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Connection between heat diffusion and heat conduction in one-dimensional systems†

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Heat and energy are conceptually different, but often are assumed to be the same without justification. An effective method for investigating diffusion properties in equilibrium systems is discussed. With this method, we demonstrate that for one-dimensional systems, using the indices of particles as the space variable, which has been accepted as a convention, may lead to misleading conclusions. We then show that though in one-dimensional systems there is no general connection between energy diffusion and heat conduction, however, a general connection between heat diffusion and heat conduction may exist. Relaxation behavior of local energy current fluctuations and that of local heat current fluctuations are also studied. We find that they are significantly different, though the global energy current equals the globe heat current.

heat diffusion, heat conduction, correlation

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1 Introduction

By definition, it is clear that heat and internal energy are conceptually different. Internal energy is referred to as the total kinetic and potential energy of a system, which is a function of the system state, while heat is a quantity that characterizes a process. For one-dimensional (1D) systems, combining the continuous equations of energy and mass, such that: $\frac{\partial e(x,t)}{\partial t} + \frac{\partial}{\partial x} j^e(x,t) = 0$ and $\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x} p(x,t) = 0$, one can obtain

$$\frac{\partial}{\partial t}\left[e(x,t) - \frac{(e+P)\rho(x,t)}{\rho}\right] + \frac{\partial}{\partial x} j^q(x,t) = 0, \qquad (1)$$

and thus introduce the heat density function [1–4] as:

$$q(x,t) = e(x,t) - \frac{(e+p)\rho(x,t)}{\rho}. \qquad (2)$$

Here $e(x,t)$, $\rho(x,t)$, $p(x,t)$, $j^e(x,t)$, and $j^q(x,t)$ represent, respectively, the density of energy, mass, momentum, energy current, and heat current; e (ρ) and P represent, respectively, the spatially averaged energy (mass) density and the internal pressure of the system at the equilibrium state. The local heat current is related to the local energy current as:

$$j^q(x,t) = j^e(x,t) - \frac{e+P}{\rho} p(x,t). \qquad (3)$$

Therefore, the physical meaning of the change rate of $q(x,t)$ is definite: it represents the divergence of the local heat current. Conversely, the value of $q(x,t)$ itself lacks specific meaning. Usually $q(x,t)$ is negative, because $P > 0$ and $\langle \rho(x,t)/\rho \rangle = 1$. Indeed, following eq. (1), the heat density can be defined as $q(x,t) + c$ with an arbitrary constant c. Energy contains two parts, corresponding to regular and irregular motions, respectively, but heat is consistently related to thermal processes that feature random motions.

However, in some previous studies energy and heat are

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not distinguished. An example is in the study of the relation between anomalous diffusion and transport properties in low-dimensional (one- and two-dimensional) systems [5,6]. It is well known that in bulk (three-dimensional) materials the thermal conductivity κ and the heat diffusion coefficient D can be generally related by $\kappa = \rho c_P D$, where c_P is the constant pressure specific heat. This relationship does not hold in low-dimensional systems. In recent decades, stimulated by the rapid progress in nanoscience [7–11], transport properties of low-dimensional systems has attracted intensive research efforts [5,6,12–16]. It has been found that in general diffusion and transport are abnormal in low-dimensional systems. In particular, in 1D momentum conserving systems, the heat conductivity diverges with the system size L as $\kappa \sim L^{\alpha}$ and the heat diffusion coefficient diverges with time as $D \sim t^{\beta-1}$ (α and β are constants). In some studies [17,18] the heat diffusion behavior has been assumed, implicitly, to be the same as the energy diffusion behavior, and the exponent β is calculated by tracing energy diffusion instead.

It has been conjectured that there exists a general relation between exponents α and β. Two formulae, $\alpha = 2 - 2/\beta$ by Li and Wang [19] and $\alpha = \beta - 1$ by Denisov et al. [20], have been proposed. It is worth noting that in these studies [19,20] the researchers did not distinguish heat diffusion and energy diffusion and treated them identically. Though this is valid for the specific example systems they studied where energy and heat are coincidentally the same, we emphasize that in principle β involved in these two formulae should be the exponent that characterizes heat diffusion, rather than that of energy diffusion. This is particularly critical for clarifying which one of these two formula is correct. In our very recent study [21], it has been shown that the diffusion behaviors of energy and heat can be qualitatively different, suggesting that there should be no general relation between energy diffusion and heat conduction, but a general relation between heat diffusion and heat conduction may exist and can be established.

This paper is an effort to verify this conjecture. We will attempt to first ascertain a correct way for calculating the exponent β, so as to validate the study. So far there are two classes of methods for probing diffusion processes, that is, the equilibrium [18,21,22] and non-equilibrium [17,23–27] methods. With both methods, the probability density function (PDF) of local fluctuations of interested physical quantities are calculated. The space variable of the PDF should correctly give the positions of local fluctuations, but in practice the indices of particles are often taken as the space variable as substitute to facilitate the simulations [17,18]. In doing so, the underlying idea is that the index of a particle is equivalent to the position in 1D systems, as the particle simply moves around the equilibrium position. As we herein demonstrate, this is not the case: Using the index variable may result in not only quantitative but also qualitative deviations, which may be responsible for the confusing results of β reported previously. By taking the correct space variable and the equilibrium method (which has been shown to be more efficient and accurate [21,22]), we can calculate the exponent β of heat diffusion with high precision in a 1D hard-point gas model [17,28–30]. By comparing it with the values of the exponent α obtained in previous studies [30–33] we will show that the anomalous heat diffusion and heat conduction can be accurately connected by the formula $\alpha = 2 - 2/\beta$.

In addition, we also discuss the behaviors of the local heat current and the local energy current. By properly setting the coordinate system to guarantee the system has a vanishing total momentum, we find that although the total heat current is always equal to the total energy current, the relaxation behaviors of local currents of energy and heat can be remarkably different.

Herein, the model to be studied will be described and the methods for probing energy and heat diffusion will be detailed.

2 Models

We consider two paradigmatic 1D models extensively employed for studying transport properties of low-dimensional systems. Each model is composed of N point particles arranged in order. We denote by m_k, x_k, v_k, and p_k, respectively, the mass, the position, the velocity, and the momentum of the kth particle.

The first model is a 1D hard-point gas [17,28–30] with alternative mass m_o for odd-numbered particles and m_e for even-numbered particles. We set $m_o = 1$ and $m_e = 3$, the same as used by Cipriani et al. [17] for comparison. The particles travel freely except for elastic collisions with the nearest neighbors. After a collision between the kth particle and the $(k+1)$th particle, the velocities change to

$$v'_k = \frac{m_k - m_{k+1}}{m_k + m_{k+1}} v_k + \frac{2m_{k+1}}{m_k + m_{k+1}} v_{k+1}, \tag{4}$$

$$v'_{k+1} = \frac{2m_k}{m_k + m_{k+1}} v_k - \frac{m_k - m_{k+1}}{m_k + m_{k+1}} v_{k+1}. \tag{5}$$

Another model is a 1D lattice; i.e., the well known Fermi-Pasta-Ulam (FPU) model defined by the Hamiltonian:

$$H = \sum_k \frac{p_k^2}{2m_k} + \frac{1}{2}(x_k - x_{k-1} - 1)^2 + \frac{1}{4}(x_k - x_{k-1} - 1)^4, \tag{6}$$

where the masses of all particles are set to unity.

In our simulations the periodic boundary condition is applied and the system size L is set to be the same as the particle number N, so that the averaged particle number density is unity. The local temperature is defined as $T_k \equiv \frac{\langle p_k^2 \rangle}{k_B m_k}$, where k_B (set to be unity) is the Boltzmann constant and $\langle \cdot \rangle$ stands for the ensemble average. For both models the average energy per particle is fixed to be unity, corresponding to a system temperature $T = 2$ in the gas model and $T \approx 1.2$ in the FPU model.

3 Methods

In principle, one can probe the diffusion behavior directly by adding an external perturbation to the equilibrium system and observing the ensuing relaxation process [24–26]. This method requires demanding computing resource, so that a satisfactory precision is usually difficult to attain [22]. A more effective method [18,21] is instead to study the properly rescaled spatiotemporal correlation functions of fluctuations in the equilibrium state. The basic idea of this method is detailed in the following.

Let $A(x,t)$ represents the density distribution function of a physical quantity $\mathcal{A}$. In numerical simulations, in order to calculate the spatiotemporal correlation function of fluctuations of $\mathcal{A}$, we have to discretize the space variable initially. Thus, we divide the space occupied by the system into $N_b = L/b$ bins of equal size of b. The total quantity of $\mathcal{A}$ in the kth bin, denoted by $A_k(t)$, is defined as $A_k(t) \equiv \int_{x\in k\text{th bin}} A(x,t)\mathrm{d}x$. As such $A_k(t)/b$ gives the coarse-grained density of $\mathcal{A}$ in the kth bin. The fluctuations of $\mathcal{A}$ are therefore captured by $\Delta A_k(t) \equiv A_k(t) - \langle A\rangle$, where $\langle A\rangle$ represents the ensemble average of $A_k(t)$. The positions of the bin centers can then be used as the coarse-grained space variable.

For a conserved physical quantity $\mathcal{A}$, it has been derived elsewhere [21] that the PDF corresponding to a local fluctuation initially located in the kth bin, which is specified by $\Delta A_k(0)$, can be calculated as:

$$\rho_A(\Delta x_{k,l}, t) = \frac{\langle \Delta A_l(t)\Delta A_k(0)\rangle}{\langle \Delta A_k(0)\Delta A_k(0)\rangle} + \frac{1}{N_b - 1} \tag{7}$$

if the microcanonical ensemble is considered, and

$$\rho_A(\Delta x_{k,l}, t) = \frac{\langle \Delta A_l(t)\Delta A_k(0)\rangle}{\langle \Delta A_k(0)\Delta A_k(0)\rangle} \tag{8}$$

if the canonical ensemble is considered. Here $\Delta x_{k,l}$ denotes the displacement from the kth bin to the lth bin, that is, $\Delta x_{k,l} \equiv (l-k)b$. For consistency, in the following we will use x to denote $\Delta x_{k,l}$ without confusion. The spatiotemporal correlation function defined above gives the causal relation between a local fluctuation and the effects it induces at another position and at a later time, thus effectively equivalent to the PDF that describes the diffusion process of the fluctuation. In order to facilitate numerical simulations, we suggest considering the microcanonical ensemble where all systems are isolated from the environment. Hence one does not have to simulate the environment, which reduces simulation time.

In previous studies [17,18,25–27], the authors constantly use the indices of particles to represent the space variable. In particular, the value of $\mathcal{A}$ of the kth particle, denoted by $A_k^{\mathrm{ind}}(t)$, is adopted to represent the density distribution of $\mathcal{A}$ at the position of kL/N, and $\langle \Delta A_l^{\mathrm{ind}}(t)\Delta A_k^{\mathrm{ind}}(0)\rangle$ is assumed to represent the correlation between two positions with a distance of $x = (l-k)L/N$ and a time delay of t. In the following, we will refer to this coordinate as the index variable. Although the index represents the mean position of a particle in the equilibrium state, it by no means gives the position of the particle at instant times that is critical for correctly calculating the spatiotemporal correlation functions. For this reason, Dhar [34] questioned the effectiveness of the index variable because it may result in large position fluctuations. We find that it is more pronounced: the deviations caused by using the index variable is not only quantitative, but also qualitative.

Taking the energy fluctuations as an example, we show that indeed the index variable may lead to qualitatively incorrect results. We denote the spatiotemporal correlation function obtained by using the coarse-grained space variable and the index variable as $\rho_e(x,t)$ and $\rho_e^{\mathrm{ind}}(x,t)$, respectively. The 1D gas model is considered first. To prepare an equilibrium gas, the system is efficiently simulated for a sufficient time by using the event-driven algorithm that employs the heap data structure to identify the collision times [30]. Then $\rho_e(x,t)$ and $\rho_e^{\mathrm{ind}}(x,t)$ are calculated with $N = 4000$ and $b = 1$. Figures 1(a) and (b) show the results. One can see that they are remarkably different: with the coarse-grained space variable, the spatiotemporal correlation function has two peaks, while with the index variable it has three peaks. The two peaks of $\rho_e(x,t)$ move outwards with a constant speed $v = 1.75$, which can be readily shown to be the sound speed [21]. The two side peaks of $\rho_e^{\mathrm{ind}}(x,t)$ move outwards with the same speed. The center peak of $\rho_e^{\mathrm{ind}}(x,t)$ does not move but broadens as $\Delta w \sim t^{0.67}$, where Δw represents the half-height width. It can be thought that the two side peaks represent the sound mode and the center peak represents the heat mode, as in the case of the mass fluctuations that gives the dynamic structure factor of the system [4]. However, we find the ratio of the area of the center peak to that of the two side peaks equals $1/2$, while it should equal 2, that is, the Landau-Placzek ratio [35,36] of an ideal gas, if it characterizes the dynamic structure factor [4]. As will be discussed in the next section, the decaying behavior of the center peak is also different from the heat mode. Therefore, $\rho_e^{\mathrm{ind}}(x,t)$ fails to capture the properties of the heat mode. It can be noted that the three peak structure has also been reported in other studies of the gas model by using the index variable [17,26,27].

As mentioned above, diffusion properties can also be investigated directly by observing the evolution of an added perturbation to the system. We find that by applying this method, one can obtain the same results (See Figures 1(c) and (d)). In addition, we find that in the 1D FPU model (see Figures 1(e) and (f)), the qualitative difference between $\rho_e(x,t)$ and $\rho_e^{\mathrm{ind}}(x,t)$ is also readily apparent [21]. These results suggest clearly that the position of a particle at instant times cannot be approximated by the equilibrium position in order to correctly calculate spatiotemporal correlation functions.

4 Results and discussions

In Figure 1(a), it is clearly shown that the energy fluctuations transport ballistically in the 1D gas model, implying that the mean square displacement of the transported energy increases

in time as $\langle x^2(t)\rangle \sim t^2$. And the heat conduction properties of this model have been extensively studied [28–30]. It has been found that the heat conductivity κ diverges with the system size L as $\kappa \sim L^\alpha$ with $\alpha = 1/3$ [30–33], suggesting that heat diffuses in a supperdiffusive manner rather than ballistically. Therefore, energy diffusion and heat conduction do not fall into the same anomalous class. We then calculate the PDF of heat fluctuations, that is, $\rho_q(x,t)$, following eq. (2) and present the results in Figure 2. It can be seen that the profile of $\rho_q(x,t)$ differs completely from that of energy fluctuations, $\rho_e(x,t)$ (see Figure 1(a)), the former having only one single peak. This feature has been reported elsewhere [21], but here we perform the simulation with a larger system size of $N = 4096$ which allows us to measure the decaying rate of $\rho_q(x,t)$ more accurate. As presented in Figure 2(b), we obtain that the height of the peak of $\rho_q(x,t)$ is $h = \rho_q(0,t) \sim t^{-\lambda}$ with $\lambda = 0.60$. As heat is a conserved quantity, the peak of $\rho_q(x,t)$ must keep the area unchange, and as a consequence the half-height width should broaden as $\Delta w \sim t^{-0.60}$. As such $\rho_q(x,t)$ at different time may be rescaled onto a common function. This is confirmed by our study presented in Figure 2(c): $\rho_q(x,t)$ is indeed invariant upon rescaling $x \to t^\lambda x$ so that $t^\lambda \rho_q(x,t) = t_0^\lambda \rho_q(x_0,t_0)$ for $x = (t/t_0)^\lambda x_0$ with scaling factor $\lambda = 0.60$.

This result confirms for the first time that the relaxation of the heat mode follows the scaling law with $\lambda = 3/5$ as predicted by the hydrodynamic mode-coupling theory [37]. This scaling property implies that $\rho_q(x,t)$ relaxes as $\langle x^2(t)\rangle = \langle x_0^2(t_0)\rangle(\frac{t}{t_0})^{2\lambda}$; that is, heat fluctuations diffuse in a power law $\langle x^2(t)\rangle \sim t^\beta$ with the diffusion exponent $\beta = 2\lambda$ [21]. We obtain $\beta = 1.20$ accordingly, suggesting that heat diffusion is superdiffusive, in clear contrast with energy diffusion which is ballistic. Also, by combining $\beta = 1.20$ obtained here and $\alpha = 1/3$ obtained in previous analytical and numerical studies [30–33], we find they follow consistently the general formula proposed by Li and Wang [19] attempting to connect energy diffusion (should be heat diffusion instead) and heat conduction in 1D systems.

Note that the center peak of $\rho_e^{\rm ind}(x,t)$ (see Figure 1(a)) is also invariant upon the rescaling but with $\lambda = 0.67$ instead, which implies $\beta = 1.34$. Also note that the formula $\alpha = \beta - 1$ correctly describes the relation of energy diffusion and heat conduction in this case [17,18]. We can therefore conclude that this is a consequence by improperly replacing the space variable with the particle indices.

Finally, we study the relaxation behavior of local energy current and local heat current. We set the total momentum of the system to be zero. The global energy current always equ-

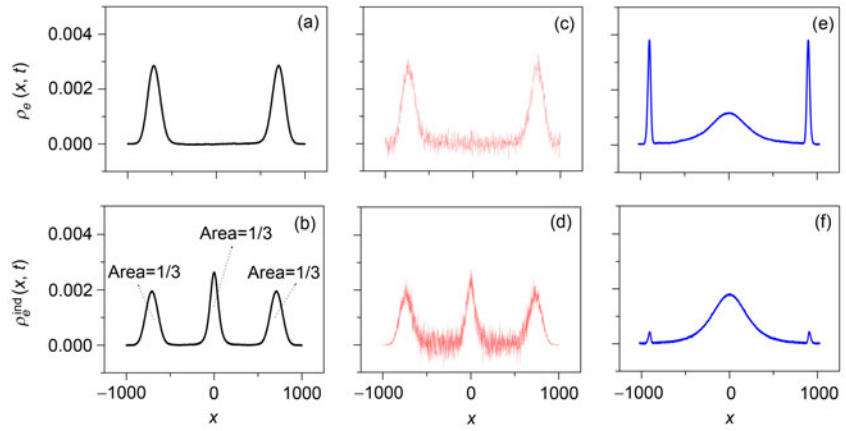

Figure 1 (Color online) Probability density distribution function of energy obtained by using correlation function method and perturbation method with space variable being, respectively, coarse-grained space variable and particle indices. (a)–(d) are for gas model at $t = 400$, obtained by (a), (b) correlation function method and (c), (d) perturbation method. (e), (f) are for FPU model at $t = 600$ by using correlation function method.

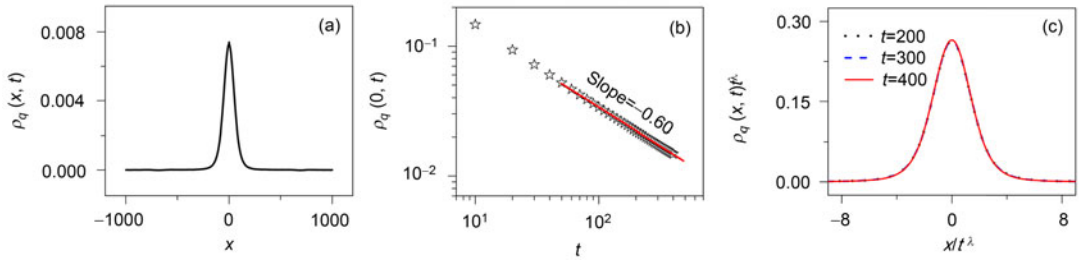

Figure 2 (Color online) Simulation results of spatiotemporal correlation function of heat fluctuations, $\rho_q(x,t)$, for 1D gas model. (a) presents a snapshot of $\rho_q(x,t)$ at time $t = 400$, and (b) shows time dependence of height of center peak of $\rho_q(x,t)$. Solid line in (b) is best linear fitting of data for revealing asymptotic characteristics, suggesting that $\rho_q(0,t) \sim t^{-0.60}$. In (c) $\rho_q(x,t)t^\lambda$ versus x/t^λ at three different times are compared with rescaling factor $\lambda = 0.60$ obtained via best linear fitting in (b). These three curves overlap perfectly verifies the scaling property of $\rho_q(x,t)$.

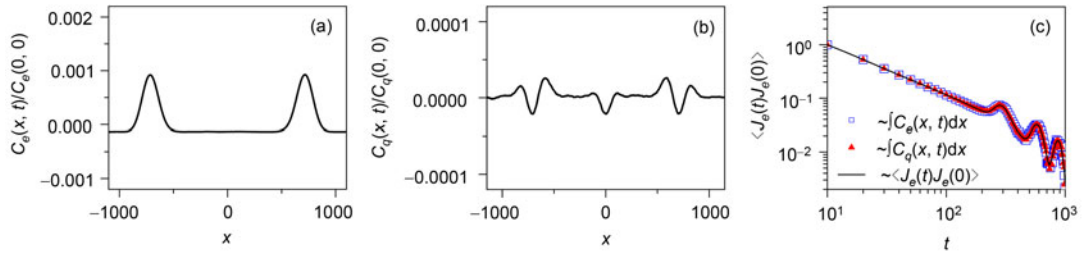

Figure 3 (Color online) Spatiotemporal correlation function of local energy current $C_e(x,t)$ (a) and of local heat current $C_q(x,t)$ (b) at time $t = 400$ for 1D gas model N=3000. In (c), autocorrelation function of globe energy current $\langle J_e(t)J_e(0)\rangle$ (solid line) is compared with $\int C_e(x,t)\mathrm{d}x$ (open squares) and $\int C_q(x,t)\mathrm{d}x$ (solid triangles). These three sets of data fall onto the same curve upon proper shifts in vertical direction, N=512.

als the globe heat current, but this fact does not imply the properties of local heat current and local energy current are identical. Figures 3(a) and (b) show the spatiotemporal correlation functions of local energy current $C_e(x,t) = \langle j_l^e(t) j_k^e(0)\rangle$ and that of local heat current $C_q(x,t) = \langle j_l^q(t) j_k^q(0)\rangle$. Here $x = (l-k)L/N$, (the size of a bin is $b = L/N$), the local energy current is defined as $j_l^e(t) = \sum_{k:x_k\in l\text{th bin}} m_k v_k^3/2$, and the local heat current is obtained by substituting $j_l^e(t)$ into eq. (3). It can be seen that $C_e(x,t)$ and $C_q(x,t)$ have remarkably different features: the former has a global negative bias, and the two peaks moving oppositely at the sound speed. The latter is more complex. There are two pulses which appear as a negative Mexican hat wavelet and move outwards at the sound speed, but there is no global bias. Instead, there is a dip at the origin. Therefore, the properties of $C_q(x,t)$ can not be probed by studying $C_e(x,t)$, and *vice versa*.

The globe energy current $J_e(t) = \sum_k j_k^e(t)$. One has $\langle J_e(t)J_e(0)\rangle = \langle \sum_k j_k^e(0) \sum_l j_l^e(t)\rangle \propto \langle j_k^e(0) \sum_l j_l^e(t)\rangle$ for any index k because of the homogeneity of the system. Thus, $\langle J_e(t)J_e(0)\rangle \propto \int C_e(x,t)\mathrm{d}x$. Because $J_e(t) = J_q(t)$ as a result of the null total momentum, we have $\int C_e(x,t)\mathrm{d}x \propto \int C_q(x,t)\mathrm{d}x$. This result implies that though the relaxation behaviors of local heat current and local energy current are different, the integrals decay in the similar way, which is also confirmed by direct simulation results shown in Figure 3(c).

5 Conclusions

We demonstrate herein that in 1D systems, using the particle indices as the space variable may result in qualitative deviations in probing the diffusion properties, and hence should be abandoned. Instead, the coarse-grained space variable is a correct and practical choice. By taking advantage of this, we have verified that in the 1D gas model, heat diffusion and heat conduction, rather than energy diffusion and heat conduction, can be connected by the formula $\alpha = 2 - 2/\beta$ [19] accurately, rather than by that proposed elsewhere [20]. Our analysis has also shown that energy diffusion and heat conduction follows $\alpha = \beta - 1$ as observed [17,18] may be a misunderstanding caused by misusing the particle indices as the space variable. We emphasize that the position of a particle at instant times cannot be approximated by the equilibrium position in probing spatiotemporal correlation functions of a system.

In addition, in the case of null total momentum, though the globe energy current equals to the globe heat current, the local energy currents differ from the local heat currents. The relaxation behavior of the former is significantly different from that of the latter as well. We conclude that in general, the relaxation and transport properties of heat can not be identified with those of energy.

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