Super heat diffusion in one-dimensional momentum-conserving nonlinear lattices

Lei Wang (王雷),* Zhiyuan Wu (吴志远), and Lubo Xu (续路波)
Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials and Micro-nano Devices, Renmin University of China, Beijing 100872, People's Republic of China
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Heat diffusion processes in various one-dimensional total-momentum-conserving nonlinear lattices with symmetric interaction and asymmetric interaction are systematically studied. It is revealed that the asymmetry of interaction largely enhances the heat diffusion; while according to our existing studies for heat conduction in the same lattices, it slows the divergence of heat conductivity in a wide regime of system size. These findings violate the proposed relations that connect anomalous heat conduction and super heat diffusion. The generality of those expectations is thus questioned.

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I. INTRODUCTION

Heat conduction in macroscopic systems is generally governed by the Fourier law, i.e., the stationary state heat current density $\vec{j}$ induced by a small temperature gradient satisfies $\vec{j} = -\kappa \nabla T$, where the heat conductivity κ is a constant independent of the system size L. It is, however, widely observed that heat conduction in one-dimensional (1D) momentum-conserving systems is anomalous, i.e., the Fourier law is violated [1,2] and the resulting heat current j decays with the system length L as $L^{-1+\alpha}$, $\alpha > 0$. Therefore, the heat conductivity κ is length dependent and diverges with L by L^{α}.

On the other hand, the heat energy diffusion process can be characterized by the evolution of the energy mean square displacement $\sigma^2(t) \sim t^{\beta}$. Here $\beta = 1$ corresponds to the normal diffusion, while $\beta > 1$ corresponds to the super diffusion [3]. Generally speaking, when the heat conduction is anomalous, the heat diffusion is also super.

The detailed connection between these two transport phenomena has attracted much interest recently. In 2003 it was proposed that the two power exponents α and β satisfy a general relation $\beta = 2/(2-\alpha)$ [4]. This relation agrees with some existing numerical simulations [5–7]. Based on noninteracting-heat-carrier and Levy-walk assumptions, another suggestion that $\beta = \alpha + 1$ was also proposed in the same year [8]. It was also supported by some numerical calculation [9,10] and theoretical analyses [11]. The points in common of the two suggestions are the following: (1) when the heat conduction in a material is normal, its heat diffusion is also normal, i.e., $\alpha = 0 \Leftrightarrow \beta = 1$; (2) when the heat conduction is ballistic, the heat diffusion is also ballistic, i.e., $\alpha = 1 \Leftrightarrow \beta = 2$; and (3) most importantly, in the anomalous transport case that $\alpha \in (0,1)$ and $\beta \in (1,2)$, the greater α the greater β.

The main objective of this paper is to systematically study the heat diffusion process in various 1D momentum-conserving nonlinear lattices and then verify the generality of these existing theoretical expectations.

*phywanglei@ruc.edu.cn

II. MODELS AND SIMULATIONS

A. Lattice models

In this paper we numerically study heat conduction and diffusion in a few one-dimensional momentum-conserving nonlinear lattices whose Hamiltonians read

$$H = \sum_i \left[\frac{\dot{x}_i^2}{2} + V(x_i - x_{i-1})\right]. \quad (1)$$

The mass of all particles has been set to unity. The potential energy between the particles i and $i-1$ is $V_i \equiv V(x_i - x_{i-1})$. The interaction force is correspondingly $f_i = -\partial V_i/\partial x_i$. The local energy that belongs to the particle i can be defined in either a symmetric form: $E_i = \frac{\dot{x}_i^2}{2} + \frac{1}{2}(V_i + V_{i+1})$, i.e., connected particles share their interaction potential energy equally, or an asymmetric form: $E_i = \frac{\dot{x}_i^2}{2} + V_i$, i.e., the interaction potential energy belongs to the particle right next to it. Similarly, the instantaneous local heat current can be defined symmetrically as $j_i \equiv \frac{1}{2}(\dot{x}_i + \dot{x}_{i+1}) f_{i+1}$, or asymmetrically as $j_i \equiv \dot{x}_i f_{i+1}$. The instantaneous global heat current is defined as $J(t) \equiv \sum_i j_i(t)$. Unless otherwise stated, we choose the symmetric definitions throughout this paper. We will discuss the difference in detail in Sec. II E.

The interaction potential takes the general form $V(x) = \frac{1}{2}k_2x^2 + \frac{1}{3}k_3x^3 + \frac{1}{4}k_4x^4$. We shall study three types of lattices: (1) the Fermi-Pasta-Ulam(FPU) -$\alpha\beta$ lattices with $k_2 = k_4 = 1, k_3 = 1$ (in short the FPU-$\alpha 1\beta$ lattice) and $k_2 = k_4 = 1, k_3 = 2$ (in short the FPU-$\alpha 2\beta$ lattice), (2) the FPU-β lattice with $k_2 = k_4 = 1, k_3 = 0$, and (3) the purely quartic lattice with $k_2 = k_3 = 0$, $k_4 = 1$. The interaction in the FPU-$\alpha\beta$ lattices is asymmetric, i.e., $V(x) \neq V(-x)$, while the interaction in the other lattices is symmetric. In the former case, the temperature pressure is nonvanishing finite in the thermodynamic limit [12].

In order for better numerical accuracy and acceptable computational cost, an embedded Runge-Kutta-Nystrom algorithm of orders 8(6) [13] is applied in Sec. II B and Sec. II C 2 for the simulations of conservative Hamiltonian systems; and a fifth-order Runge-Kutta algorithm [14] is applied in Sec. II C 1 for the dissipative systems.

B. Heat diffusion

1. Nonequilibrium direct simulation

The heat diffusion process can be simulated in two different ways, the noneqilibrium energy pulse method and the equilibrium energy correlation method. We first perform the calculate by the former way and then will compare the results from different ways later.

The simulations are carried out in lattices with periodic boundary conditions and totally N particles. A set of randomly chosen initial states are extracted from the microcanonical ensemble with zero total momentum and fixed energy density $\langle E\rangle$ which corresponds to temperature $T = 1$. At time $t = 0$, we need to inject energy into the middle particle (due to the periodic boundary conditions any particle can be regarded as this middle one). To this end, we first apply the conventional method [7]; i.e., the kinetic energy of the middle particle (labelled 0) is increased by a fixed value ΔE. The evolution of the energy profile along the lattice is then calculated afterwards. At a later time $t > 0$, the rescaled excess energy distribution in the lattice is defined as

$$\delta_{\rm E}(i,t) \equiv \frac{E(i,t) - \langle E\rangle}{\Delta E}. \quad (2)$$

It is easily confirmed that $\delta_{\rm E}(i,0) = 0$, if $i \neq 0$, and $\sum_i \delta_{\rm E}(i,0) = 1$. The width of the diffusion can be measured by the second moment of $\delta_{\rm E}(i,t)$:

$$\sigma^2(t) \equiv \sum_i \delta_E(i,t) i^2. \quad (3)$$

Existing studies basically focus on the close-to-equilibrium state, which requires that the value of ΔE should be infinitesimal so that every portion of the system is always at a local thermal equilibrium (LTE) state. This is a condition of some theoretical analyses [11]. However, the role of the magnitude of ΔE is still worth studying because a real energy pulse must be finite. And in the numerical point of view, ΔE may not be too small, otherwise the resulting energy diffusion cannot be distinguished from the background statistical fluctuations.

The excess energy distribution profiles $\delta_{\rm E}(i,t)$ at time $t = 100$ for various lattices and three different values of ΔE are plotted in Fig. 1 (left column). Each of the profiles consists of a central peak (thermal mode) and two side peaks (sound modes). Such an energy propagation can be captured by the diffusion profiles of the single-particle Levy walk approach [15]. The behaviors of the different modes have also been studied by the nonlinear hydrodynamic fluctuation analysis recently [16].

We see in the figure that the sound modes move faster in larger ΔE case, which results in a larger $\sigma^2(t)$ in short time t region. However, the difference vanishes in longer t region. It is reasonable since all the states will approach to equilibrium in long t limit. As a consequence, the resulting $\sigma^2(t)$ for different ΔE approach each other; see Fig. 1 (right column). In the numerical point of view, we found $\Delta E = 3\langle E\rangle$ is the best choice. We have also plotted the evolution of $\delta_{\rm E}(i,t)$ at long t region and the corresponding $\sigma^2(t)$, for $\Delta E = 3\langle E\rangle$ in Fig. 2.

We see in Fig. 2 that in the long t region $\sigma^2(t)$ for the lattices with symmetric interaction basically follow the same power-law divergence $\sigma^2(t) \sim t^{1.4}$, while the power exponents for the FPU-$\alpha 1\beta$ and the FPU-$\alpha 2\beta$ lattices are about 1.5 and 1.8, which are evidently greater than 1.4. The fact is clear that heat diffuses faster in lattices with asymmetric interaction, and the greater the asymmetric term k_3 the faster heat diffuses.

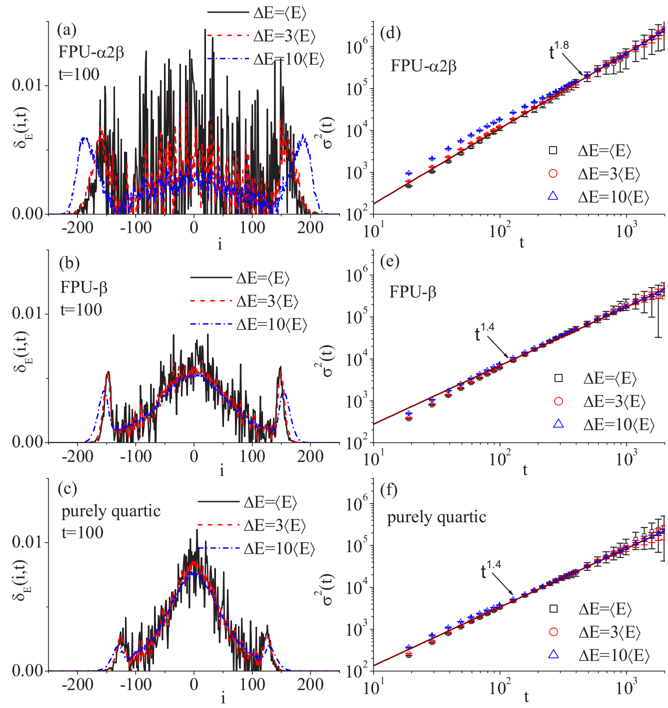

FIG. 1. (Color online) Left column: Snapshots of the rescaled excess energy distribution $\delta_{\rm E}(i,t)$ at time $t = 100$ for various lattices and three different energy pulse values. Right column: The corresponding $\sigma^2(t)$. Generally the side peaks move a little faster for the case $\Delta E = 10\langle E\rangle$, and correspondingly $\sigma^2(t)$ is also larger. The difference vanishes when t increases. It is reasonable, because the system is closer to equilibrium state as t increases. The results for $\Delta E = \langle E\rangle$ and $3\langle E\rangle$ basically overlap each other.

We note that when the kinetic energy of the central particle is changed, the velocity of the particle is also changed. Therefore, the total momentum of the lattice is no longer zero. In order to avoid any puzzle derived from, we have also tried an alternative way, i.e., at time $t = 0$, we do not change the velocity of the central particle, but change its coordinate so as to increase the total potential energy by the same value ΔE. The comparison between different results for the FPU-$\alpha 2\beta$ lattice is shown in the inset of Fig. 2(d). No evident disparity can be observed. Therefore, we conclude that the observed energy diffusion is physical.

2. Equilibrium spatiotemporal correlation of the local energy

In Ref. [9] the energy fluctuation spatiotemporal correlation function is proposed to characterize the diffusion processes. In a stationary state, the energy fluctuation spatiotemporal correlation function is defined as

$$C_{\rm EE}(i,t) \equiv \langle \Delta E_i(t) \Delta E_0(0)\rangle, \quad (4)$$

where $\Delta E_i(t) \equiv E_i(t) - \langle E_i\rangle$. In a homogeneous lattice, $\langle E_i\rangle$ is independent of the particle label i and simply equals $\langle E\rangle$.

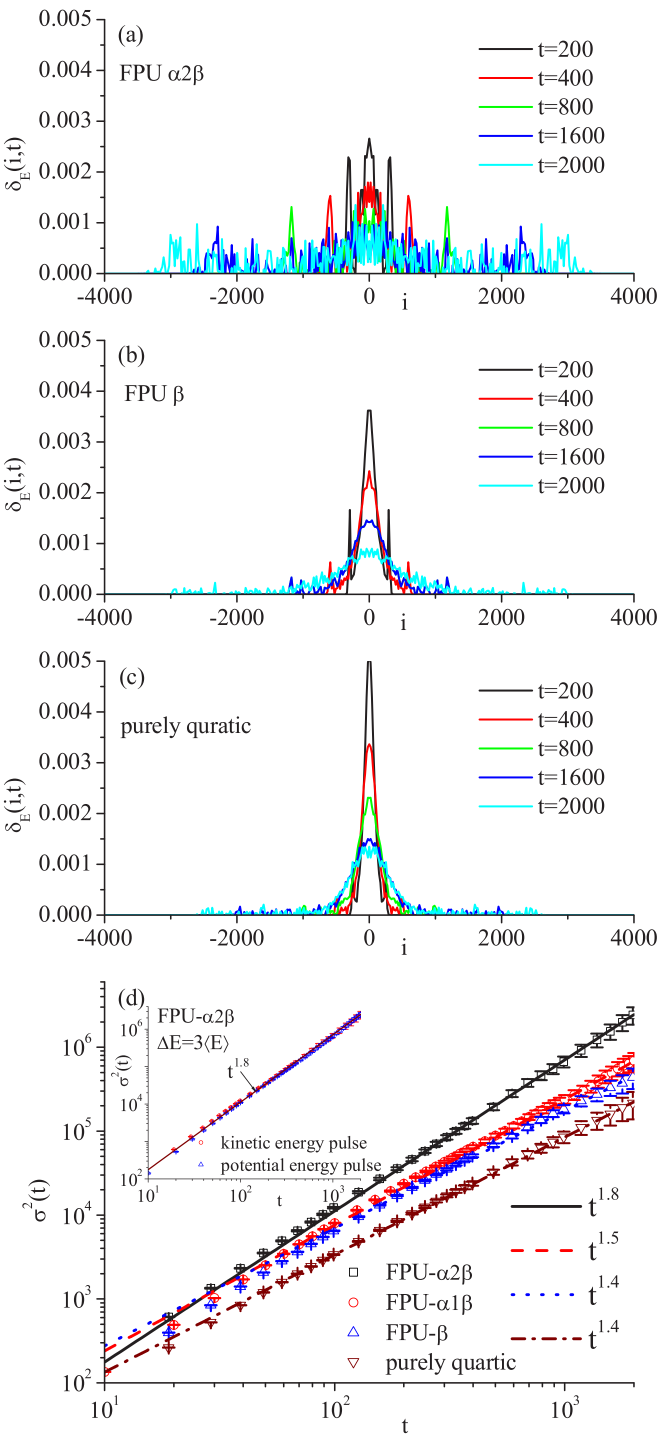

FIG. 2. (Color online) (a)–(c) Energy diffusion in various lattices, $\Delta E = 3\langle E\rangle$. Data binning over contiguous time t has been performed to reduce statistical fluctuations. (d) The corresponding $\sigma^2(t)$. Inset: The comparison between the results from different ways of energy injection, the kinetic energy and potential energy, for the FPU-$\alpha 2\beta$ lattice.

Originally, the simulation is supposed to be performed in a canonical assemble, i.e., the two ends of the lattice are coupled with two heat baths so as to keep the system at a fixed temperature [9]. However, it is much more convenient to simulate lattices in microcanonical assembles with periodic boundary condition and fixed energy density which correspond to the desired temperature T [17].

In a microcanonical assemble, due to the energy conservation, $\sum_i C_{\rm EE}(i,0) = \sum_i \langle \Delta E_i(0)\Delta E_0(0)\rangle = \Delta E_0(0)\langle \sum_i \Delta E_i(0)\rangle = 0$. Since $\langle \Delta E_0(0)\Delta E_0(0)\rangle > 0$, this induces a constant correlation between any pair of particles, even though they are far from each other and thus should have no causal relationship at the same time. Such an inherent correlation does not reflect any property of the lattice and thus should be excluded from the calculation [17]. If the asymmetric definition of local energy is applied, then there should be no causal relationship between any two different particles, while if the symmetric definition is applied, then the local energy of nearest-neighboring particles is also correlated for $t = 0$ since they share the potential energy of a same interaction. This part also contributes to the inherent correlation.

In order to remove the above mentioned inherent correlation and compare the results with those from the direct diffusion simulation, we define the rescaled local energy correlation function

$$\rho_{\rm E}(i,t) \equiv \frac{C_{\rm EE}(i,t)}{C_{\rm EE}(-1,0) + C_{\rm EE}(0,0) + C_{\rm EE}(1,0)} + \frac{1}{N}. \quad (5)$$

This definition satisfies $\rho_{\rm E}(i,0) = 0$, if $|i| > 1$, and $\sum_i \rho_{\rm E}(i,0) = 1$.

$\rho_{\rm E}(i,t)$ is expected to evolve in the same way as $\delta_E(i,t)$ does [9]. Therefore,

$$r^2(t) \equiv \sum_i \rho_E(i,t) i^2 \quad (6)$$

provides another way of calculating the width of the diffusion $\sigma^2(t)$ in Eq. (3), with much higher efficiency.

Again, we simulate the lattices at temperature $T = 1$. The evolution of $\rho_E(i,t)$ and the corresponding $r^2(t)$ are plotted in Fig. 3. Compared with those from the direct energy diffusion simulations that are plotted in Fig. 2, the curves are much smoother, and the error bars for $r^2(t)$ are much smaller.

The calculation of heat diffusion by different methods agrees with each other very well for the lattices with symmetric interaction. As for the FPU-$\alpha 2\beta$ lattice, the two sound modes are much bigger while the central peak is smaller for the latter method, compared with those for the former method. Due to the big fluctuation of $\delta_{\rm E}(i,t)$ we are not able to verify whether it would approach $\rho_{\rm E}(i,t)$ in the small ΔE limit or not. What we have observed is that the deviation between $\delta_{\rm E}(i,t)$ and $\rho_{\rm E}(i,t)$ for $\Delta E = \langle E\rangle$ is still noticeable and far beyond the statistical uncertainty. The divergence power exponents of $\sigma^2(t)$ and $r^2(t)$ are not exactly identical. However, most importantly, both of them suggest that heat diffuses in the lattices with asymmetric interaction much faster than it does in the lattices with symmetric interaction. Similar behavior has also been observed recently in a 1D hard gas model [17].

C. Heat conduction

In this subsection we will briefly review some existing calculations of the heat conductivity in those lattices.

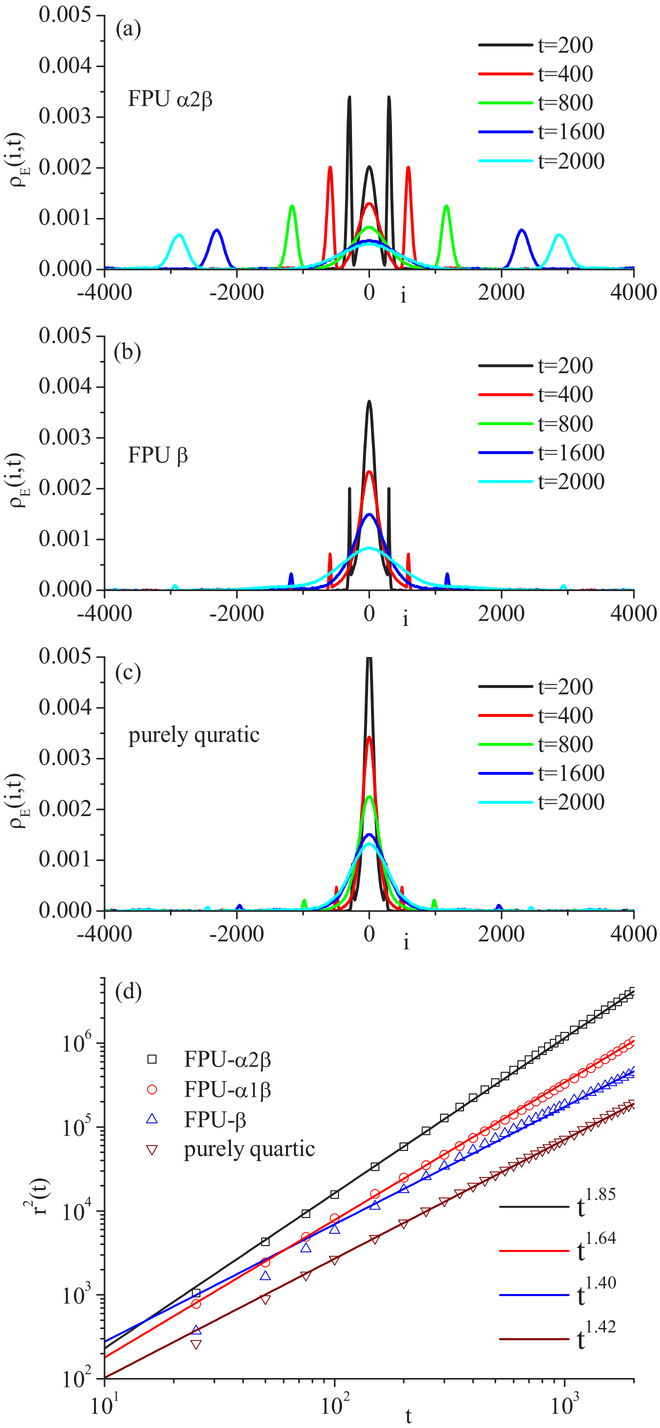

FIG. 3. (Color online) (a)–(c) The rescaled local energy correlation function $\rho_{\rm E}(i,t)$ in various lattices. (d) The corresponding $r^2(t)$. The error bars are not plotted since they are smaller than the symbol size.

1. Nonequilibrium heat bath method

The heat conductivity κ can be directly calculated by the nonequilibrium heat bath method. To this end, fixed boundary conditions are applied, and two Langevin heat baths with different temperatures 1.5 and 0.5 are coupled to the two ends of the lattice with length L. In the stationary state, time- and site-independent heat current j flows from the hot to the cold. The length-dependent heat conductivity $\kappa_{\rm NE}(L)$ is defined as $\kappa_{\rm NE} \equiv \frac{J}{dT/dL}$. Here the subscript "NE" denotes that the calculation is based on the nonequilibrium method and $\frac{dT}{dL}$ denotes the temperature gradient in the central region of the lattice.

2. Equilibrium Green-Kubo method

An alternative way of determining the dependence of heat conductivity on system length is based on the Green-Kubo formula [18]. Namely, the rescaled heat current correlation function is defined as

$$C_{JJ}(\tau) \equiv \lim_{N\to\infty} \frac{1}{k_{\rm B}T^2N} \langle J(t)J(t+\tau)\rangle_t, \tag{7}$$

where N is the total particle number. The Boltzmann constant $k_{\rm B}$ is set to unity throughout this paper. In the anomalous heat conduction case, the length-dependent heat conductivity is calculated by

$$\kappa_{\rm GK}(L) \equiv \int_0^{L/v_s} C_{JJ}(\tau)\, d\tau. \tag{8}$$

v_s is the sound velocity, which can be measured by the speed of the sound modes showing in Figs. 3 or 2. The subscript "GK" denotes that the calculation is based on the Green-Kubo formula.

The simulations are carried out in lattices with periodic boundary conditions. Microcanonical simulations are applied with zero total momentum [19] and identical energy density $\langle E\rangle$ that corresponds to the required temperature $T = 1$.

The numerical results of $\kappa_{\rm NE}$ and $\kappa_{\rm GK}$ for various lattices are plotted in Figs. 4(a) and 4(b), respectively. These data have been presented separately in several figures in Refs. [20] and [21]. We see $\kappa_{\rm NE}$ and $\kappa_{\rm GK}$ for various lattices are basically consistent with each other. In a wide range of L, κ in the FPU-$\alpha\beta$ lattices diverges so slowly that the heat conduction behaves like Fourier's law. Evidently the asymmetric interaction slows the divergence of heat conductivity. Such a phenomenon has been repeatedly observed in the same or similar lattices recently [21–25], since it was observed in a FPU-$\alpha\beta$ lattice [20] a few years ago. The physical reason is, however, still not clear. Even in an extremely long range of L which is already a macroscopic scale, the heat conductivity in the FPU-$\alpha\beta$ lattices diverging faster than in the FPU-β lattice is highly unlikely [21,26].

D. Super heat diffusion and anomalous heat conduction

The two facts that have been observed, i.e., (1) heat diffuses faster in lattices with asymmetric interaction and (2) heat conduction diverges, however, more slowly in lattices with asymmetric interaction, clearly violate the two theoretical expectations mentioned in the introduction section, both of which suggest that the faster heat diffuses, the faster heat conduction diverges. It is quite surprising that the fast heat diffusion in the lattices with asymmetric interaction does not lead to a fast-divergent heat conductivity.

We note that the two expectations consider systems in the thermodynamic limit. Therefore, although it is highly unlikely that the situation "faster heat diffuses but slower heat

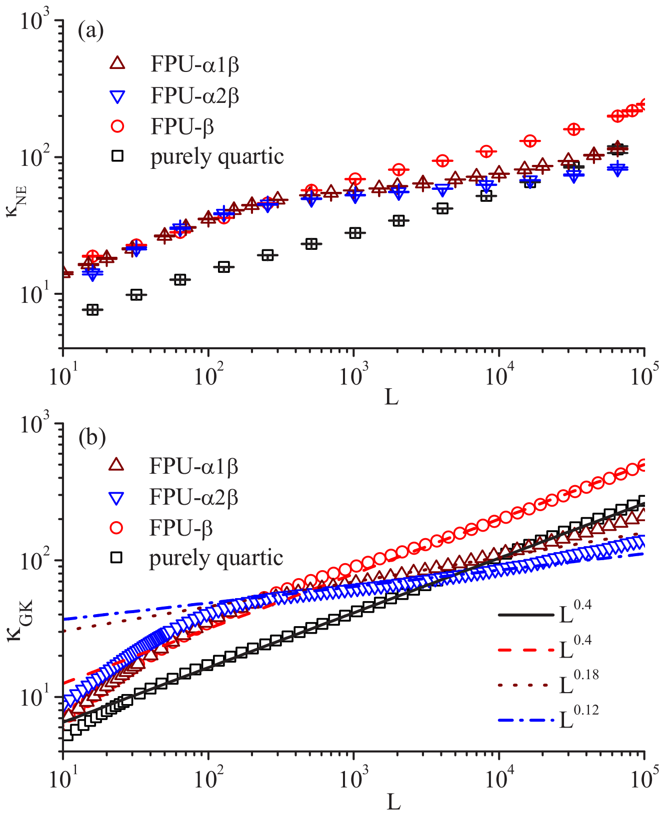

FIG. 4. (Color online) (a) $\kappa_{\rm NE}$ and (b) $\kappa_{\rm GK}$ vs lattice length L for various lattices. They basically agree with each other. These data have been published in Refs. [20,21]. The lines in (b) are the best linear fits of $\kappa_{\rm GK}$ in the middle region of L. κ diverges much more slowly in the lattices with asymmetric interaction, in a wide region of L.

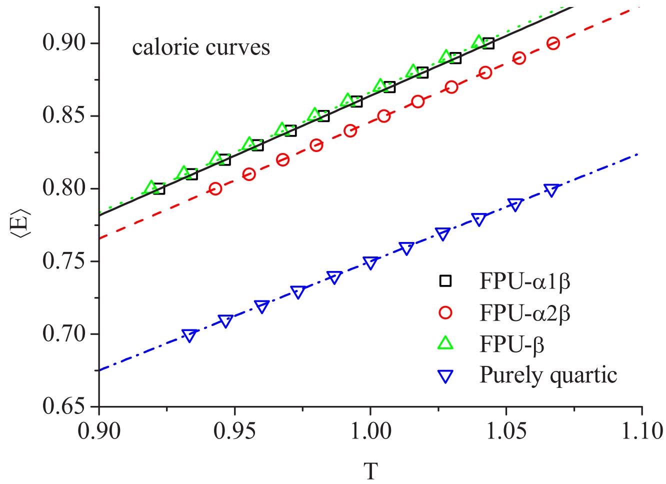

FIG. 5. (Color online) Calorie curves for the four lattices. Symbols correspond to the numerical simulations, and the lines are their linear fit around $T = 1$.

conduction diverges" would change in an extremely large time and size scale, we are still not able to completely rule out such a possibility based on the numerical simulations only. In order to study this issue more carefully, we verify a relation that was proposed very recently in Ref. [11] that heat current correlation function $C_{JJ}(t)$ and the local energy correlation function should be related rigorously by

$$\frac{d^2}{dt^2}r^2(t) = \frac{2C_{JJ}(t)}{c}. \tag{9}$$

Equation (9) is expected to be valid not only in the long t limit, but for any finite t as well. An immediate consequence of this equation is $\beta = \alpha + 1$ [11].

The specific volumetric heat capacity c can be temperature independent (in the purely quartic lattice) or temperature dependent (in other lattices). It can be calculated either directly by the local slope of the calorie curves, i.e., $c \equiv \frac{d\langle E(T)\rangle}{dT}$ (see Fig. 5), or alternatively from the relation $k_B T^2 c = \lim_{L\to\infty}\frac{1}{L}\langle \Delta E_L^2\rangle$ [11]. Results from the different methods are consistent with each other. At $T = 1$, c equals about 0.824, 0.804, 0.829, and 0.750, for the FPU-$\alpha 1\beta$ lattice, the FPU-$\alpha 2\beta$ lattice, the FPU-β lattice, and the purely quartic lattice, respectively. However, we note that the theoretical expectation $\langle E(T)\rangle = \frac{1}{2}T + \frac{\int V(x)e^{-V(x)/T}dx}{\int e^{-V(x)/T}dx}$ [11] is not valid for the lattices with asymmetric interaction.

The comparison of the left- and right-hand sides of Eq. (9) is presented in Fig. 6. The numerical simulations agree with the theoretical expectation for the FPU-β and the purely quartic lattices very well, which is also consistent with the existing numerical calculation [11]. However, Eq. (9) is violated in the lattices with asymmetric interactions, i.e., the FPU-$\alpha\beta$ lattices; and the greater the asymmetric term k_3, the larger the discrepancies. Furthermore, such an inconsistency does not vanish in the long t limit. These findings are consistent with the observations in Secs. II B and II C that the asymmetry of interaction enhances the heat diffusion while reducing the heat conduction.

E. Definitions of local energy and local heat current

It is worth mentioning that the definitions of the local heat current j_i and the local energy E_i must be consistent with each other, i.e., satisfies the continuity equation $\dot{E}_i = j_{i-1} - j_i$ [1], which is a precondition of Eq. (9) [11]. The symmetric definitions that we used meet this requirement. If we define the local energy asymmetrically as $E_i \equiv \frac{\dot{x}_i^2}{2} + V_i$, then the local heat current should be defined accordingly as $j_i \equiv \dot{x}_i f_{i+1}$. Note that under different definitions of j_i, the values of the instantaneous global heat current $J(t) \equiv \sum_i j_i(t)$ are not necessarily the same. Their resulting correlation C_{JJ} might also be different. If such asymmetric definitions of E_i and j_i are simultaneously applied, Eq. (9) is also satisfied for the lattices with symmetric interaction. However, the results are not exactly the same as those from the symmetric definitions; see Fig. 6(b). They oscillate in the short t region first, then approach those from the symmetric definitions in the large t region. In contrast to the heat-current correlation loss that are induced by finite-size effects [26], we have confirmed that these oscillations behave the same in long and short lattices, and thus they are not induced by the finite length of the lattice. These oscillations are unlikely to be physical and must be attributed to the asymmetric definitions. That is why we choose the symmetric definitions in this paper, although the

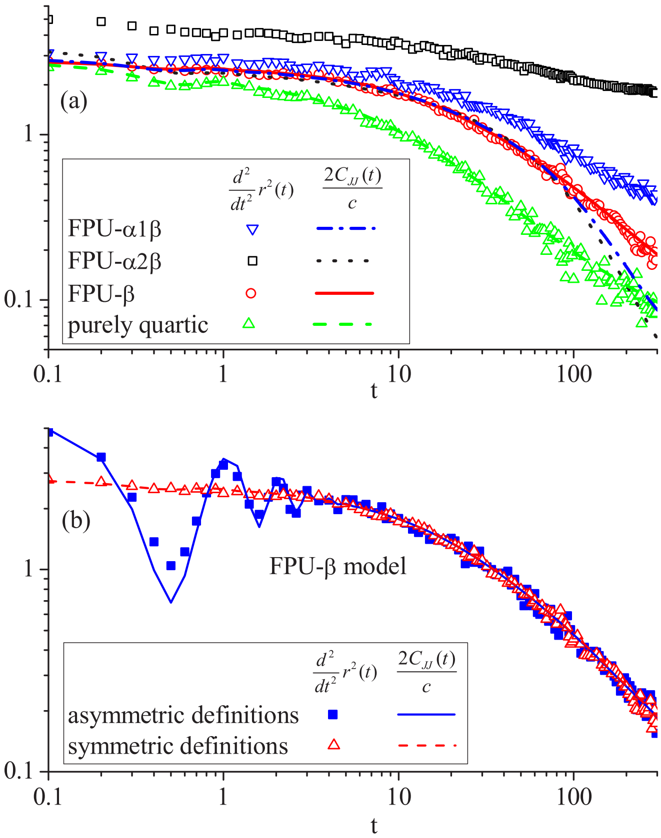

FIG. 6. (Color online) (a) Comparison between the left-hand (symbols) and right-hand (curves) sides of Eq. (9) for various lattices. The agreement for those with symmetric interaction (the FPU-β and the purely quartic lattices) is very good. However, evident discrepancies are observed for the lattices with asymmetric interaction, i.e., the FPU-$\alpha\beta$ ones. (b) Comparison between the results from different definitions of the local energy E_i and the local current j_i for the FPU-β lattice. Symbols and curves correspond to the left- and right-hand sides of Eq. (9), respectively.

asymmetric ones have been applied even more widely due to their simplicity [10,27].

III. SUMMARY AND DISCUSSIONS

We have carried out calculation for heat diffusion in a few 1D momentum-conserving nonlinear lattices, including two lattices with symmetric interaction (the FPU-β and the purely quartic lattices) and two with asymmetric interaction (the FPU-$\alpha\beta$ lattices). We have compared the results from two different methods, the nonequilibrium energy pulse method and the equilibrium local energy correlation method. In the former case, we have also studied the role of the magnitude of the injected energy. It is found that in a short time, the larger the injected energy, the faster it diffuses. However, the difference decays as in the long time limit.

According to the comparison between the above mentioned two methods, we found their results agree with each other quite well for the lattices with symmetric interaction. The agreement is not so good for the FPU-$\alpha 2\beta$ lattice. The two sound modes are much higher while the central peak is a little lower for the latter method, compared with those for the former method. Due to the big fluctuation, we are not able to verify whether such a disparity decays or not in the small ΔE limit. Both methods suggest that the heat diffuses in the lattices with asymmetric interaction much faster than does it in the lattices with symmetric interaction. Interestingly, existing calculation of heat conductivity indicates that κ in the lattices with asymmetric interaction diverges not as fast as it does in the lattices with symmetric interaction. This phenomenon violates both of the two existing theoretical expectations mentioned in the introduction. The asymmetric interaction should be responsible for it.

A recently proposed relation $\frac{d^2}{dt^2}r^2(t) = \frac{2C_{JJ}(t)}{c}$ has been checked. Again, the relation is satisfied in the lattices with symmetric interactions (the FPU-β and the purely quartic lattices) while it is violated in the FPU-$\alpha\beta$ lattices whose interaction is asymmetric.

In summary, the effects of the asymmetric interaction that are observed in this paper include (1) the greater ΔE dependence of $\delta_{\rm E}(i,t)$ [Fig. 1(a)]; (2) the disparities between $\delta_{\rm E}(i,t)$ and $\rho_{\rm E}(i,t)$ [Figs. 2(a) and 3(a)]; (3) the faster heat diffusion [Figs. 2(d) and 3(d)] but slower heat-conductivity divergence [Fig. 4]; and (4) the violation of Eq. (9) [Fig. 6]. More studies are necessary to understand all these interesting phenomena, in particular, why the fast heat diffusion does not contribute to heat conduction.

It has been suggested recently by Chen *et al.* that the conventional definition of the heat current [1,2], which is applied in this paper, is actually the energy current, and the heat current should be defined differently [17]. Furthermore, they claimed that if that different definition of heat current is applied, then one of the connection formulas, $\beta = 2/(2-\alpha)$, will be correct for the 1D hard gas model [28].

ACKNOWLEDGMENTS

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