Diffusion of heat, energy, momentum, and mass in one-dimensional systems

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We study diffusion processes of local fluctuations of heat, energy, momentum, and mass in three paradigmatic one-dimensional systems. For each system, diffusion processes of four physical quantities are simulated and the cross correlations between them are investigated. We find that, in all three systems, diffusion processes of energy and mass can be perfectly expressed as a linear combination of those of heat and momentum, suggesting that diffusion processes of heat and momentum may represent the heat mode and the sound mode in the hydrodynamic theory. In addition, the dynamic structure factor, which describes the diffusion behavior of local mass density fluctuations, is in general insufficient for probing diffusion processes of other quantities because in some cases there is no correlation between them. We also find that the diffusion behavior of heat can be qualitatively different from that of energy, and, as a result, previous studies trying to relate heat conduction to energy diffusion should be revisited.

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I. INTRODUCTION

In recent years, stimulated by the rapid progress in both theoretical and experimental studies, the nonequilibrium transport properties in low-dimensional systems have become a favored research topic. In principle, based on the linear response theory [1], these properties can be revealed by studying the evolution of spontaneous fluctuations in equilibrium systems. However, in general how a spontaneous fluctuation may evolve is still an open question. For example, if a local fluctuation will simply relax until it vanishes or spread (diffuse) into other parts of the system, and if fluctuations of different physical quantities may evolve in the same way, are unclear yet.

To study relaxation processes is of fundamental importance. The conventional hydrodynamic theory predicts that a perturbation may induce a heat mode and a sound mode [2], hence the relaxation of a fluctuation may be understood as a combination of such two types of hydrodynamic modes. However, in recent decades, it has been found that the linearized hydrodynamic description may be invalid in low-dimension systems [3–5]. Therefore, it is necessary to investigate, by direct simulations, the particular properties of the hydrodynamic modes and show how they manifest themselves in different systems. This kind of first-hand information can be very helpful for checking the deviations from the hydrodynamic transport theories and shed light on how to improve them.

Numerical simulations have special advantages for this aim, because they are applicable to a large variety of relaxation processes, many of which are not accessible by present laboratory experiments. Indeed, among various quantities, at present only the evolving process of the mass density fluctuations can be measured in laboratories by inelastic neutron or x-ray scattering experiments in terms of the dynamic structure factor. The dynamic structure factor is defined as the Fourier transform of a spatiotemporal correlation function of local mass density fluctuations [2]. It can be applied to probe the information of the interparticle interactions and

their time evolution, and thus has been widely studied via theoretical, experimental, and numerical methods [2,6–9]. Therefore, verifying the existence of correlation between the relaxation processes of a given physical quantity and that of the local mass density fluctuations has practical importance as well. If they are correlated and the correlation is made clear by simulations, then with the existing experimental techniques the relaxation behavior of the given quantity can be obtained by measuring the dynamic structure factor. If there is no correlation, then numerical simulations would be the main tool to explore the former.

Another instance requiring us to clarify if there is any correlation between relaxation processes of different quantities is encountered in the study of heat conduction in low-dimensional systems [10,11]. Heat conduction is closely related to the heat relaxation behavior. It is known that the heat current and the energy current are conceptually different [12,13], but they may have the same value at nonequilibrium stationary states [10,14]. In the literature [15–19], sometimes heat relaxation has been assumed, implicitly, to be the same as energy relaxation, and the heat conduction properties are thus deduced based on energy relaxation instead. Given this, to clarify if heat and energy follow the same relaxation law is a necessary task.

This work is an effort towards filling these gaps. We shall focus on the evolution of local fluctuations of energy, heat, momentum, and mass, and pay particular attention to their correlations. We shall consider three typical one dimensional (1D) systems as examples to show the system-dependent relaxation properties. The rest of this paper is organized as follows: The models to be studied will be described in the next section, and the method we use to probe the evolution of local fluctuations will be detailed in Sec. III. The main results will be provided and discussed in Sec. IV, followed by a brief summary in the last section.

As we find that most relaxation processes in our study have characteristics of generalized diffusion—i.e., the corresponding fluctuations do not decay to zero but spread across the system—in the following we refer to them as diffusion for the sake of simplicity. For example, by "diffusion of energy" we mean the evolution process of local energy fluctuations.

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II. MODELS

We study three paradigmatic 1D models that have been shown very useful for exploring the dynamic implications on thermodynamic properties: one gas model and two lattice models. The gas model [18,20–22] is a simplified representative of 1D fluids which consists of N hard-core point particles arranged in order in a 1D box of length L with alternative mass m_o for odd-numbered particles and m_e for even-numbered particles. The particles travel freely except for elastic collisions with their nearest neighbors. The two lattice models are the Fermi-Pasta-Ulam (FPU) model [23] and the lattice ϕ^4 model [24], representing lattices with and without the momentum conserving property, respectively. Their Hamiltonian is $H = \sum_i H_i$ with $H_i = \frac{p_i^2}{2m_i} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}(x_i - x_{i-1})^4$ for the FPU model and $H_i = \frac{p_i^2}{2m_i} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}x_i^4$ for the lattice ϕ^4 model, where H_i, p_i, m_i, and x_i represent, respectively, the energy, the momentum, the mass, and the displacement from its equilibrium position of the ith particle.

In our simulations, the system size L is set to be equal to the particle number N, so that the averaged particle-number density is unity. The local temperature is defined as $T_i \equiv \frac{\langle p_i^2 \rangle}{k_B m_i}$, where k_B (set to be unity) is the Boltzmann constant and $\langle \cdot \rangle$ stands for the ensemble average. For the 1D gas model, we take $m_o = 1$ for odd-numbered particles and $m_e = 3$ for even-numbered particles as in Ref. [18] for the sake of comparison, and the average energy per particle is unity so that the system temperature $T = 2$. For the FPU model and the lattice ϕ^4 model, all particles have a unit mass and the system temperature is $T = 0.5$.

III. METHOD

In the equilibrium state, the diffusion behavior of a physical quantity can be probed by studying the properly rescaled spatiotemporal correlation function of its density fluctuations [19,25,26]. The method given in Ref. [19] will be detailed and extended to microcanonical systems in the following.

We assume that the systems are microcanonical with periodic boundary condition and the physical quantity to be considered, denoted by $\mathcal{A}$, is conserved. The density distribution function of $\mathcal{A}$ is denoted by $A(x,t)$, where x and t are the space and the time variables, respectively. In numerical simulations, in order to calculate the spatiotemporal correlation function of $A(x,t)$, we have to discretize the space variable. For this aim we divide the space range of a system into $N_b = \frac{L}{b}$ bins of equal size b. The total quantity of $A(x,t)$ in the jth bin is denoted by $A_j(t)$, defined as $A_j(t) \equiv \int_{x \in j\text{th bin}} A(x,t)dx$. The fluctuation of $A(x,t)$ in the jth bin is thus $\Delta A_j(t) \equiv A_j(t) - \bar{A}$, where $\bar{A}$ is the ensemble average of $A_j(t)$. These N_b bins serve as the coarse-grained space variable.

The diffusion characteristics of $\mathcal{A}$ can be captured by the spatiotemporal correlation function defined as

$$\rho_A(\Delta x_{i,j}, t) \equiv \frac{\langle \Delta A_j(t) \Delta A_i(0) \rangle}{\langle \Delta A_i(0) \Delta A_i(0) \rangle} - C_{\text{inh}}, \quad (1)$$

where $\Delta x_{i,j}$ denotes the displacement from the ith bin to the jth bin, i.e., $\Delta x_{i,j} \equiv (j - i)b$. The constant C_{inh} represents the

inherent correlation resulting from the fact that $\mathcal{A}$ is conserved, which has nothing to do with the causal correlation and hence must be deducted [19]. For a microcanonical system we have $\sum_j \Delta A_j(0) = 0$ due to the fact that $\mathcal{A}$ is conserved, therefore $\sum_{j \neq i} \Delta A_j(0) \Delta A_i(0) = -\Delta A_i(0) \Delta A_i(0)$ and

$$\sum_{j \neq i} \langle \Delta A_j(0) \Delta A_i(0) \rangle = -\langle \Delta A_i(0) \Delta A_i(0) \rangle. \quad (2)$$

As $\langle \Delta A_j(0) \Delta A_i(0) \rangle$ is statistically equivalent for all $j \neq i$ due to the homogeneity of space and time, we have

$$\langle \Delta A_j(0) \Delta A_i(0) \rangle = -\frac{1}{N_b - 1} \langle \Delta A_i(0) \Delta A_i(0) \rangle. \quad (3)$$

At $t = 0$, there should be no causal relationship between two different bins, i.e., $\rho_A(\Delta x_{i,j}, 0) = 0$ for $i \neq j$; we can then obtain that $C_{\text{inh}} = -\frac{1}{N_b - 1}$. Because the inherent correlation remains unchanged in time, the spatiotemporal correlation function

$$\rho_A(\Delta x_{i,j}, t) = \frac{\langle \Delta A_j(t) \Delta A_i(0) \rangle}{\langle \Delta A_i(0) \Delta A_i(0) \rangle} + \frac{1}{N_b - 1} \quad (4)$$

thus defined can then accurately capture the causal correlation induced by an initial fluctuation of $\mathcal{A}$ in microcanonical systems. It is slightly different from the spatiotemporal correlation function defined in canonical systems, in which the inherent correlation C_{inh} vanishes [19]. For the sake of convenience, in the following the notation x will be used to replace $\Delta x_{i,j}$ without confusion. Because the spatiotemporal correlation function defined above gives the causal relation between a local fluctuation and the effects it induces at another position (with a displacement x) and at a later time (with a time delay t), it is in essence equivalent to the probability density function that describes the diffusion process of the fluctuation.

It should be noted that the coarse-grained space variable we have taken is important for obtaining the correct spatiotemporal correlation function. If the indexes of particles are used as the space variable, the corresponding correlation function could be dramatically different, because the indexes do not reflect the real physical positions of the particles and thus may cause large position fluctuations [27]. Indeed, as will be presented in the next section, the 1D gas model's spatiotemporal correlation function of energy has a two-peak structure [see Fig. 1(b)]. But if the indexes of particles are used, it shows a three-peak structure instead [18,28]. We therefore emphasize that the coarse-grained space variable is essential for studying the *spatial* diffusion, which is exactly our aim here.

The 1D gas model is efficiently simulated by using the event-driven algorithm that employs the heap data structure to identify the collision times [20]. For the FPU model and the lattice ϕ^4 model, a Runge-Kutta algorithm of 7th to 8th order is adopted for integrating the motion equations, and the Andersen thermostat [29] is utilized to thermalize the system for preparing the equilibrium systems. In calculating the spatiotemporal correlation functions a periodic boundary condition is applied and $N = 4000$ particles are considered, but we have checked and verified that for larger N the simulation results remain the same. For all three models the equilibrium systems are prepared by evolving the systems for a long enough time ($> 10^8$ time units of the models)
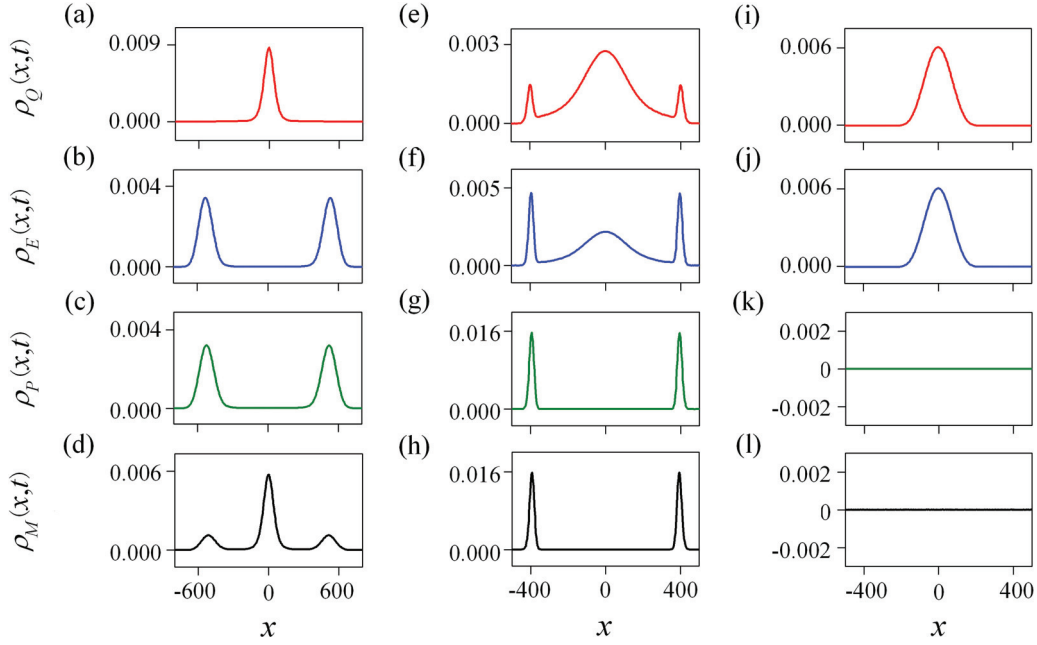
FIG. 1. (Color online) The spatiotemporal correlation functions of heat, energy, momentum, and mass, denoted by $\rho_Q(x,t)$, $\rho_E(x,t)$, $\rho_P(x,t)$, and $\rho_M(x,t)$, respectively, for the 1D gas model (a)–(d), the FPU model (e)–(h), and the lattice ϕ^4 model (i)–(l) at $t = 300$.

from properly assigned random states [30], then the system is evolved in isolation. The size of the ensemble for averaging is larger than 10^{10}.

IV. RESULTS AND DISCUSSIONS

We probe the diffusion behavior of a given physical quantity by studying its spatiotemporal correlation function. We are particularly interested in the diffusion behaviors of heat, energy, momentum, and mass, whose density functions are respectively denoted by $Q(x,t)$, $E(x,t)$, $P(x,t)$, and $M(x,t)$, and the corresponding spatiotemporal correlation functions are denoted by $\rho_Q(x,t)$, $\rho_E(x,t)$, $\rho_P(x,t)$, and $\rho_M(x,t)$. For 1D systems, the heat density function is defined as $Q(x,t) = E(x,t) - \frac{(\bar{E}+\bar{F})M(x,t)}{\bar{M}}$ [31], where $\bar{E}$ ($\bar{M}$) and $\bar{F}$ are, respectively, the spatially averaged energy (mass) density and the internal pressure of the system in equilibrium state. In our simulations, the density functions $E(x,t)$, $P(x,t)$, and $M(x,t)$ are numerically measured first, based on which $Q(x,t)$ is obtained as well. Then the corresponding spatiotemporal correlation functions are evaluated straightforwardly.

The spatiotemporal correlation functions of all three models at an example time $t = 300$ are shown in Fig. 1. It can be seen that the diffusion behavior of the same quantity may vary from system to system (see, e.g., any row in Fig. 1 for a comparison) and in the same system different quantities may have dramatically different diffusion properties as well, though for some of them, such as energy and momentum in the gas model, the diffusion behaviors could be the same. Also, it can be found that except for $\rho_P(x,t)$ and $\rho_M(x,t)$ for the lattice ϕ^4 model, all other spatiotemporal correlation functions conserve their total volume, i.e., $\int \rho_A(x,t)dx = 1$, and we can identify either one standing center peak, or two moving side peaks, or the "superposition" of them. In every case where two

side peaks appear, we find that the centers of the side peaks move outwards at a constant speed. More specifically, the side peaks move outwards at a speed $v = 1.75$ in the gas model and at $v = 1.32$ in the FPU model. In the lattice ϕ^4 model where the total momentum is not conserved due to existence of on-site potentials, we find that $\rho_P(x,t)$ and $\rho_M(x,t)$ decay exponentially and relax to zero rapidly. This is the reason why in Figs. 1(k) and 1(l) no structure is identified.

We find that both $\rho_M(x,t)$ and $\rho_E(x,t)$ can be perfectly expressed as a linear combination of $\rho_Q(x,t)$ and $\rho_P(x,t)$. Our data show that in the gas model $\rho_M(x,t) = \frac{2}{3}\rho_Q(x,t) + \frac{1}{3}\rho_P(x,t)$ and $\rho_E(x,t) = \rho_P(x,t)$, while in the FPU model we have $\rho_M(x,t) = \rho_P(x,t)$ and $\rho_E(x,t) = 0.78\rho_Q(x,t) + 0.22\rho_P(x,t)$, and in the lattice ϕ^4 model $\rho_E(x,t) = \rho_Q(x,t)$ and $\rho_M(x,t) = \rho_P(x,t) = 0$.

We conjecture that functions $\rho_Q(x,t)$ and $\rho_P(x,t)$ can be identified with the heat mode and the sound mode, respectively. Indeed, the function $\rho_Q(x,t)$ represents the heat mode because by definition it describes the motion of heat exclusively [31]. The function $\rho_P(x,t)$ describes the collective motion carrying the memory of the initial moving directions of the particles. In both the gas and the FPU models, $\rho_P(x,t)$ has a bimodal structure and the peaks move outwards at a constant speed, hence can be reasonably related to the sound mode. To make our conjecture more convincing, we study the dynamic structure factor represented by the function $\rho_M(x,t)$. In the gas model, we have measured with high precision the volume of the center peak (i.e., the area enclosed by the center peak curve and the abscissa) of the function $\rho_M(x,t)$, finding it to be $\frac{2}{3}$, and that of the two side peaks to be $\frac{1}{3}$ [see Fig. 1(d)]; the ratio of them equals 2, which is unchanged in time and is in perfect agreement with the Landau-Placzek ratio [32,33] of an ideal gas. In addition, if we multiply $\rho_M(x,t)$ by a factor of 3, its side peaks will overlap with $\rho_P(x,t)$. Similarly, multiplying
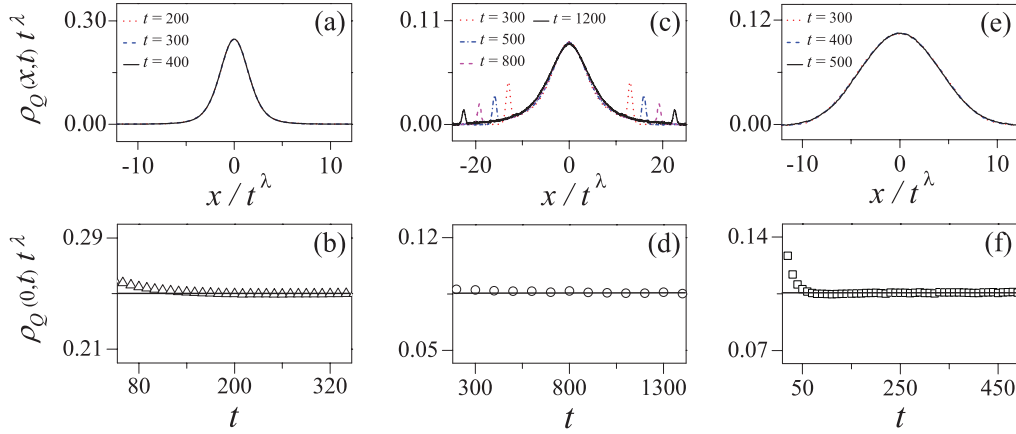
FIG. 2. (Color online) Rescaled profiles of the spatiotemporal correlation function of heat $\rho_Q(x,t)$ for all three models. (a)–(b) are for the gas model with rescaling factor $\lambda = 0.59$ obtained via best fitting. In (a) $\rho_Q(x,t)t^\lambda$ vs x/t^λ at three different times are compared and in (b) $\rho_Q(0,t)t^\lambda$ vs time is shown. (c)–(f) are the same as (a) and (b) but for the FPU model with rescaling factor $\lambda = 0.60$ and the lattice ϕ^4 model with rescaling factor $\lambda = 0.50$ respectively. As a result of rescaling, three curves in (a) and (e) overlap and are indistinguishable. In (c), on each curve there are two side peaks symmetric with respect to $x = 0$, which from the center to the two sides are at $t = 300$, 500, 800, and 1200, respectively.

$\rho_M(x,t)$ by $\frac{3}{2}$, its center peak will overlap with $\rho_Q(x,t)$. These facts convincingly suggest that $\rho_Q(x,t)$ and $\rho_P(x,t)$ represent the heat mode and the sound mode. In the FPU model, there are only two side peaks on $\rho_M(x,t)$, therefore the ratio of the area of the center peak to that of the two side peaks is zero, which is also in agreement with the Landau-Placzek ratio of this model. The function $\rho_M(x,t)$ thus represents only the sound mode. The function $\rho_P(x,t)$ represents the sound mode as well, because it is identical to $\rho_M(x,t)$ as shown in Figs. 1(g) and 1(h).

As a consequence, diffusion properties of heat and momentum can characterize all others diffusion processes. Let us first discuss diffusion of heat by considering $\rho_Q(x,t)$. We find that there is an interesting scaling property in $\rho_Q(x,t)$ in all three systems, i.e., $\rho_Q(x,t)$ is 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 $x = (\frac{t}{t_0})^\lambda x_0$ [see Figs. 2(a) and 2(e)]. For the gas model and the lattice ϕ^4 model $\rho_Q(x,t)$ is a unimodal function; the simulation results suggest that $\lambda = 0.59$ for the former and $\lambda = 0.50$ for the latter. Neglecting the decaying side peaks, $\rho_Q(x,t)$ of the FPU model has the same scaling invariance property with $\lambda = 0.60$ [see Fig. 2(c)]. As $\rho_Q(x,t)$ conserves its volume, we have $\rho_Q(x,t)dx = \rho_Q(x_0,t_0)dx_0$, which leads to the result that the variance of $\rho_Q(x,t)$ goes in time as $\langle x^2(t) \rangle = \langle x_0^2(t_0) \rangle (\frac{t}{t_0})^{2\lambda}$; i.e., a heat fluctuation diffuses in a power law $\langle x^2(t) \rangle \sim t^\beta$ with the diffusion exponent $\beta = 2\lambda$. Thus, we obtain $\beta = 1.18$, 1.20, and 1.00 for the gas model, the FPU model, and the lattice ϕ^4 model, respectively, indicating that a heat fluctuation undergoes superdiffusion in the gas model and the FPU model but normal diffusion in the lattice ϕ^4 model. As mentioned above, the center peak of $\rho_M(x,t)$ in the gas model can be rescaled and overlap perfectly with $\rho_Q(x,t)$. So can the center peak of $\rho_E(x,t)$ in the FPU model and in the ϕ^4 model. To summarize, these peaks relax in the same manner as that of $\rho_Q(x,t)$.

Now let us turn to the sound mode. If $\rho_A(x,t)$ has two side peaks moving at a constant speed v and conserving their

volumes, then $\langle x^2(t) \rangle \sim \int_{vt-\Delta x}^{vt+\Delta x} (vt)^2 \rho_A(x,t)dx \sim t^2$, where Δx represents the width of the peaks. Hence all the processes that involve the sound mode should fall into the class of ballistic diffusion, including the diffusion processes of energy, momentum, and mass density in the gas model and in the FPU model. Particularly, for $\rho_E(x,t)$ in the FPU model we have $\langle x^2(t) \rangle \sim at^{1.20} + ct^2$ since $\rho_E(x,t) = 0.78\rho_Q(x,t) + 0.22\rho_P(x,t)$ as mentioned above, where a and c are constants. Therefore, though the center peak relaxes in a superdiffusive manner, its asymptotic diffusion behavior will be dominated by $\langle x^2(t) \rangle \sim ct^2$ even if a is much larger than c.

The peaks of $\rho_P(x,t)$ disperse while moves ballistically. The dispersion reveals the information of the sound attenuation. Similarly, as for the center peak of $\rho_Q(x,t)$, we find that there is also an interesting scaling property of the side peaks of $\rho_P(x,t)$, i.e., the side peak, taking the right one for example, of $\rho_P(x,t)$ is invariant upon rescaling $\bar{x} \to t^\delta \bar{x}$, where $\bar{x} = x - vt$ (v is the speed of the side peak), so that $t^\delta \rho_P(\bar{x},t) = t_0^\delta \rho_P(\bar{x}_0,t_0)$ for $\bar{x} = (\frac{t}{t_0})^\delta \bar{x}_0$, where $\bar{x}_0 = x - vt_0$. As shown in Fig. 3 for the gas model and the FPU model, the simulation results suggest that $\delta = 0.64$ for the former and $\delta = 0.50$ for the latter.

The above results have some important implications. For example, they indicate that the dynamic structure factor is not sufficient to capture all diffusion processes. In the gas model, as $\rho_M(x,t) = \frac{2}{3}\rho_Q(x,t) + \frac{1}{3}\rho_P(x,t)$ and $\rho_E(x,t) = \rho_P(x,t)$, indeed energy and momentum diffusion can be revealed by the side peaks of $\rho_M(x,t)$ and heat diffusion can be extracted from the center peak of $\rho_M(x,t)$. But in the FPU model, though the dynamic structure factor may characterize the momentum diffusion because $\rho_M(x,t) = \rho_P(x,t)$, it is useless for exploring energy and heat diffusion. In the lattice ϕ^4 model, the function $\rho_M(x,t)$ does not give any interesting information [See Fig. 1(l)]. Therefore, it is necessary to investigate the diffusion behavior of other physical quantities case by case, not only when they have no correlation with the diffusion behavior of mass density so that they can not be probed by the dynamic
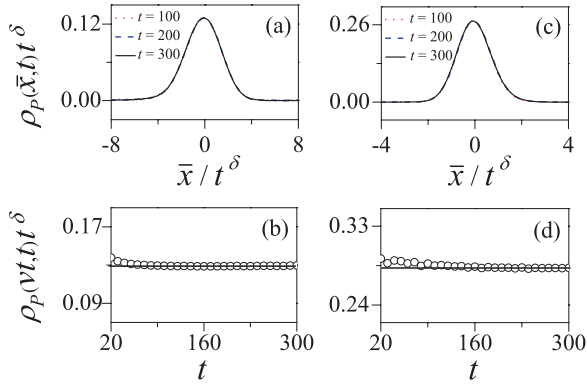
FIG. 3. (Color online) Rescaled profiles of the side peaks on the spatiotemporal correlation function of momentum $\rho_P(x,t)$ for the gas model and the FPU model. (a) and (b) are for the gas model with rescaling factor $\delta = 0.64$ obtained via best fitting. In (a) $\rho_P(\bar{x},t)t^\delta$ vs $\bar{x}/t^\delta$ at three different times are compared, where $\bar{x} = x - vt$ (v is the speed of the side peak). In (b) $\rho_P(vt,t)t^\delta$ vs time is shown. (c) and (d) are the same as (a) and (b) but for the FPU model with rescaling factor $\delta = 0.50$. The fact that three curves in (a) and (c) overlap and are indistinguishable indicates the perfect scaling properties of the side peaks of $\rho_P(x,t)$.

structure factor, but also when the correlation exists but we want to ascertain how to extract the relaxation properties of other quantities from the dynamic structure factor.

Another important implication is that there is no definite correlation between diffusion of heat and energy. The results presented in Fig. 1 also suggest that, in a system, diffusion behavior of energy can be completely different from that of heat and hence may not provide any information of the latter. For example, in the gas model [see Figs. 1(b) and 1(a)], there are two moving peaks in the spatiotemporal correlation function of energy $\rho_E(x,t)$, but there is only one standing peak in that of heat $\rho_Q(x,t)$. In the FPU model, though at an early stage both $\rho_E(x,t)$ and $\rho_Q(x,t)$ have a three-peak structure [see Figs. 1(f) and 1(e)], there is a significant difference between them: while the former keeps its three-peak structure throughout, the two side peaks in the latter keep shrinking and

asymptotically $\rho_Q(x,t)$ becomes unimodal. To scrutinize this difference, we compare in Fig. 4 the time evolution of $\rho_Q(x,t)$ and $\rho_E(x,t)$. We find in both of them the half-height width of the side peaks widens as $l \sim t^{0.50}$, but their height decays as $h \sim t^{-1.31}$ in $\rho_Q(x,t)$ rather than $h \sim t^{-0.50}$ as in $\rho_E(x,t)$. As a result the side peaks of $\rho_E(x,t)$ keep their volumes unchanged since lh is time independent, in clear contrast to those of $\rho_Q(x,t)$ that keep shrinking as $lh \sim t^{-0.81}$. Hence over time $\rho_Q(x,t)$ and $\rho_E(x,t)$ will become qualitatively different. Of all three models we find that only in the lattice ϕ^4 model are the diffusion behaviors of energy and heat the same [see Figs. 1(i) and 1(j)].

These results suggest that the previous studies trying to establish a universal connection between *energy* diffusion and *heat* conduction [18,19] should be revisited. Conceptually, it is heat diffusion, rather than energy diffusion, that should and can be meaningfully related to heat conduction. For 1D momentum conserving systems, it has been found that generally the heat conductivity κ diverges in the thermodynamic limit as $\kappa \sim L^\alpha$ with $0.25 \leqslant \alpha \leqslant 0.5$ [10,11,13,20,34–39], and on the other hand, energy diffuses in time as $\sim t^\beta$. Two formulas, $\alpha = \beta - 1$ [15] and $\alpha = 2 - \frac{2}{\beta}$ [16], have been proposed to connect the two exponents α and β universally. But as shown in our gas model, the energy fluctuations spread ballistically and thus the diffusion of energy is characterized by $\beta = 2$, such that α and β definitely do not agree with either of the two formulas. In the FPU model, due to the ballistic behavior of the two side peaks on $\rho_E(x,t)$, β will asymptotically saturate at $\beta = 2$, again disobeying the two formulas.

From the hydrodynamic point of view, the reason why there is no universal connection between energy diffusion and heat conduction is conceptually easy to understand: the former is also affected by advection, i.e., the sound mode. This has been well shown by our simulation results that, in all three models, the diffusion process of energy can be perfectly expressed as a linear combination of those of heat and momentum.

V. SUMMARY

The method for calculating the spatiotemporal correlation functions in microcanonical systems has been shown to be
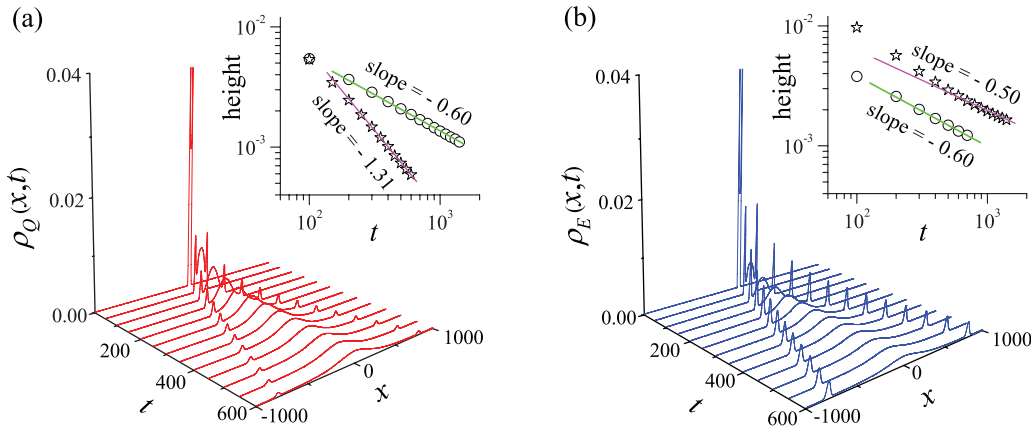

FIG. 4. (Color online) (a) The spatiotemporal correlation function of heat, $\rho_Q(x,t)$, for the FPU model. The inset shows the log-log plot of time dependence of the heights of the center peak (open circles) and the side peaks (open stars). (b) The same as (a) but for the spatiotemporal correlation function of energy, $\rho_E(x,t)$, of the FPU model.

effective in probing the diffusion processes in equilibrium systems. By this method, the diffusion processes of local fluctuations of heat, energy, momentum, and mass in three one-dimensional systems are explored in detail. It is found that diffusion of energy and mass can be expressed as a linear combination of $\rho_Q(x,t)$ and $\rho_P(x,t)$, which we conjecture to be representatives of the heat mode and the sound mode, respectively. There is a scaling in function $\rho_Q(x,t)$, i.e., $\rho_Q(x_0,t_0) = (\frac{t}{t_0})^\lambda \rho_Q((\frac{t}{t_0})^\lambda x_0,t)$, in all three models. For the lattice ϕ^4 model, $\lambda = 0.5$, indicating normal diffusion. For the gas model and the FPU model, $\lambda = 0.59$ and 0.60, respectively, indicating superdiffusion. The function $\rho_P(x,t)$ vanishes in the lattice ϕ^4 model due to the momentum-nonconserving property. For the gas model and the FPU model, $\rho_P(x,t)$ conserves its volume and follows the scaling relation $\rho_P(\overline{x}_0,t_0) = (\frac{t}{t_0})^\delta \rho_P((\frac{t}{t_0})^\delta \overline{x}_0,t)$ with $v = 1.75$, $\delta = 0.64$ in the gas model (at temperature $T = 2$) and $v = 1.32$, $\delta = 0.50$ in the FPU model.

We have revealed correlations between different diffusion processes. It is found that the diffusion behaviors of different physical quantities may be distinctively different, and the correlations between them could be very complex. The diffusion behavior of a physical quantity may vary from system to system, hence they should be studied case by case. Diffusion of heat, energy, and momentum is correlated with that of mass density fluctuations in the gas model, which implies that they can be probed by measuring the dynamic structure factor. In the two lattice models, the dynamic structure factor provides no information of heat diffusion.

A particular finding is that diffusion of energy can be qualitatively different from that of heat, hence a universal connection may not exist between energy diffusion and heat conduction (though we conjecture that instead of energy diffusion, a universal connection may be established between *heat* diffusion and *heat* conduction). This is different from the relationship between the energy current and the heat current [12,13], which turns out to be the same [10] at nonequilibrium stationary state.

We have not studied two- and three-dimensional systems. In one of our studies [30] it has been shown that the particle diffusion can be qualitatively different from the energy diffusion in a two-dimensional gas with Lennard-Jones interactions, but the relaxation behavior of heat has not been studied yet. In previous studies heat diffusion has constantly been *assumed* to be normal in three-dimensional systems, including the three-dimensional gases with Lennard-Jones interactions [40,41]. What we have learned in this work suggests that it is very necessary to check if this is the case.

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