrium phenomenon and the direct simulation method (NEMD) of the heat transfer problem is much more preferred. It has been shown that NEMD methods are faster and efficient in terms of computer time as compared to EMD methods. Various past MD simulation investigations on the thermal conductivity are based on generally three NEMD techniques that use a temperature gradient, a heat energy flux, and a homogeneous field (external force) technique. The first two computer simulation methods have some disadvantages that are reported by Ciccottia et al. In the last mentioned technique, the impose forces are used in the equations of motion to generate a required heat energy flow and the thermal conductivity is then obtained from the heat energy flux and external force field relationship.

In the last 15–20 years survey of the theoretical perspective, we give a short overview of computer simulation techniques that can be used to overcome the thermal transport barriers in order to compute the thermal conductivity in linear and nonlinear regimes. This paper also provides the comprehensive results that help to review a current picture of modification in the model of thermal conductivity for different ranges of plasma state points of the strongly coupled Yukawa fluids (SCYFs). In a non-Newtonian fluid, the thermal conductivity ($\lambda$) may vary with the applied field (external) strength, where as in the Newtonian fluid it does not happen. Hoover and Ashurst reported calculations of thermal conductivity through their model based on the temperature gradient. Soon after, Evans introduced an improved HNEMD method to calculate the thermal conductivity, with a low value of external perturbation of the LJ fluid, through the autocorrelation function of the microscopic heat energy current. A considerable amount of theoretical studies and computer simulations have been done to understand the thermal conductivity in simple and molecular liquids and their reference herein. The 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, and Mandadapu et al. 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, Wang et al. and Mandadapu et al. 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 two-dimensional (2D) and three-dimensional (3D) SCYFs. Pierleoni et al. 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 SCYFs was calculated by GKR–EMD simulation of and an extended variational procedure (VP) of Faussurier and Murillo, and inhomogenous NEMD (InHNEMD) work of Donkó and Hartmann. Very recently, Shahzad and He have employed the homogenous perturbed MD (HPMD) and HNEMD methods and computed the thermal conductivity of 3D SCYFs. Moreover, numerous calculations of the thermal properties have been studied for the behavior of 2D SCYFs in Refs. 8 and 27, and their reference herein, and transport properties have been considered for the behavior of 3D SCYFs. A full understanding of 3D thermal conductivity and even of 2D strongly coupled dusty systems is still lacking. This shows the ongoing debate on the existence and nature of thermal coefficients in the linear and nonlinear regimes of 3D SCYFs with Yukawa interactions and it indicates current extension in the field of applied plasma physics.

The main targets of this reported work are to study the effects of external force field strengths on plasma thermal conductivity ($\lambda_0$) of SCYFs at the corresponding plasma state points ($\Gamma$, $\kappa$) and to enlarge and find out the linear regime of external force fields by employing the same approach as
introduced in our earlier work\textsuperscript{26,27} with suitable higher system sizes (N). Moreover, it is for the first time to delve the understanding of linearity behaviors in 3D SCYFs along with the calculations of near-equilibrium plasma thermal conductivity. Recently, we have been reported the numerical results for 3D strongly coupled dusty plasmas in literature studies,\textsuperscript{26,34} where we have published data with constant force fields (\(F_0 = 0.002\) and 0.005) and some preliminary results\textsuperscript{35} for the thermal conductivity. In this paper, we extend our numerical results for the estimations of plasma \(\lambda_0\) for a wide range of external force fields (\(F_0\)) than those employed in former known simulation results of the 3D SCYFs\textsuperscript{23–26,34,35} and at different higher system sizes (N). This range of external force fields is acceptable for the computation of near-equilibrium outcomes of plasma \(\lambda_0\) for the complete and higher range of plasma parameters (\(\Gamma, \kappa\)). Moreover, we estimate the effect of screening parameter \(\kappa (\equiv 1, 6)\) of dust on the plasma \(\lambda_0\) with different system sizes and system temperatures (1/\(\Gamma\)). The influence of external force field along with \(\kappa\) on the plasma \(\lambda_0\) of the 3D strongly coupled plasma system of dust particles is another motivating task that is examined for near-equilibrium conditions.

II. NUMERICAL METHOD

A. Theory and HNEMD algorithm

To simulate the behavior of dust particles in a dusty plasma, the determination of a suitable interaction potential is critical. The Yukawa interaction potential, a screened Coulombic potential, is the most common model that is currently employed for investigating the interaction between charged dust grains (particles) in a dusty plasma\textsuperscript{7,23–27,32–35}

\[
\phi_y(|r|) = \frac{Q_d^2}{4\pi\varepsilon_0} \frac{e^{-|r|/\lambda_D}}{|r|},
\]

where \(\lambda_D\) represents the Debye screening length, \(r\) represents the interparticle spacing (of the dust particles), and \(Q_d\) is the charge on the dust particle. The Ewald Summations is used to account for the pairwise interactions between particles and further details can be found in Refs.\textsuperscript{25–27 and 36}. In addition to being used to describe the pairwise interaction between dust particles, this interaction model is also used to describe the interactions that are present in many practical (physical) systems of interest, including biomedicine, astrophysics, chemical and biological systems, physics of polymers, hydrodynamics, and aerodynamics, and materials for energy generation.

A well known form, Green-Kubo equations (GKEs) for the thermal conductivity parameter of uncharged particles,\textsuperscript{6} of the relevant transport equations with screened interaction models can minimize the difficulties typically encountered when using MD simulation to study transport processes in dusty plasmas. These GKEs have been applied to understand the behavior of charged particles in a dusty plasma\textsuperscript{7,9,22–27}. The GKEs of a simple liquid have been employed to estimate the thermal conductivity, shear viscosity, and diffusion coefficients, respectively, of 2D and 3D SCYFs and weakly coupled plasmas\textsuperscript{8,32–36}

\[
\lambda = \frac{1}{3k_B T V^2} \int_0^\infty \langle \mathbf{J}_Q(t) \mathbf{J}_Q(0) \rangle dt,
\]

where in Eq. (2), \(T\) and \(V\) are the absolute temperature and volume of the system, respectively, and \(k_B\) represents the Boltzmann’s constant. In our MD simulation, the angular brackets estimate the average over all dust particles (ensemble average) in the simulation domain. The microscopic heat flux vector \(\mathbf{J}_Q(t)\) is given by the expression

\[
\mathbf{J}_Q(i)V = \sum_{i=1}^{N} E_i \frac{\mathbf{p}_i}{m} - \frac{1}{2} \sum_{i \neq j} r_{ij} \left( \frac{\mathbf{p}_i}{m} \cdot \mathbf{F}_{ij} \right),
\]

where \(r_{ij}(t) = r_i(t) - r_j(t)\) and \(\mathbf{F}_{ij}(t)\) are the interparticle separation (position vector) and total interparticle force at time \(t\), respectively, on particle \(i\) due to \(j\), and \(\mathbf{p}_i\) is the momentum vector of the \(i\)th particle. Further details on the thermal transport equations can be found in Refs.\textsuperscript{6–9}, and a detailed discussion of the microscopic expression has been reported in Refs. \textsuperscript{26 and 27} for the heat flux vector (\(\mathbf{J}_Q\)) of Yukawa potential. The sum of kinetic Energy \((p_i^2/2m)\) and potential energy \((1/2 \sum \phi_y)\) is the total energy \(E_i\) of particle \(i\), given by

\[
E_i = \frac{p_i^2}{2m} + \frac{1}{2} \sum_{j \neq i} \phi_y,
\]

where \(\phi_y\) is the Yukawa pair potential between particle \(i\) and \(j\) and given by Eq. (1). The Evan’s non-Hamiltonian linear response theory (LRT) has been used for a system showing equations of motion

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

\[
\dot{\mathbf{p}}_i = \sum_{j=1}^{N} \left[ \mathbf{F}_i + \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i).\mathbf{F}_i(t) \right] - 2\mathbf{p}_i,
\]

where \(\alpha\) is the Gaussian thermostat multiplier that maintains the system temperature, and it is given as

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

\(\mathbf{F}_i(=-\partial\phi_y/\partial\mathbf{r}_i)\) is the total interparticle force acting on particle \(i\) and \(\mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i)\) is the tensor phase variable that gives the coupling of system to the fictitious external force field \(\mathbf{F}_i(t)\). Recently, we have reported a detail examination on the Yukawa conductivity outcomes and discussed the tensor \(\mathbf{D}_i = \mathbf{D}_i(\mathbf{r}_i, \mathbf{p}_i)\) element in terms of Ewald-Yukawa sums for the case of microscopic heat flux vector \(\mathbf{J}_Q(t)\) for a Yukawa system.\textsuperscript{7,26} The LRT is applied in a simple method for a system given in Ref. \textsuperscript{6}. The external force field \(\mathbf{F}_i(t)\) that performs the work done on the system and equilibrium is maintained by applying the thermostat \(\alpha\), given by Eq. (7).\textsuperscript{12,15} The external force field parallel to the z-axis is of
the form $F_\alpha(t) = (0, 0, F_z)$, in the limit $t \to \infty$, therefore, the plasma thermal conductivity is computed as

$$\lambda = \frac{1}{3k_BT^2} \int_0^\infty \langle J_Q(t)J_Q(0) \rangle dt = \lim_{F_z \to 0} \lim_{t \to \infty} \frac{-\langle J_Q(t) \rangle}{TF_z}, \quad (8)$$

where $J_Q(t)$ is the z-component of the heat flux vector. The plasma parameters of SCYFs can be explained by three normalized parameters: the first is the plasma coupling parameter $\Gamma = (Q^2/4\pi a^3)ak_BT$, where $T$ is the system temperature (in energy units), $k_B$ is the Boltzmann’s constant, and $a_w=(3/4\pi n)^{1/3}$ is the Wigner–Seitz (WS) radius (average separation between the nearest dust) with $n=N/V$ being the number density of the dust particle, the second is the Debye screening parameter $\kappa \equiv a_w/\lambda_D$, where $\lambda_D$ is Debye screening, and third is the external force field strength $F^*=(F_z)/(a_wJ_Qz)$, where $J_Qz$ is the heat current (thermal energy) and the external force field strength $F_e(t) = (F_z)$.7–9,26,27,34

B. Simulation technique and parameters

In this section, we present the modeling and implementation features of our presented HNEMD simulation to calculate the thermal transport coefficients of 3D SCYFs. This HNEMD simulation employed an improved effective potential to allow researchers to recognize the underlying mechanism(s) that govern the thermal transport properties and the effect that the non-Newtonian behaviors have on the equilibrium and non-equilibrium dynamics. This simulation method also provides a guide for the experimental efforts that will determine the appropriate simulation parameters for implementing our improved techniques.

The simulations of this plasma system involve particle number, $N$, from 500 to 4000–13 500. For this plasma system, the pairwise Yukawa interaction has already been described (see Sec. II A) that computed the periodic boundary conditions with the minimum image convention for the dust particles. The edge size of the simulation box is calculated as $L/a_w$, and the number of particles is chosen to be sufficiently large such that the results are independent of the size effects (earlier simulations have shown that the particle range is sufficient when using the Yukawa interaction model).7,9,26,34,35 The total interaction force, $F_i = -\frac{\partial U}{\partial r_i}$, is computed on an individual dust particle and the corresponding acceleration of the i\textsuperscript{th} particle is calculated using the Newton’s second law of motion, $a_i = F_i/m_i$.37 Using an MD simulation step $dt$, the measured acceleration is used to find the particle’s velocity and position at the next time. This process is repeated for every particle in the system. These steps are continued for a given number of simulation time steps. It is noted that the calculation of these interaction forces needs more than 75% to 80% of the computational time due to the fact that the pair interactions between the plasma particles need be computed. In the current simulations, the time steps are 0.005 $\omega_0^{-1} \leq dt \leq 0.001 \omega_0^{-1}$, where $\omega_0 = (Qz^2/4\pi a^3m^2)^{1/2}$ is the plasma frequency of the dust particles and $m$ is the mass of the dust particle.7–9,26,27,34,35 A predictor-corrector method is used when solving these equations numerically to calculate the desired forces and the Ewald sums scheme is used to account for the long-range interactions of plasma particles.36,37 Further details related to the Ewald sums approach SCYFs can be found in Ref. 36. In our simulation, the algorithm for the transport equations modeling (i.e., the pairwise plasma particle interaction forces, heat energy, etc.) is employed as a $\kappa$-dependent cutoff radius technique. The output steps are estimated between simulation time steps of $3.0 \times 10^7/\omega_0$ and $1.5 \times 10^7/\omega_0$ for the investigation of transport data. These calculations are employed over a wider range of plasma parameters of $1 \leq \Gamma \leq 300$ and $1 \leq \kappa \leq 6$ using improved fast effective algorithms for extended $F^*$.

III. RESULTS AND DISCUSSION

In this part, we present the numerical results obtained by using the HNEMD approach [Eq. (8)] for the thermal transport coefficient ($\lambda$) of 3D SCYFs as a function of system temperature ($\equiv 1/\Gamma$) and external force field strength $F^* = (F_z/a_wJ_Qz)$ at different Debye screening parameters ($\kappa$) and number of particles ($N$). The thermal conductivity is reported here with suitable normalization ($\omega_0$), in the limit of an appropriate linear range of low normalized external force field $F^*$, for a wide range of plasma states of Coulomb coupling ($\Gamma \geq 1$) and Debye screening ($\kappa \geq 1$). This normalization has been widely employed for the estimation of thermal conductivity of the earlier studies of one component complex plasmas (OCPPs)22 and SCYFs 7–9,23–29,32–36. The presented HNEMD approach to 3D SCYFs makes it possible to investigate all the possible ranges of plasma state points ($\Gamma, \kappa$) for different $F^*$ and $N$. The thermal conductivity reported here can be normalized as $\lambda_0 = \lambda/nk_BTQz^2$ (by the plasma frequency, $\omega_0$). It has been demonstrated that the Einstein frequency decreases with an increase of $\kappa$, $\omega_E-\omega_0/3$ as $\kappa \to 0$ and $\lambda_0 = \lambda^*/(3\omega_E/\omega_0)$.7,26 The normalized thermal conductivity with various applied external force field strengths is compared and discussed. In the present case, we simulate a set of heat (thermal) fluxes by an external force field using the HNEMD (Evans’) approach for the SCYFs and disturb the system with normalized force of strength $F_z$. Moreover, the Gaussian thermostat is used in order to maintain the temperature of SCYFs prior to the switching on of the external force field $F^*$ that generates the canonical ensemble given in Eq. (9) of Ref. 26. Practically, it is essential for the NEMD approach to be thermostated in order to remove the heat due to the work done by the external force field strength $F^*$. For efficient simulation, and in order to obtain data from the present homogenous NEMD technique, we need to consider different parameters. In our case, these parameters including screening strength ($\kappa$), plasma coupling (system temperature $\equiv 1/\Gamma$), system size ($N$), external field strength ($F^*$), thermostat ($x$), simulations proceeded length (total run time), and simulation step time ($\Delta t$) are varied to compute how these parameters can influence the thermal conductivity of SCYFs.

In the present work, we have implemented the recently developed relation for the heat (thermal) flux7,26 to estimate the thermal conductivity of strongly coupled dusty plasmas through the classical HNEMD method. Now, we focus our attention to the simulation results, shown in Figs. 1–6, where we obtained the plasma thermal conductivity during
HNEMD simulations of standard dust particles in 3D within the strongly coupled regime for different $\Gamma$ and $N$ at $\kappa = 1, 2, 3, 4, 5,$ and $6$. These figures illustrate the key results for the plasma thermal conductivity as well as the earlier simulation results taken from Salin and Caillol (Ref. 23); GKR-EMD (SC), Inhomogenous NEMD of Donkô and Hartmann (Ref. 25); InHNEMD ($N = 1600$ and 6400), homogenous perturbed MD of Shahzad and He (Ref. 7); HPMD (SH), and a theoretical variational procedure of Faussurier and Murillo (Ref. 24); VP (FM). The dashed (central) lines represent the reference set of data ($\lambda_{\text{REF}}$) that are taken from Ref. 26. The dotted lines show $\pm 20\%$ deviation of our presented data from the $\lambda_{\text{REF}}$. (b) Variation of the obtained results $\lambda_0$ ($F^*, \Gamma$) as a function of $\Gamma$ (vertical) and $F^*$ (horizontal) at $\kappa = 1$ and 2 ($N = 500$). The horizontal axes are multiplied by a factor (10 000 and 20 000) which magnifies the $F^*$.
lower and higher than the $F^*$ values shown in panels (a) are also checked for various combinations of plasma states in order to found the linear range for the homogenous plasma $\lambda_0$. The external force filed of $F^* < 0.001$ and $F^* > 0.1$ give very noisy measurements for both lower and higher $\Gamma$ values, respectively. Our simulation data of $\lambda_0$ are in nearly satisfactory agreement with earlier simulation data performed by different research groups based on different numerical approaches and show that the presented HNEMD approach and earlier GKR-EMD and PHMD methods have equivalent performance, all yielding the close investigations for the plasma $\lambda_0$ with different $N$.

$\lambda_0$ ($\Gamma, F^*$), shown in Figs. 1–6, are performed for $N = 500$ and 4000 ($\kappa = 1, 2, 3$ and 4) and $N = 13 500$ (for $\kappa = 1, 2, 3, 4, 5$ and 6) particles at varying values of $F^*$. Figures 1 and 2 display the plasma thermal conductivity $\lambda_0$ ($\Gamma$) normalized by plasma frequency $\omega_0$, as a function of plasma coupling ($\Gamma$) for $\kappa = 1$ and 2, respectively. For both cases, the SCYF system is composed of a total of $N = 500$ and 4000 particles and a sequence of nine different calculations (total of 36 simulations) is performed with varying external force field strengths. Performing HNEMD computations with various system sizes for varying $F^*$, we examined the accuracy and consistency of the plasma $\lambda_0$ investigations. For these two
In cases, we compare the thirty six different simulation data sets, together with previous 3D computation data points, covering from the nonideal position ($C_1 = 1$) to nearly strongly coupled positions ($C_1 = 100$ for $\kappa = 1$ and $C_1 = 300$ for $\kappa = 2$). The graphs illustrate the reasonable agreement among the different numerical results and the uncertainties inherent to the different techniques are comparable. Here in these graphs, the results obtained with $N = 13500$ for $F^* = 0.005$ are taken as the reference results and calculate the other numerical results normalized by these reference results ($\lambda_{\text{REF}}$) (as explained above). The previous numerical results of GKR-EMD,\textsuperscript{23} InHNEMD,\textsuperscript{25} HPMD,\textsuperscript{7} and VP\textsuperscript{24} are also normalized by these reference results ($\lambda_{\text{REF}}$) shown in Figs. 1(a) and 2(a), except the data at $\Gamma = 200$ and 300 ($N = 4000$) and $\kappa = 2$ ($F^* = 0.005$) because the earlier results are not accessible. These data points ($\Gamma = 200$ and 300) are normalized by a reference set of results ($\lambda_{\text{REF}}$) taken as the results from HPMD at $N = 13500$ for $P_{ex} = 0.005$ and are reported in Ref. 26. It is examined
that our HNEMD simulation results are generally in fair agreement with parts of GKR-EMD and InHNEMD results for the complete plasma range and the graphs show overall the same behaviors as expected in the earlier simulation methods for 3D Yukawa systems. For most of plasma states of \( 1 \leq \Gamma \leq 100 \) \((N = 500 \text{ and } 4000, \text{ at } \kappa = 1 \text{ and } 2)\), the presented simulation results match well with each other, earlier simulation results and reference set of data, and the plasma \( \lambda_0 \) is normally overpredicted, depending upon the combination of plasma state points \((\Gamma, \kappa)\). However, in the case of \( \Gamma > 100 \) \((N = 500 \text{ and } 4000, \text{ at } \kappa = 2)\), our results of plasma \( \lambda_0 \) are underpredicted and most of the present data points are within less than a 20% range around the reference set of data (dotted lines shown in graphs). Moreover, it is to be noted that very noisy measurements of plasma \( \lambda_0 \) are generated at the normalized force field strength range of \( 0.007 \leq F^* \leq 0.009 \) \((\Gamma = 300 \text{ and } N = 500), 0.001 \leq F^* \leq 0.004, \text{ and } 0.005 \leq F^* \leq 0.009 \) \((\Gamma = 300 \text{ and } N = 4000)\) at \( \kappa = 2 \). It is further examined that the complete normalized force field \( F^*(0.001–0.1) \) generates very noisy measurements of plasma \( \lambda_0 \) mainly at the lower \( \Gamma < 1 \) and

**FIG. 4.** (a) Comparison of measured results of normalized plasma \( \lambda_0/k_{\text{REF}} \) \((k)\) by the presented HNEMD approach at screening \( \kappa = 3 \) and 4 \((N = 4000)\) for different plasma coupling \( \Gamma \) \((\equiv 1, 300)\) and varying external force fields \( F^* \) \((\equiv 0.001, 0.009)\); for details, see the caption of Fig. 1. Variation of obtained results \( \lambda_0 \) \((F^*, \Gamma)\) as a function of \( \Gamma \) (vertical) and \( F^* \) (horizontal) at \( \kappa = 3 \) and 4 \((N = 4000)\). The horizontal axes are multiplied by a factor \((10000)\) which magnifies the \( F^* \).
higher \( \Gamma > 300 \) for \( N = 500 \) and 4000 and \( \kappa = 1 \) and 2. The simulation observable linear regime of \( F^* \) is established between 0.001 \( \leq F^* \leq 0.009 \), as shown in Figs. 1(a) and 2(a) for \( \kappa = 1 \) and 2, where plasma \( \lambda_0 \) is independent of \( F^* \) within limited statistical uncertainties. Exterior to this regime, the plasma \( \lambda_0 \) is strongly dependent on \( F^* \) and linearity is not maintained. These Figs. 1(a) and 2(a) suggest that all the presented investigations lie within less than a \( \pm 20\% \) range around the reference set of points \( \lambda_{0,\text{REF}} \).

Parts (b) of Figs. 1 and 2 show the variation of plasma \( \lambda_0 \) (\( \Gamma, F^* \)) with different plasma couplings \( \Gamma \) and normalized force fields \( F^* \) for SCYF at \( \kappa = 1 \) and 2. There are various multiplication factors that are to be considered in order to obtain the best results of plasma \( \lambda_0 \) by the HNEMD technique. In our present case, a factor of (10 000) is multiplied to the external force field strength \( F^* \) values that field strength is magnified for plotting as shown in graphs (b) for \( \kappa = 1 \) (\( N = 500, 4000 \)) and 2 (\( N = 4000 \)). For \( \kappa = 1 \) (\( N = 500 \)), we multiply a factor of (20 000) to the force field \( F^* \) that magnifies the plotting axis apparently. It is to be noted that the system size \( (N) \), field strength \( (F^*) \), system temperature \( (\Gamma) \), and screening strength \( (\kappa) \) are the major
parameters for investigating the plasma $\lambda_0$. These parts (b) of both figures illustrate the variation of plasma $\lambda_0$ with an increase of $F^*$ for different combinations of plasma states of $\Gamma \equiv (1, 300)$, $\kappa \equiv (1, 2)$, and for $N = 500$ and 4000, keeping linearity in the framework of the linear response theory.\(^6\) It is observed from these two parts (b) of Figs. 1 and 2 that the plasma $\lambda_0$ values remain nearly straight for lower $\Gamma$ ($\equiv 1, 2$) and the $\lambda_0$ gradually seems wavy for intermediate $\Gamma$ ($\equiv 5, 10$). It is an interesting case where the combined effect of $F^*$ and lower $\Gamma$ shows the maximum value of plasma $\lambda_0$ in the SCYS over the complete range of force field $F^*$. Moreover, these wavy shapes show that the plasma $\lambda_0$ remains close to each other and the reference set of data $\lambda_{REF}$ for varying $F^*$ corresponding to each low values of $C$ and linearity is maintained. It is clearly depicted that there is no significant effect of external force field $F^*$ on plasma $\lambda_0$ showing increasing or decreasing behaviors of $\lambda_0$ at lower values of $\Gamma$ (system temperature $\equiv 1/\Gamma$). However, instead, constant plasma $\lambda_0$ is observed for
intermediate to higher $\Gamma$ (≈ 20, 100) that is initially growing and then decreasing finally with increasing $F^*$. It is examined from the affected region (shown off white) that the plasma $\lambda_0$ increases for the range of $0.001 \leq F^* \leq 0.007$ ($\kappa = 1$, $N = 500$ and 4000), $0.001 \leq F^* \leq 0.002$ ($\kappa = 2$, $N = 500$), and $0.001 \leq F^* \leq 0.004$ ($\kappa = 2$, $N = 4000$), and decreases for the range of $0.007 \leq F^* \leq 0.009$ ($\kappa = 1$, $N = 500$ and 4000), $0.002 \leq F^* \leq 0.009$ ($\kappa = 2$, $N = 500$), and $0.004 \leq F^* \leq 0.009$ ($\kappa = 2$, $N = 4000$) with an increase of $F^*$. It is noted that a decreasing behavior is shifted towards higher $\Gamma$ with an increase in $\kappa$, but within a relatively limited statistical uncertainty.

Two sets of Figs. 3 and 4 show the plasma $\lambda_0$ obtained from the ratio of heat flux and external force field ($J_{Q2}(t)/F_2$) as a function of plasma coupling $\Gamma$, setting $N=500$ and 4000 particles for the cases of $\kappa = 3$ and 4, respectively. The parts (a) of these figures illustrate the main results and also show the numerical calculations taken from the 3D GKR-EMD work of Ref. 23, InHNEMD investigations of Ref. 25, HPMD simulations of Ref. 7, and VP results of Ref. 24. For both cases, we compare the total of thirty six different HNEMD computation data sets with each other corresponding to varying external force fields, and these data sets are normalized with the reference set (as explained above) of data ($\lambda_{0\text{REF}}$), and together with earlier normalized numerical results. Figures 3(a) and 4(a) provide a normally excellent agreement of our numerical results with different data of GKR-EMD, InHNEMD, and HPMD simulations. It is observed that most of the plasma $\lambda_0$ data points match well with each other and reference set of data, and $\lambda_0$ is usually overpredicted at the low $\Gamma$ (1, 5) and high $\Gamma$ (50, 100) and underpredicted at intermediate $\Gamma$ (10, 20) for $N=500$ ($\kappa = 1$). However, the plasma $\lambda_0$ state points matched the reference data line for $N=4000$ ($\kappa = 1$) excellently. In the case of $\kappa = 2$ ($N=500$ and 4000), the presented simulation results closely match the reference set of data (dotted lines as shown) and the majority of data points are underpredicted for $1 \leq \Gamma \leq 100$. At higher $\Gamma$ (200, 300), some of the data points of plasma $\lambda_0$ are overpredicted for both cases. Furthermore, it is observed that noisy calculations of plasma $\lambda_0$ are observed mainly at higher $\Gamma$ (200, 300) for $N=500$ and 4000 ($\kappa = 3$). The linear regime in the HNEMD approach is found computationally in the range of $0.001 \leq F^* \leq 0.009$ for both the cases. It is noticed that most of the presented simulation results fall within less than ±20% range around the reference set of points ($\lambda_{0\text{REF}}$), regardless of the external force field strengths in the HNEMD method. Figures 3(b) and 4(b) show the variation of plasma $\lambda_0$ versus different combinations of $\Gamma$ and $F^*$ for $N=500$ and 4000 at $\kappa = 3$ and 4, respectively. For $N=500$ and $\kappa = 3$ (4) case, a factor of 20 000 (30 000) is multiplied to normalized $F^*$ values that force field is magnified for scaling along the horizontal axis (i.e., $x$-axis) and we multiply a factor of (10 000) to $F^*$ for $N=4000$ and $\kappa = 3$ (4) case. It is to be noted from these parts (b) that the plasma $\lambda_0$ decreases with increasing $\Gamma$ and $F^*$ and combined effect of higher $\Gamma$ and $F^*$ demonstrates the decreasing trend for $\kappa = 3$ ($N=500$). It is clearly shown from parts (b) of Figs. 3 and 4 that the affected region (shown off white) of plasma $\lambda_0$ reduces gradually as we move towards higher $\kappa$ (from $\kappa = 1$ to 4).

The HNEMD simulated results for plasma $\lambda_0$ as a function of $\Gamma$ are plotted in Figures 5 and 6, for lower and higher $\kappa$, respectively, under varying force field strengths. The simulations are performed with extended number of particles up to $N=13 500$ and Debye screening strength up to $\kappa = 1, 2, 3, 4, 5, 6$. It is to be noted that different sequences of simulations are carried out with various values of external force field, ten for $\kappa = 1$ and 3, eleven for $\kappa = 2, 5$ and 6, and twelve for $\kappa = 4$. For both figures, we evaluate sixty five different simulation results with each other and earlier numerical results. Here, it is recalled that all present and earlier data sets are normalized by a reference set of data points ($\lambda_{0\text{REF}}$), as explained earlier. It is remarkable that the presented HNEMD approach provides computations for plasma $\lambda_0$ within the limited statistical uncertainties for the wide range of appropriate system sizes ($N=500$ to 13 500) and have significant results for higher screening parameters. It is observed that the presented plasma $\lambda_0$ results lie more close to earlier GKR-EMD,$^{23}$ InHNEMD,$^{25}$ and HPMD$^7$ simulations and are significantly higher than the earlier prediction results of VP, expect at $\kappa = 2$ where the present results are close to theoretical estimations. From Figs. 5 and 6 it is found that the range of normalized $F^*$ is extended up to 0.001 $\leq F^* \leq 0.05$ ($\kappa = 1$ and 3), 0.001 $\leq F^* \leq 0.1$ ($\kappa = 2, 5$ and 6), and 0.001 $\leq F^* \leq 0.5$ ($\kappa = 4$). It is interesting that our results of normalized plasma $\lambda_0$ fall very close to the reference line $\lambda_{0\text{REF}}$ (reference set of data) and mainly normalized data points are very close to each other and normally underpredicted, for higher number of $N$. However, it is noted that our simulation data are slightly overpredicted at higher $\kappa$ (=5 and 6) for a lower range of force field 0.001 $\leq F^* \leq 0.004$. Furthermore, it is examined during simulation run that very noisy calculations are observed at the normalized $F^*$ regime of 0.006 $\leq F^* \leq 0.5$ at $\kappa = 1, 2, 3$ and 4 for $\Gamma = 1$, and $\Gamma = 300$ ($\kappa = 4$). We have checked that the normalized $F^*$ is independent of $\Gamma$ and $\kappa$ with following conditions: $0.008–0.05$ at $\Gamma = 50$ ($\kappa = 1$), $F^*$ is extended up to 0.009–0.05 at $\Gamma = 100$ ($\kappa = 1$), and $F^*$ is extended up to 0.001–0.5 at lower $\Gamma < 2$ ($\kappa = 5$ and 6) gives noisy measurements. In addition, only a few plasma $\lambda_0$ calculations are found at higher $F^*$ (0.05 to 0.5), where signal-to-noise ratios are acceptable, for different combinations of plasma parameters ($\Gamma, \kappa$). It is concluded from Figs. 5(a) and 6(a) that the linear response theory is valid for 0.001 $\leq F^* \leq 0.1$, where plasma $\lambda_0$ is independent of $F^*$ within limited statistical uncertainties, and the linear regime is extended with increasing $N$ (=13 500). It is important to note from figures that the presented plasma $\lambda_0$ uncertainty decreases as the external force field $F^*$ increases with the same simulation time, confirming numerical results.$^7$ The deviation of the presented data from the reference line is still satisfactory and again nearly all the plasma data fall within a ±20% range around the reference line ($\lambda_{0\text{REF}}$) for the both figures.

Figures 5(b) and 6(b) demonstrate that the variance of plasma $\lambda_0$ as a function of $F^*$ along the horizontal axis and $\Gamma$ along the vertical axis for $N=13 500$ at $\kappa = 1, 2, 3, 4, 5, 6$. In these cases ($\kappa = 1$ to 6), a constant factor of 10 000 is multiplied to normalized $F^*$ ($\times 10$ 000) in order to...
to magnify the values of $F^*$ along the horizontal-axis. It is significant that we have extend the external force field very broadly for $N = 13,500$ as compared to the number of particles for $N = 500$ and 4000. For the force filed range of $F^* = (0.001–0.009)$, the wavy shape of plasma $\lambda_0$ is formed at nearly $\Gamma (\equiv 5, 10)$ and remains straight nearly at $\Gamma (\equiv 1, 2)$. For this mentioned range of $F^*$, it is observed that the affected region (shown off white) of plasma $\lambda_0$ decreases with increasing $\kappa (\equiv 1–4)$ and this region contains maximum values of plasma $\lambda_0$. It is clearly seen from parts (b) of Figs. 5 and 6 that the overall trend of plasma $\lambda_0$ corresponding to $\Gamma$ is the same as in Figs. 1–4, for the force field range of $F^* = (0.001–0.009)$. Unlike to earlier cases of lower $N$, it is interesting to note that there is a significant effect of $F^*$ on plasma $\lambda_0$ that showing the overall decreasing behavior of $\lambda_0$ at lower $\Gamma (\equiv 1, 10)$, intermediate $\Gamma (\equiv 20, 50)$, and higher $\Gamma (\equiv 100, 200)$ for higher $F^* = (0.01–0.05)$ with $\kappa (\equiv 1, 2$ and 3) and $F^* = (0.005–0.05)$ with $\kappa (\equiv 4)$. However, it is noted that plasma $\lambda_0$ further increases with an increase in $F^* (0.05–0.1)$ for $\kappa = 2$ at lower, intermediate, and higher $\Gamma$. Figure 6(b) shows that the plasma $\lambda_0$ clearly decreases with an increase of $F^*$ for the complete range of $\Gamma$ at higher $\kappa (\equiv 5$ and 6).

**IV. CONCLUSIONS**

We have computed the plasma thermal conductivity of 3D strongly coupled complex plasmas (Yukawa fluids) over a wide range of plasma coupling $\Gamma (\equiv 1, 300)$ and screening parameters $\kappa (\equiv 1, 6)$. We have performed a total of one hundred and thirty seven different HNEMD simulations with different system sizes under varying force field strengths for all possible combinations of plasma parameters $(\Gamma, \kappa)$. Our calculations show that the plasma thermal conductivity $\lambda_0(F^*, \Gamma)$ depends on both the plasma parameters. Within relatively limited statistical uncertainty, it has been found that the overall decreasing behavior of plasma thermal conductivity is seen from the results obtained through the presented HNEMD approach. The simulated results obtained through the presented HNEMD approach and those obtained through GKR-EMD, PHMD, and InHNEMD computations for SCYFs are found to be in reasonable agreement, generally overpredicted (1% to 24%) and underpredicted (1% to 27%) within statistical limits, depending on plasma parameters $(\Gamma, \kappa)$. Further, comparison illustrates that the new simulations with different system sizes and varying force fields fall within less than $\pm 20\%$ around the reference line that show the excellent performance (its accuracy and consistency) of the presented HNEMD techniques and earlier GKR-EMD and InHNEMD methods. It is demonstrated that we have explored a wide range of external force fields for plasma thermal conductivity and it can be used to calculate the plasma conductivity data for the whole range of plasma parameters $(\Gamma, \kappa) \equiv (1–300, 1–6)$ than those used in earlier studies. Finally, it is concluded that the improved Evan’s approach is excellent in its significant higher range of external force field, and it is a best substitute option to investigate the overall behavior and effects of plasma thermal conductivity under varying force effects for SCYFs. For future work, it will be interesting to analyze a system in 3D complex plasma experiments, which under the influence of dissipation (internal friction), can be simulated by a presented HNEMD approach with proper modification of the dust particle equation of motion.

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