Simulational Study on Dimensionality-Dependence of Heat Conduction

Takashi Shimada*, Teruyoshi Murakami†, Satoshi Yukawa‡, Keiji Saito§, and Nobuyasu Ito**

Department of Applied Physics, School of Engineering,
The University of Tokyo, Bunkyo-ku, Hongo, Tokyo 113-8656, Japan
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Heat conduction phenomena are studied theoretically using computer simulation. The systems are crystal with nonlinear interaction, and fluid of hard-core particles. Quasi-one-dimensional system of the size of $L_x \times L_y \times L_z (L_x \gg L_y, L_z)$ is simulated. Heat baths are put in both end: one has higher temperature than the other. In the crystal case, the interaction potential $V$ has fourth-order non-linear term in addition to the harmonic term, and Nose-Hoover method is used for the heat baths. In the fluid case, stochastic boundary condition is charged, which works as the heat baths. Fourier-type autocorrelation function of heat flux is also observed and long-time tails of the form of $\sim t^{-d/2}$, where $d$ denotes the dimensionality of the system, are confirmed.

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The normal heat conduction, which is described by the Fourier heat law

$$J = -\kappa \cdot \text{grad}(T)$$

(1)

where $J$ and $T$ denote the heat flux and the temperature respectively, is one of the most fundamental nonequilibrium phenomena. However the microscopic origin of it has not been clarified completely. Unlike the Debye’s theory for the specific heat in equilibrium solids, this phenomena cannot be modeled by the harmonic chain [1]. In the harmonic chain, global internal temperature gradient is not formed, so that the thermal conductivity diverges. Disorder of mass of particles in the system does not give the saturated thermal conductivity in the thermodynamic limit [2]. This behavior attributes to the lack of scattering process between modes in the system. On the other hand, some chaotic systems realize the Fourier heat law [3,4,5]. Thus the nonintegrability of the system which causes scattering between modes is one of crucial elements for the Fourier heat law. It is worth stressing that all these chaotic models and the Lorentz-gas model, which is used as the model of the heat conduction in metals or diluted gas [3,4,5], are characterized by the nature that the total momentum is not conserved in the bulk.

Recent studies for total momentum conserving system by Lepri et al. shed a light on another crucial aspect, that is, dimensionality [6]. They first study the thermodynamic behavior of energy transport in the one-dimensional Fermi-Pasta-Ulam (FPU) $\beta$ lattice numerically and analytically investigated the dimensionality-dependence. In the numerical investigation for the one-dimensional case, they found numerically that the thermal conductivity diverges as $N^\alpha$ where $N$ is the number of oscillators and $\alpha$ is estimated roughly to be $1/2$. They also calculated the power spectrum $S(\omega)$ of the global heat flux in the equilibrium and found its power-law divergence as $\omega^{-0.37}$ in the low-frequency region. It corresponds to a slow decay of autocorrelation function of globally averaged heat flux $C_j(t)$ as $t^{-0.63}$. This power-law decay of the autocorrelation function implies the divergence of the thermal conductivity as $\kappa \sim N^{\alpha \approx 0.37}$ by applying the Green-Kubo formula $\kappa = \frac{1}{k_B T^2} \int_0^\infty C_j(t)dt$, (2)

because the upper limit of the time integration is expected to be proportional to the system size. Moreover they took an analogy with the hydrodynamical systems where the velocity autocorrelation function decays slowly as $t^{-d/2}$ ($d$ is the dimensionality of the system) when the density is high [7,8]. In those systems, the autocorrelation function of heat flux also has the long-time-tails of the same exponent. From this analogy, they conjectured the logarithmic divergence in two-dimensional system and the converging thermal conductivity in three-dimensional system [9]. Following these studies, Hatano reported a diverging result in the one-dimensional diatomic Toda lattice [10] and recently Lippi and Livi confirmed their prediction for the two-dimensional FPU-$\beta$ lattice and Leonard-Jones 6/12 lattice [11].

Although the analogy with dense-fluids is plausible for one and two-dimensional system, there has been no direct study on either three dimensional lattices or dense fluids system. Thus in the following we investigate the dimensionality dependencies of heat conduction on three-dimensional nonlinear lattice and dense fluid of hard-core particle.

Our model for crystal is coupled three-dimensional FPU-$\beta$ lattice with Nosé-Hoover thermostats at both sides. Hamiltonian of this system is represented as follows,

$$\mathcal{H}_0 = \sum_{i=1}^{N} \frac{p_{ij}^2}{2} + \sum_{i,j,n,n} V_{ij},$$

(3)

$$V_{ij} = \frac{1}{2}(dq_{ij})^2 + \frac{q}{4}(dq_{ij})^4 \quad (dq_{ij} = |q_i - q_j| - l_0),$$

(4)

where $N, l_0, g$ denote the number of particles, natural length of the bond and the coefficient of the fourth order nonlinear term respectively. Mass of the particles are
uniformly 1. Here dynamical variables $p_i = (p_{ix}, p_{iy}, p_{iz})$ and $q_i = (q_{ix}, q_{iy}, q_{iz})$ are three-dimensional. The summation over $V_{ij}$ takes only for nearest neighbor pairs. In this system, the total momentum is conserved in the bulk since potential is simply the function of distance between two particles. We will study two kinds of lattices: one is one-dimensional-like ($1 \times 1 \times N_z$) lattices, and the other is three-dimensional-like one ($3 \times 3 \times N_z$) where $N_z$ is taken to be from 8 to 256. In the following we will call the former as 1D-lattice and the latter as 3D-lattice; although the 3D-lattice is actually quasi-one-dimensional, we will see this system maintains the three-dimensionality later. We take periodic boundary condition to the bonds vertical to $N_z$-direction. Note that our model have no long-distance-correlations. Nosé-Hoover thermostats \cite{19,20} act on each particle in both ends condition to the bonds vertical to $N_z$-direction. \( T_0 \) is the temperature of the heat bath \( T = 1 \). Here dynamical variables of $p_i$ and $q_i$ move as follows;

\[
\dot{q}_i = p_i, \quad (\text{in the bulk}) \tag{5}
\]
\[
\dot{p}_i = \left\{ \begin{array}{ll}
-\frac{\partial q_{il}}{\partial q_i} - \zeta_i p_i & (\text{at the both ends}) \nonumber
\end{array} \right.
\]

and thermostat variables move as follows;

\[
\zeta_i = \frac{1}{Q} \left( \frac{p_i^2}{3k_B T} - 1 \right). \tag{6}
\]

Here $T$ is the temperature of the heat bath($T_L$ or $T_R$) and $Q$ is the parameter of coupling between the thermal bath and the system. In this study we set $Q = 1$ in order that the response time of the thermostats($\sim 1/\sqrt{Q}$) becomes the same order as the original time scale of the lattice. The value of other parameters are chosen as follows;

\[
k_B = 1, \quad T_L = 152/3, \quad T_R = 8, \quad g = 0.1, \quad l_0 =100.
\]

Under this condition, system is fully chaotic \cite{21}. The 3D-lattice corresponds to the van-der-Waals solids since the natural length is enough long comparing with the displacement of particles which is usually smaller than 10, in other words, nonlinearity comes from the presence of the natural length is negligible, however it changes the strongest coupling combination of the displacements. We used the fourth-order predictor-corrector method to integrate the differential equations. Time step we use($10^{-3}$) for integration provides the total energy conservation with a relative accuracy $10^{-7}$ in the isolated system for the time corresponds to the longest simulation.

We define the local temperature as

\[
T(i) = < p_i^2 / 3 >, \tag{7}
\]

where $< \cdot >$ means average over long time. The local heat flux $j_{kl}$ is defined as the energy transfer per unit time from the $k$th particle to the nearest particle $j$ as

\[
j_{kl} = -p_k \cdot \frac{\partial V_{kl}}{\partial q_i}. \tag{8}
\]

For the 3D-lattice, we will treat only fluxes flow along the $N_z$-direction bonds. Then we can represent the flux from the $k$th particle to the next particle in $N$-direction simply as $j_k$. The average of these heat flux $j_k$ over time and whole system is calculated as

\[
<j > = < \frac{1}{N^2} \sum_k j_k > \tag{9}
\]

where $N'$ is equal to $(N - 1)$ for 1D-lattice and $(N - 9)$ for 3D-lattice.

It was confirmed that the temperature profile takes a linear form and the effect of boundary with thermostats was negligible in both ends. From this fact we reasonably define the global thermal conductivity as

\[
\kappa = < j > / N_z \frac{T_L - T_R}{N_z}, \tag{10}
\]

by substituting $(T_L - T_R)/N_z$ for the temperature gradient in Eq.(8).

Size-dependence of the thermal conductivity $\kappa$ is shown in FIG.1. In the 1D-lattice, thermal conductivity diverges as $\sim N_z^{0.4}$ showing a good agreement with the study by Lepri et al. \cite{24}. However, in the 3D-lattice, the result makes a sharp contrast with the 1D-lattice(FIG.1). The thermal conductivity converges although the systems are actually quite narrow especially for large $N_z$ and system become 1D-lattice like in the infinite size limit($N_z \to \infty$).

![FIG. 1. Size dependence of the thermal conductivity in lattice systems is given in log scale. Boxes denote the one in 1D-lattice ($1 \times 1 \times N_z$) and circles denote the one in 3D-lattice ($3 \times 3 \times N_z$). Error bars show $2\sigma$ error regions. The dotted line is proportional to $N_z^{0.38}$ which is obtained from a best fit by the power law for 5 points without the smallest system’s one.](image-url)
In order to check the analogy with hydrodynamical system, we also calculate temporal autocorrelation functions of average heat flux in the isolated systems. In this case the boundary conditions are periodic for all directions. These systems have no contact with the heat bath and the energy density is chosen to the value corresponding to \((T_L + T_R)/2 = 88/3\). In FIG. 2, we can see that the autocorrelation function of 1D-system decays as \(t^{−0.65}\) and the one of 3D-system decays \(t^{−1.5}\) asymptotically. Thus these results show the agreement with the Lepri et al.’s conjecture.

\[ \tag{11} f(v) = \frac{1}{T} (2\pi T)^{−d/2} |v_z| \exp\left(-\frac{v_z^2}{2T}\right), \]

Next, to study the thermal conductivity of fluid, the system of hard-core particles is simulated. The particles, with the uniform radius \((\sigma = 0.1)\) and mass \((m = 1)\), collide elastically with each other. It is clear that this system also conserves the total momentum in the bulk. The dimension of the objective systems are two \((L_x \times L_z)\) and three \((L_x \times L_y \times L_z)\) where \(L_x\) and \(L_y\) is fixed to 1 and \(L_z\) is taken to be from 2 to 20. The fixed width of the system \((L_x, L_y)\) is chosen from following condition; it must be large enough comparing with the radius of the particles, and on the other hand, it should be small to eliminate the hydrodynamic flow since we are interested in the Fourier type heat conduction. The left and right sides of the system are the walls with temperature \(T_L = 6\) and \(T_R = 2\) (again \(T_L > T_R\)), and the boundary conditions for other directions are periodic. If a particle comes to the left or right end, where the stochastic heat bath is acting, velocity is randomly chosen according to the equilibrium distribution

\[ T(z) = \frac{1}{d} \left\langle \sum_{z−\epsilon < \ell^i < z+\epsilon} \langle v^2 \rangle \right\rangle / \left\langle \sum_{z−\epsilon < \ell^i < z+\epsilon} 1 \right\rangle, \tag{12} \]

in the same way as the lattice case (Eq. (11)). Both in the two and three dimensional systems, temperature profiles have linear forms except for the area nearby boundary. For this reason, we use the temperature gradient obtained by the fitting in the bulk for the \(\text{grad}(T)\) in Eq. (11) to calculate the thermal conductivity of the system. The global heat flux is measured as the energy received by the cold bath per unit time in the steady state.

Size-dependence of the thermal conductivity \(\kappa\) is again investigated. In the two-dimensional system, \(\kappa(L_z)\) diverges as \(\sim L_z^\alpha\) where \(\alpha\) is estimated less than 0.2. This result is consistent with the logarithmic divergence in lattice system \([18]\). On the other hand, as shown in FIG. 3, \(\kappa(L_z)\) saturates to a constant value in the three-dimensional system.

The autocorrelation function of heat flux in the two and three-dimensional isolated systems is also observed. In this observation we chose the global density to the same value as the one of nonequilibrium steady state and apply the periodic boundary condition to all direction. The function shows power-law decay as \(\sim t^{-1}\) and \(\sim t^{-1.5}\).
$t^{-1.5}$ asymptotically in the two and the three-dimensional system, respectively.

In summary, using non-linear lattice and hard-core fluid we have confirmed normal Fourier-type heat conduction in three-dimension. The 1D-lattice shows the power-law divergence of the thermal conductivity as same as other one-dimensional chains. In the two-dimensional fluid system, thermal conductivity slowly diverges in thermodynamic limit. In the three-dimensional systems, the thermal conductivity converges in both lattice and fluid. We have also investigated the autocorrelation function of the heat flux and confirmed the long time tails whose exponent is $-d/2$. These results mean that the divergence behavior of thermal conductivity can be understood by the analogy with hydrodynamical system [15,18]. It is remarkable that the quasi-one-dimensional total momentum conserving system shows the normal Fourier-type heat conduction.

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