THERMAL PROPERTIES OF SIMULATED NON-IDEAL SYSTEMS

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PACS 52.27.Lw, 52.27.Gr, 52.35.Fp

The dependence of the thermal conductivity on the temperature is studied for a simulated non-ideal Yukawa system by means of the Green–Kubo formula in a wide range of parameters. The phase state of the system under study is changed from a strongly coupled 2D-solid to a low-coupled hot liquid. A method of calculation of the thermal conductivity for 2D-systems via the Green–Kubo formula is developed.

1. Introduction

Examination of thermodynamic properties of non-ideal systems of interacting particles is of significant interest in various fields of science and technology (plasma physics, medical industry, physics of polymers, *etc.*). The main issue involved in the studies of these systems is associated with the absence of an analytically justified theory of liquid, which could provide simple parametric expressions for its equations of state, thermodynamic characteristics, and kinetic coefficients. To predict the physical properties of non-ideal systems, various semiempirical approaches and computer simulations of particle's dynamics involving the various models for their interaction potentials are widely used [1–11].

Dusty plasma (consisting of electrons, ions, neutral gas, and solid macroparticles of micron sizes) is a good experimental model for studying the non-ideal systems, including the verification of the existing analytical approaches and the development of new models in the theory of liquid. In a gas discharge plasma, the non-emitting micron-size grains acquire a significant negative charge, eZ (where e is the electron charge), and can form three-dimensional (3D-) or the two-dimensional (2D) structures similar to a liquid or a solid. The quasi-2D-structures, which consist of from 1 to 10 layers of grains, are typical of the plasma of a radio frequency (RF-) discharge [8–11]. The basic attention is given to a screened Coulomb potential of the Yukawa type that is of particular interest in the context of the investigation of dusty plasma [8–10] and colloid systems (including medical and biological systems and polymer structures) [2, 7]. Respectively, the effective coupling parameter for these Yukawa systems can be rewritten as

$$\Gamma^* = c_1\Gamma\left(1+\kappa+\frac{\kappa^2}{2}\right)\exp(-\kappa), \tag{1}$$

where $\Gamma = (Ze)^2/Tl_p$ is the Coulomb coupling parameter, and $\kappa = l_p/r_D$ is the screening factor. Then the characteristic frequency ω^* can be presented as

$$\omega^* = \left[\frac{c_2(eZ)^2\left(1+\kappa+\frac{\kappa^2}{2}\right)\exp(-\kappa)}{l_p^3\pi M}\right]^{1/2}. \tag{2}$$

2. The Method

To simulate a 2D-system of interacting particles, we write the pair interaction potential as

$$\phi(r) = \frac{(eZ)^2}{r}\exp\left(-r/r_D\right), \tag{3}$$

where eZ is a particle's electric charge considered constant and equal for all particles, and r_D is the screening length. It is assumed that the particles are propagating in a viscous medium. The interaction of particles with this medium is described simply by introducing the collision frequency $\nu_{\rm fr}$ and the stochastic force R caused by random collisions of particles with medium's molecules. The simulation is fulfilled by the molecular dynamics method with periodic boundary conditions and the Langevin equations of motion:

$$M\ddot{q}_{\alpha i} = -\nu_{\rm fr}\dot{q}_{\alpha i} + \sum_{j\neq 1} f_{\alpha ij} + R_\alpha. \tag{4}$$

Here, $\alpha = x, y$, M is particle's mass considered constant and equal for all particles, $\nu_{\rm fr}$ is the collision frequency that causes the velocity-linear friction, f_{ij} is the pair

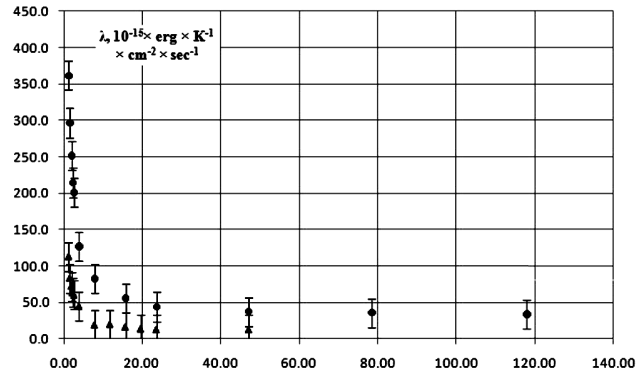

Fig. 1. Dependence of the thermal conductivity on the parameter Γ^* for $\xi = 0.33$ (▲) and $\xi = 1$ (●)

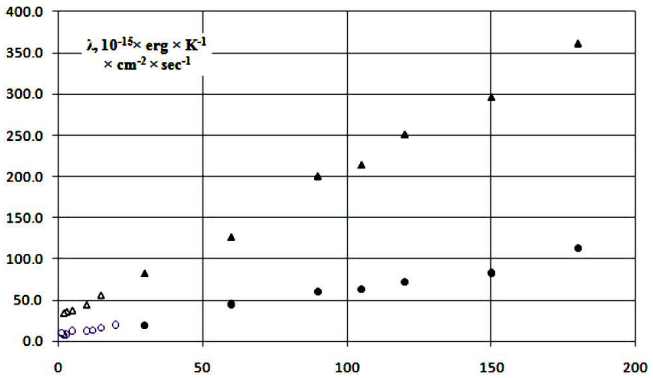

Fig. 2. Dependence of the thermal conductivity on the temperature (in ergs$\times 10^{-11}$) for $\xi = 0.33$ (● – solid, ● – transitional phase, and ○ – liquid) and $\xi = 1$ (▲ – solid, ▲ – transitional phase, and △ – liquid)

interaction force for i and j particles, and $\mathbf{R}_\alpha$ is the random force. The factor for this force can be written [12] as

$$C_{\rm Br} = \sqrt{2\tau\nu_{\rm fr}h}, \tag{5}$$

where $\tau = T/M$, T is the temperature (in ergs), and h is the time integration step. Influence of the stochastic force is allowed for by adding a correction to particle's velocity vector. This correction is determined as a normally distributed random number with dispersion $C_{\rm Br}$. The integration step h is found according to the rule

$$h = \frac{1}{20\max\{\nu_{\rm fr}; \omega^*, \}}, \tag{6}$$

where

$$\omega^* = eZ\left[2\left(1+\kappa+\frac{\kappa^2}{2}\right)\frac{\exp(-\kappa)}{\pi M l_p^3}\right]^{1/2}. \tag{7}$$

Here, l_p is the average interparticle distance.

The system consists of $N = 256$ particles. The screening factor $\kappa = 2$. The scaling parameter ξ is equal to 0.33 and 1. The interparticle distance $l_p = 0.1$ cm is taken equal to the value commonly observed in experiments with dusty plasma in RF discharges. The cut distance value is chosen equal to $2/3L$, where $L = 1.6$ cm is the calculation cell size. The connection between the effective non-ideality parameter and the temperature of the system reads

$$\Gamma^* = \frac{3}{2}(eZ)^2\left(1+\kappa+\frac{\kappa^2}{2}\right)\frac{\exp(-\kappa)}{Tl_p}. \tag{8}$$

Solving the equations of motion is fulfilled numerically within the Runge–Kutta approach with 4th-order accuracy. According to the Green–Kubo formula [5], the expression for the thermal conductivity coefficient is written as

$$\lambda = \frac{k_{\rm B}}{T^2}\lim_{t\to\infty}\int\limits_{t_0}^{t_0+t}\langle J_{Q\alpha}(t')J_{Q\alpha}(t_0)\rangle dt', \tag{9}$$

where

$$J_{Q\alpha}(t) = \frac{n}{N}\left[\sum_{i=1}^{N} e_i v_{i\alpha} + \sum_{i=1}^{N}\sum_{j=i+1}^{N}(\mathbf{r}_{ij}\mathbf{v}_{ij})\phi'_{ij}\frac{\mathbf{r}_{ij}}{|r_{ij}|}\right]. \tag{10}$$

Here, n is particles' concentration, $e_i = Mv_i^2/2 + \sum_{j=1}^{N}\phi_{ij}$ is particle's energy, ϕ is the pair interaction energy, ϕ' is the first derivative of (3) at the point $|r_{ij}|$, and $\mathbf{r}_{ij}$ and $\mathbf{v}_{ij}$ are the mutual distance and the relative velocity of particles i and j.

The data on the coordinates and the velocities of particles collected during the simulation were processed to yield values of the function $J_{Q\alpha}(t)$. Then the average values $\langle J_{Q\alpha}(t')J_{Q\alpha}(t_0)\rangle$ over the ensemble are computed. This allows us to calculate integral in (9). Since the system under study is considered being isotropic, the results for the X and Y directions are averaged.

3. Results

The resulting dependence of the thermal conductivity λ on the parameter Γ^* found after calculations is shown in Fig. 1. Our main result is the dependence $\lambda(\Gamma^*)$. For strongly-coupled states, this dependence monotonically decreases with increase of the parameter Γ^*. For

strongly-coupled states, the derivative $\lambda'(T)$ changes sign and becomes positive.

A similar behavior for the considered dependence is observed for both values of the scaling parameter ξ. More details of the λ dependence on T are easily seen in Fig. 2. Leaps can be observed at the points $T \sim 100$ and $T \sim 30$, erg$\times 10^{-11}$ which are considered by some authors as phase transition points [13].

4. Conclusion

Thermal conductivity of a simulated strongly coupled 2D-system with pair interaction potential is studied for a wide range of temperatures (solid, transitional, and liquid states are involved). Simple properties of the dependence of the thermal conductivity on the temperature are detected and described.

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Received 19.01.11

ТЕПЛОВІ ВЛАСТИВОСТІ МОДЕЛЬОВАНИХ НЕІДЕАЛЬНИХ СИСТЕМ

Ю.В. Хрустальов, О.С. Вауліна, О.Ф. Петров, В.Е. Фортов

Р е з ю м е

Вивчено температурну залежність теплопровідності модельної неідеальної системи Юкава для широкого діапазону параметрів з використанням формули Гріна–Кубо. Фазовий стан системи змінюється від сильнозв'язаного двовимірного твердого стану до слабозв'язаної гарячої рідини. Розвинуто метод обчислення теплопровідності двовимірних систем з використанням формули Гріна–Кубо.