# Anomalous energy diffusion in two-dimensional nonlinear lattices

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Heat transport in one-dimensional (1D) momentum-conserved lattices is generally assumed to be anomalous, thus yielding a power-law divergence of thermal conductivity with system length. However, whether heat transport in a two-dimensional (2D) system is anomalous or not is still up for debate because of the difficulties involved in experimental measurements or due to the insufficiently large simulation cell size. Here we simulate energy and momentum diffusion in the 2D nonlinear lattices using the method of fluctuation correlation functions. Our simulations confirm that energy diffusion in the 2D momentum-conserved lattices is anomalous and can be well described by the Lévy-stable distribution. As is expected, we verify that 2D nonlinear lattices with on-site potentials exhibit normal energy diffusion, independent of the dimension. Contrary to the hypothesis of a 1D system, we further clarify that anomalous heat transport in the 2D momentum-conserved system cannot be corroborated by the momentum superdiffusion any longer. Our findings offer some valuable insights into mechanisms of thermal transport in 2D system.

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## I. INTRODUCTION

Fourier's law [1] has witnessed a good validation in the three-dimensional (3D) bulk systems, where thermal conductivity  $\kappa$  is an intrinsic property of a material. However, the breakdown of Fourier's law has recently been confirmed [1–7] in low-dimensional systems. For the one-dimensional (1D) system, thermal conductivity  $\kappa$  in the 1D Fermi-Pasta-Ulam  $\beta$ (FPU- $\beta$ ) nonlinear lattices was first found [8] to diverge with the system size N as  $\kappa N^{\alpha}$  with  $0 < \alpha < 1$ . Similar lengthdependent thermal conductivity was further observed in the FPU chains [9-12], the diatomic Toda lattice [13-16], and random collision model [17]. This non-Fourier heat transport is referred to as anomalous heat transport. Although many efforts such as mode-coupling theory [18], hydrodynamical theory [19], and nonlinear fluctuating hydrodynamics [20,21] have been made, the origin of anomalous heat transport [5] still remains unclear. Normal heat conduction obeying Fourier's law has been demonstrated in the 1D Frenkel-Kontorova lattices [10,22] and  $\phi^4$  lattices [23,24], where the total momentum is not conserved. Therefore, it was once assumed that momentum conservation leads to [25] anomalous heat conduction in low-dimensional lattices. However, a contradictory result is founded in the 1D coupled rotator lattices [26] which reveal normal heat conduction in spite of their momentum conservation. A further hypothesis [27] that normal (anomalous) spread of excess momentum density gives rise to normal (anomalous) heat conduction was made for 1D nonlinear lattices.

Furthermore, understanding thermal transport in twodimensional (2D) systems is not only of theoretical interests [1-3,5], but also of great importance to the possible technological applications [5–7]in two dimensions realistic materials such as graphene [28,29]. However, heat transport in 2D systems is far from being clear. Based on the modecoupling theory [2,3,5], it has been conjectured that thermal conductivity in the 2D nonlinear lattices with the conserved momentum will diverge logarithmically with system size. Numerical simulations in the 2D FPU- $\beta$  nonlinear lattices [30] and in the disk lattices [31] with vector displacements verified such logarithmical divergences. But a power-law divergence of thermal conductivity with system size is observed [32] in the 2D FPU- $\beta$  nonlinear lattices. A recent study with scalar displacements [33] reveals a power-law divergence in the 2D FPU- $\beta$  nonlinear lattices and a logarithmically divergent thermal conductivity for the purely quartic lattices, respectively. In contrast, normal heat conductivity was observed [34] in the 2D scalar lattices. A possible explanation for the difference among these simulation results maybe lies in the strong finitesize effects [33] within affordable computational resources.

Energy diffusion [5,15,20,21,27,35–41] acts as another important approach to understanding heat transport in 1D systems since this diffusion method can circumvent the finitesize problem. Nevertheless, the approach of energy diffusion is difficult to be utilized in 2D nonlinear lattices on account of theoretical difficulties or of heavy computations. No investigation of energy diffusion has been made in 2D nonlinear lattices. To overcome this obstacle of heavy computations, our present work has successfully accelerated the computation through a graphics processing unit [42] (GPU). The aim of this paper is to investigate energy and momentum diffusion in the 2D nonlinear lattices. Our simulations confirm that energy diffusion in the 2D momentum-conserved lattices is

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anomalous and can be well described by the Lévy-stable distribution. We clarify that anomalous heat transport can no longer be corroborated by the momentum superdiffusion in the 2D system, in contrast to the hypothesis [27] for the 1D nonlinear lattices.

The paper is organized as follows. In Sec. II, we first introduce three typical models of 2D nonlinear lattices and then describe the adopted simulation approach using the energymomentum fluctuation correlation function. In Sec. III, we present our main results of energy and momentum diffusions for the three 2D nonlinear lattices, accompanied by a discussion on the possible mechanism in terms of Lévy walk distributions. Finally, conclusions are drawn in Sec. IV.

#### **II. MODELS AND METHODS**

#### A. Models

Here we consider energy diffusion in the 2D square lattices made of  $N_x \times N_y$  atoms with a vector displacement of  $\mathbf{q}_{i,j}$ .  $N_x$ and  $N_y$  denote the number of atoms in the *x* and *y* direction, respectively. The equilibrium positions of the atoms coincide with the lattice sites, labeled by a pair of integer indices  $\{(i, j), i = 1, N_x; j = 1, N_y\}$ . For simplification, each atom in those lattices only interacts with its nearest neighbors that characterize the short-range interatomic forces in real solids. The general Hamiltonian for the adopted 2D nonlinear lattices can be written as

$$H = \sum_{i=1}^{N_y} \sum_{j=1}^{N_y} \left[ \frac{\mathbf{p}_{i,j}^2}{2m} + V(|\mathbf{q}_{i+1,j} - \mathbf{q}_{i,j}|) + V(|\mathbf{q}_{i,j+1} - \mathbf{q}_{i,j}|) + U(\mathbf{q}_{i,j}) \right], \quad (1)$$

where  $\mathbf{q}_{i,j}$  is the vector displacement from its equilibrium position of the atom on the (i, j) lattice site and  $\mathbf{p}_{i,j}$  corresponds to its momentum vector. m is the atom mass and has been set m = 1 without loss of of generality. The interaction potential is taken as  $V(r) = \frac{1}{2}kr^2 + \frac{1}{4}\beta r^4$ . The term  $U = \frac{1}{4}gr^4$  denotes the on-site potential, which breaks the momentum conservation. To compare our results of energy diffusion to previous simulations [30,32-34,43] of heat conduction, we consider three typical types of 2D nonlinear lattices: the FPU- $\beta$  model with  $k = 1, \beta = 1, g = 0$ ; the purely quartic lattice with  $k = 0, \beta = 1, g = 0$ ; and the  $\phi^4$  model with  $k = 1, \beta = 0, g = 1$ . The FPU- $\beta$  model has been widely used [30,32,33,43] for studying nonlinear behaviors and heat transport in low-dimensional nonlinear lattices. The purely quartic lattice can be regarded as [5,33] the high temperature limit of the FPU- $\beta$  lattice. The  $\phi^4$  model [23,24,44] without the momentum conservation is studied to demonstrate the effect of the momentum conservation on energy diffusion in 2D nonlinear lattices. To show the dimensional crossover of energy diffusion in the 2D nonlinear lattices, the length  $N_x$ is fixed to be 1023, while the lattice width  $N_v$  varies from 1 (1D) to 1024 (2D). Consequently, the largest number of particles in the nonlinear lattices is up to 1 047 552 during our simulations.

#### **B.** Methods

To make a direct comparison to the hydrodynamics theory [20,21], we focus on energy and momentum diffusion in the above 2D nonlinear lattices. The nonlinear hydrodynamic fluctuation theory states [20,21,45] that anomalous energy-momentum diffusion in nonlinear lattices can be characterized by the scaling forms of the space-time correlation of fluctuation functions. Here we define the spatiotemporal correlation of fluctuation function [35,36] of energy  $\rho_E(i, t)$  and momentum  $\rho_P(i, t)$  fluctuation for a microcanonical system as

$$\rho_E(\Delta x_{i,j}, t) = \frac{\langle \Delta H_i(t) \Delta H_j(0) \rangle}{\langle \Delta H_0(0) \Delta H_0(0) \rangle} + \frac{1}{N_b^x - 1}, \quad (2a)$$

$$\rho_P(\Delta x_{i,j}, t) = \frac{\langle \Delta P_i(t) \Delta P_j(0) \rangle}{\langle \Delta P_0(0) \Delta P_0(0) \rangle} + \frac{1}{N_h^x - 1}.$$
 (2b)

The spatial coarse-graining of local energy density  $H_i(t)$  and momentum density  $P_i(t)$  are summed over the atoms inside the *i*th column of bin with respect to the position *x* of an atom on the 2D nonlinear lattice at time t, separately. The energymomentum fluctuation corresponds to  $\Delta H_i(t) = H_i(t) - \bar{H}_i$ and  $\Delta P_i(t) = P_i(t) - \bar{P}_i$ . The notations  $\bar{H}_i$  and  $\bar{P}_i$  denote the averaged local density of energy and momentum, respectively. For simplicity, the number of bins  $N_b^x$  is equal to the number of lattice sites  $N_x$  along the x direction. As a result of the spatial and time translational invariance in equilibrium states, we can write energy  $\rho_E(\Delta x_{i,j}, t)$  and momentum  $\rho_P(\Delta x_{i,j}, t)$ fluctuation as  $\rho_E(i, t)$  and  $\rho_P(i, t)$  without confusion. The spatiotemporal average  $\langle \cdot \rangle$  in Eq. (2) is also performed along the x direction with time. Here we investigate the spatiotemporal correlation of the energy-momentum fluctuation along the xdirection. The investigation on energy diffusion along one direction may contribute to understanding the measurement of thermal transport in experiments, where the sample is placed between a heat source and a heat sink. A complete two-dimensional description of the spatiotemporal correlation of fluctuation is desirable, but this calculation of twodimensional point to point is beyond our present computation capability. We will pursue it in the future.

From the perspective of hydrodynamics theory, the spatiotemporal correlation function  $\rho_E(i, t)$  and  $\rho_P(i, t)$  can be viewed as the fingerprint for the behaviors of energy and momentum diffusion, corresponding to the correlation of heat modes and sound modes, respectively. To quantify the energy diffusions of heat modes on lattices, we also calculated the mean-square deviation (MSD) of energy  $\langle \Delta x^2(t) \rangle_E$  as

$$\langle \Delta x^2(t) \rangle_E = \sum_i i^2 \rho_E(i,t), \tag{3}$$

where the index *i* is summed in the range of heat modes for the energy fluctuation correlation.

During the numerical simulations, periodic boundary conditions are applied in the both x and y directions. The energy and momentum fluctuation correlation function are calculated in the equilibrium state at average energy density  $\varepsilon = 0.5$  per site for a purely quartic lattice and the FPU- $\beta$  model, and  $\varepsilon = 3.0$  per site for the  $\phi^4$  model. The system is relaxed to equilibrium state with 10<sup>6</sup> time steps from properly assigned random states that has the zero total momentum and the given average energy density per site. The number of the ensemble-



FIG. 1. The spatial profiles of the energy fluctuation correlation function  $\rho_E(i, t)$  for (a, b) the purely quartic lattices; (c, d) the FPU- $\beta$  lattices; (e, f) the  $\phi^4$  lattices with the width  $N_y = 1$ , i.e., 1D lattices, and  $N_y = 1024$ . The spatial profiles of  $\rho_E(i, t)$  at times t = 10, 50, 200 are labeled by the black solid, red dashed, and green dotted lines, respectively, as indicated in the figure.

averaging in the spatiotemporal correlation function of Eq. (2) is up to  $10^8$  after an equilibrium state is first prepared. The velocity-Verlet algorithm is adopted for integrating the motion equations with the time step h = 0.005. Owing to the heavy computations from the large system of 2D lattices, we employ the graphics processing unit (GPU) to implement the parallel acceleration.

### **III. RESULTS AND DISCUSSIONS**

We probe the diffusion behavior of energy and momentum by simulating the spatiotemporal fluctuation correlations in three typical nonlinear lattices: the purely quartic lattices, the FPU- $\beta$  lattices, and the  $\phi^4$  model. The purely quartic lattices and the FPU- $\beta$  lattices hold the momentum conservation while the  $\phi^4$  model breaks the conservation of momentum owing to the on-site potential. To demonstrate the dimensional crossover of energy diffusion from one to two dimensions, we increase the lattice width  $N_y$ , varying from 1 to 1024 with a fixed length  $N_x = 1023$ . We first present energy diffusion in three types of nonlinear lattices, elucidating the nature of heat mode in 2D nonlinear lattices. Next we investigate the diffusion of momentum to understand the dimensionalcrossover features of sound modes.

### A. Profiles of energy fluctuation correlation function

# 1. Spatial profiles of energy fluctuation correlation

The spatial profiles of the energy fluctuation correlation function  $\rho_E(i, t)$  with varying width for the purely quartic lattices, the FPU- $\beta$  lattices, and the  $\phi^4$  lattices are depicted in Fig. 1. As is shown in the figures, there is a prominent central peak in each spatial profile of  $\rho_E(i, t)$ , which corresponds to the heat mode according to the hydrodynamical theory [20,21,45]. For the 1D nonlinear lattices, i.e.,  $N_y = 1$ , our calculated  $\rho_E(i, t)$  is qualitatively consistent with the previous results [15,27,35,36,38,40,41,44]. In addition, there are two observable right- and left-moving side peaks along both sides of the central heat mode. These side peaks originate from a strong coupling [45] between the heat modes and the sound



FIG. 2. The decay of the peak height of the energy fluctuation correlation function  $H_C^E$  as a function of time (a) for the purely quartic lattice and (b) for the FPU- $\beta$  lattices. The decay of height is fitted to a power-law distribution  $H_C^E \sim t^{-1/\gamma}$  as shown in the figure.

modes by the mode cascade theory [46]. Thus, it can be inferred from the prominent side peaks that the energy and momentum transport are strongly coupled in the momentumconserved 1D nonlinear lattices. This strong coupling between heat and sound modes may contribute to anomalous energy transport by the mode cascade theory [46]. In contrast, it can be seen from Fig. 1 that these side peaks become weakened for both the purely quartic lattices and the FPU- $\beta$  lattices with width  $N_v = 1024$ . Such a disappearance of the side peaks for the wider lattices may result from the vertically summed energy along the x direction. On the other hand, for the  $\phi^4$  lattices, there are no side peaks in Figs. 1(e) and 1(f), independent of the lattice width. This observation of the  $\phi^4$  lattice with the on-site potential is in agreement with the previously reported spatial profiles of the energy fluctuation correlation function [35,44] for the 1D  $\phi^4$  model. We think that the side peak generally does not occur for the lattices without the conserved momentum, where heat transport may be carried out mainly in terms of heat diffusion. The prominent cental peak of heat modes in the spatial profiles of Fig. 1 dominates the feature of energy diffusion in low-dimensional lattices. Next, we characterize the features of these central peaks based on the Lévy walk theory using the scaling analysis.

# 2. Decay of peak height of heat modes

To investigate the probability character of the central peak of the heat mode, we first turn to the predictions of 1D nonlinear lattice by the recent nonlinear fluctuating hydrodynamic theory [20,21,45], which relates its heat and sound modes to the fluctuation correlations of three conserved quantities: energy, momentum, and stretch. Generally, this spatial-temporal fluctuation correlation function such as  $\rho_E(i, t)$  is subject to a scaling invariant relationship [47] as

$$t^{\frac{1}{\gamma}}\rho_E(i,t) \simeq \rho_E(i/t^{\frac{1}{\gamma}},t), \qquad (4)$$

with the scaling exponent  $1 \le \gamma \le 2$ . Different behaviors of diffusion can be characterized [48] by the exponent  $\gamma$ : ballistic diffusion  $\gamma = 1$ , superdiffusive diffusion  $1 < \gamma <$  2, and normal diffusion (i.e., Gaussian distribution)  $\gamma = 2$ . Phenomenologically, the dynamics of the diffusion process can be modelled [48] by the Lévy walk using the Lévy-stable distribution  $f_{LW}^{\gamma}(i, t)$  that is the Laplace-Fourier transform of the Lévy characteristic function  $e^{-|k|^{\gamma}t}$ . To put it more straightforwardly, the diffusion property of the fluctuation correlation function such as  $\rho_E(i, t)$  is determined by the scaling exponent  $\gamma$  and has the same mathematical property as the Lévystable distribution  $f_{LW}^{\gamma}(i, t)$ . The anomalous energy diffusion in our simulations can be identified through the superdiffusive diffusion  $1 < \gamma < 2$ . For the conserved quantity, the scaling exponent  $\gamma$  can be extracted [27,35] from the height of the central peak in the fluctuation correlation function. Now we start to clarify the diffusion property of heat mode using the above approach. For the purely quartic lattices and the FPU- $\beta$ model with the conserved momentum, we extract the scaling exponent  $\gamma$  from the decay of peak height  $H_c^E$  of the central heat mode. The log-log plots of the peak height  $H_c^E$  as a function of time are depicted in Fig. 2, respectively. As can be seen from the figure, a power-law decay  $H_c^E \sim t^{-1/\gamma}$  can be explicitly fitted. The rate of decay  $1/\gamma$  of  $H_c^E$  for the purely quartic lattices decreases from  $1/\gamma = 0.670 \pm 0.001$ for  $1D(N_y = 1)$  to  $1/\gamma = 0.550 \pm 0.003$  for 2D ( $N_y = 1024$ ) as illustrated in Fig. 2(a). In contrast, the decay rate  $1/\gamma$  of the central peak for the FPU- $\beta$  lattices is about 0.688  $\pm$  0.002 for the 1D chain and shows no significant change with the increase of lattice width.

### 3. Rescaled energy fluctuation correlation function

Furthermore, to identify the diffusion property of heat modes, the rescaled energy fluctuation correlation functions  $t^{1/\gamma} \rho_E(i/t^{1/\gamma}, t)$  with the varying width for the purely quartic lattices and the FPU- $\beta$  model are depicted in Fig. 3. The scaling exponent  $\gamma$  is obtained from the relation  $H_c^E \sim t^{-1/\gamma}$  shown in Fig. 2. To further confirm the superdiffusive property of  $\rho_E(i, t)$ , the Lévy-stable distribution [47,48]  $f_{LW}^{\gamma}(i, t)$  with the same scaling exponent  $\gamma$  is also plotted by the solid line in each figure. From the figure, we can find that the collapse of the central heat mode at different times after scaling is very good according to the scaling invariant in Eq. (4). The fitting



FIG. 3. The rescaled energy fluctuation correlation function  $t^{1/\gamma} \rho_E(i/t^{1/\gamma}, t)$  in the (a, b) purely quartic lattices and (c, d) the FPU- $\beta$  lattices with the width  $N_y = 1$ ,  $N_y = 1024$ . Here the exponent  $\gamma$  is obtained by fitting the decay height of the energy fluctuation correlation function to the power-law distribution  $\sim t^{-1/\gamma}$  shown in Fig. 2. The black solid line in the figure denotes the fit to the Lévy-stable distribution  $f_{LW}^{\gamma}(i, t)$ .

to the corresponding Lévy-stable distribution is also quite fine. In addition, as can be seen from Figs. 3(a) and 3(c), the side peak in the 1D system does not follow the same scaling property of heat mode as predicted by the nonlinear fluctuating hydrodynamic theory [21,45]. Here we focus on the scaling property of the heat modes. The nonlinear hydrodynamic fluctuation theory [20,21,45] predicts that the scaling exponent  $\gamma$ scales according to the Lévy-3/2 distribution (i.e.,  $\gamma = 3/2$ ) for the 1D momentum-conserved nonlinear lattices with an even potential at zero pressure, like the purely quartic lattice and the FPU- $\beta$  model. As indicated in the figure, our obtained values of the scaling exponent  $\gamma$  agree well with the prediction of nonlinear hydrodynamic fluctuation theory, with  $\gamma =$  $3/2(1/\gamma = 0.670 \pm 0.001)$  for the 1D purely quartic lattice and  $\gamma = 1.454(1/\gamma = 0.688 \pm 0.002)$  for the FPU- $\beta$  model. When the lattice width  $N_v$  is increased to 1024, the scaling exponent  $\gamma$  reaches  $\gamma = 1.818(1/\gamma = 0.550 \pm 0.003)$  for the purely quartic lattice and  $\gamma = 1.504(1/\gamma = 0.665 \pm 0.006)$ for the FPU- $\beta$  model, respectively. All values of the scaling exponent  $\gamma$  with different lattice width fall into the range 1 <  $\gamma < 2$ , thus confirming the superdiffusive property of heat modes for both the purely quartic 2D lattice and the FPU- $\beta$ 2D model. Our simulations exhibit a slower energy diffusion

with the dimensional crossover from one to two dimensions in the momentum-conserved nonlinear lattices.

Finally, as can be seen in Figs. 1(e) and 1(f), a Gaussian distribution function (normal diffusion) of the heat mode can be observed for the  $\phi^4$  model with an on-site potential, which breaks the conservation of momentum. Its profile of the energy fluctuation correlation function  $\rho_E$  can be perfectly well described by the Gaussian distribution  $\rho_E \sim e^{-i^2/4\pi D_E t}/\sqrt{4\pi D_E t}$ , where  $D_E$  denotes the diffusion constant for the heat mode. The normal heat diffusion has been well verified [35,44] in the 1D lattices with a  $\phi^4$  potential. After numerically examining the Gaussian distribution correlation function  $\rho_E$  satisfies the Gaussian distribution both for the 1D and 2D  $\phi^4$  model. Actually, this result is obvious and generally assumed beyond any doubt [35,44].

In addition, the MSD of energy distribution  $\langle \Delta x^2(i, t) \rangle_E$ (i.e., the second moments of energy in terms of the probability function) can explicitly characterize energy diffusion in the asymptotic time limit and is related to heat conduction. Next, we quantitatively characterize heat transport by calculating the MSD of energy distribution  $\langle \Delta x^2(t) \rangle_E$  given by Eq. (2) for the central heat modes.

#### B. Mean square deviation of energy distribution

Heat conduction in the 1D system can be directly related to the energy diffusion process. According to the connection theory [37], the MSD in the 1D system obeys the second order differential equation with time as

$$\frac{d^2 \langle \Delta x^2(t) \rangle_E}{dt^2} = \frac{2C_{JJ}(t)}{k_B T^2 c},\tag{5}$$

where c is the specific heat capacity and  $k_B$  is the Boltzmann constant. The autocorrelation function of heat currents  $C_{JJ}(t)$ is related to thermal conductivity  $\kappa$  through the Green-Kubo formula [1–3] given by  $\kappa = \frac{1}{k_B T^2} \int_0^\infty dt C_{JJ}(t)$ . If the MSD of an energy conserved distribution  $\langle \Delta x^2(t) \rangle_E$  is assumed to scale as  $\langle \Delta x^2(t) \rangle_E \sim t^{\beta}$ , the behavior of the diffusion process for a conservation quantity can be categorized [37,47] with regard to the exponent  $\beta$ : the normal diffusion when  $\beta = 1$ , the superdiffusion when  $\beta > 1$ , and the subdiffusion when  $\beta < 1$ . For example, the MSD  $\langle \Delta x^2(t) \rangle_E$  will be proportional to time t, i.e.,  $\langle \Delta x^2(t) \rangle_E \sim t$  when the energy fluctuation correlation function  $\rho_E$  is the Gaussian distribution like the  $\phi^4$  model. Thus the normal energy diffusion will give rise to finite thermal conductivity, indicating normal heat conduction. Furthermore, if the profile of the energy fluctuation correlation function  $\rho_E$  belongs to the Lévy-stable distribution, the MSD will spread faster than the normal diffusion and exhibits the superdiffusion with  $\beta = 3 - \gamma$  given by the Lévy walk theory [47,48]. Anomalous heat conduction has been verified in the 1D momentum-conserved nonlinear lattices [15,27,35,36,38,40,41] such as the FPU- $\beta$  and purely quartic lattices. This relation [37] of the energy diffusion to heat transport has been quantitatively verified in the 1D nonlinear lattice with symmetrical potential. As for 2D nonlinear lattices, there is no strict theoretical relationship between energy diffusion and heat transport, but we can still employ energy diffusion to qualitatively identify whether heat transport is normal or anomalous.

The calculated distributions of MSD energy  $\langle \Delta x^2(t) \rangle_E$  of heat modes versus evolving time t are plotted in Figs. 4, 5, and 6 for the purely quartic lattices, the FPU- $\beta$  lattices, and the  $\phi^4$  model with the varying width, respectively. As can be seen from Figs. 4 and 5, the MSD of energy on the purely quartic and FPU- $\beta$  model shows the superdiffusion behavior. We can find that the diffusion exponent  $\beta$  decreases with the increase of lattice width. For example, the diffusion exponent  $\beta$  for the purely quartic lattices is reduced from  $\beta = 1.415 \pm 0.003$  for  $N_v = 1$  to  $\beta = 1.269 \pm 0.003$  for  $N_{\rm v} = 1024$ . The obtained  $\beta$  of 1.419  $\pm$  0.003 for the 1D chain  $N_v = 1$  is consistent with the previously reported [27,35,36] diffusion coefficient 1.4. When the width is increased to 1024, the diffusion exponent decreases to  $\beta$  of  $1.269 \pm 0.003$  as shown in Fig. 4, still implying an anomalous heat conduction in the 2D quartic lattices. As for the 2D systems, the mode-coupling theory [2,3] predicts that the autocorrelation function of heat currents  $C_{JJ}(t)$  decays as  $t^{-1}$ , which leads to the logarithmic divergence of thermal conductivity with system size N as  $\kappa \propto \ln N$ . If the connection theory Eq. (5) is still valid in 2D systems, the MSD of energy will change over time as  $\langle \Delta x^2(t) \rangle_E \sim t \ln t$ . To compare to the powerlaw relationship, we plotted the function of  $t \ln t$  in Fig. 4



FIG. 4. The MSD of energy  $\langle \Delta x^2(t) \rangle_E$  of heat modes as a function of time for the purely quartic lattices with width  $N_y$  varying from 1 to 1024 as shown in the figure. The fittings of MSD to a power-law distribution  $\sim t^{\beta}$  for the lattices of the width  $N_y = 1$  and  $N_y = 1024$  are plotted in the figure, respectively. The red dashed line in the figure represents the function of  $t \ln t$ .

using the red dashed line. As illustrated in the figure, the discrepancy in the scaling behavior between the power-law  $\sim t^{1.269\pm0.003}$  and the function of  $\sim t \ln t$  is so small that it is difficult to numerically determine whether the observed MSD of the energy distribution conforms to the power-law  $\sim t^{1.269\pm0.003}$  or to the function of  $\sim t \ln t$  in the asymptotic time limit. A logarithmically divergent thermal conductivity with the system size *N* is recently reported [33] in the purely quartic lattice has a vector displacement field. Note that our purely quartic lattice has a vector displacement. Considering the good numerical fitting as the power-law in Fig. 4, our results of energy diffusion may be in favor of a logarithmic



FIG. 5. The MSD of energy  $\langle \Delta x^2(t) \rangle_E$  of heat modes as a function of time for the FPU- $\beta$  lattices with width  $N_y$  varying from 1 to 1024 as shown in the figure. The fittings of MSD to a power-law distribution  $\sim t^{\beta}$  for the lattices of the width  $N_y = 1$  and  $N_y = 1024$  are plotted in the figure, respectively. The red dashed line in the figure represents the function of *t* ln *t*.



FIG. 6. The MSD of energy  $\langle \Delta x^2(t) \rangle_E$  of heat modes as a function of time for the  $\phi^4$  lattices with width  $N_y$  varying from 1 to 1024 as shown in the figure. The fittings of MSD to a proportional relationship  $\sim t$  for the lattices of the width  $N_y = 1$  and  $N_y = 1024$  are plotted in the figure, respectively.

divergence of thermal conductivity with size in the purely quartic lattices with a vector displacement. At the same time, we cannot exclude that this may be a numerical coincidence. But, the calculated distributions of MSD energy  $\langle \Delta x^2(t) \rangle_E$ for energy diffusion in Fig. 4 assuredly confirms that heat transport in the 2D purely quartic lattices is anomalous. In addition, it can be seen from the figure that the dimensional crossover from one to two dimensions with the varying width occurs rapidly such that the diffusion exponent  $\beta$  for  $N_y = 16$ almost converges to the value of  $1.269 \pm 0.003$ . This rapidly convergent tendency is consistent with the direct simulation of thermal conductivity [34], where the converged results are obtained when the width  $N_y > 32$ .

A similar superdiffusive time dependence of the MSD energy distribution can be observed for the FPU- $\beta$  model in Fig. 5. A fast superdiffusive energy spreading, growing as  $\langle \Delta x^2(t) \rangle_E \sim t^{1.598 \pm 0.004}$ , is observed for the 1D lattices in Fig. 5. When the width is increased to 1024, the diffusion exponent  $\beta$  converges rapidly to  $\beta = 1.509 \pm 0.003$ . To compare to the prediction of logarithmical divergency by the mode-coupling theory, a function of  $\sim t \ln t$  is also illustrated in Fig. 5 by the red dashed line. By contrast, a significant difference exits between the power-law scale  $\sim t^{\beta=1.509\pm0.003}$  and the function of  $\sim t \ln t$ . Therefore, a powerlaw relationship can be assumed for the anomalous energy diffusion in the 2D FPU- $\beta$  lattices. If the connection theory of Eq. (5) is still valid in the 2D system, our energy diffusion yields that thermal conductivity  $\kappa$  will diverge as  $\kappa \sim N^{0.51}$ , which qualitatively coincides with the power-law divergence of thermal conductivity [32] of the 2D FPU- $\beta$  lattices with a vector displacement by the direct simulation of thermal conductivity. In contrast, as shown in Fig. 6, a normal MSD energy diffusion  $\langle \Delta x^2(t) \rangle_E \sim t$  can be observed in the  $\phi^4$ lattices with an on-site potential, irrespective of the varying width. Put differently, we extend the conclusion from 1D to 2D systems that nonlinear lattices with a  $\phi^4$  on-site potential will exhibit normal energy diffusion and thus give rise to the

Fourier law of heat transport. The normal energy diffusion in the  $\phi^4$  lattices obviously originates from the explicit Gaussian distributions of energy fluctuation correlation functions, as depicted in Figs. 1(e) and 1(f). To sum up, our MSD energy distribution strongly confirms anomalous energy diffusion in both the 1D and 2D momentum-conserved lattices of the purely quartic and FPU- $\beta$  model and normal energy diffusion in the  $\phi^4$  2D system. Next, we turn to the characteristics of momentum diffusion in the 2D lattices.

#### C. Momentum diffusion

According to the nonlinear fluctuating hydrodynamic theory [20,21,45], the full three normal modes (one heat mode and two sound modes) determined heat transport in the 1D nonlinear lattice. Sound mode or momentum diffusion can be related [20,21,45] to the momentum fluctuation correlation. Among the three types of nonlinear lattices considered, momentum diffusion cannot be well defined in the  $\phi^4$  model, owing to its nonconserved momentum. Therefore, we focus on the behavior of momentum diffusion in the purely quartic lattices and the FPU- $\beta$  lattices. Momentum diffusion is represented by the momentum fluctuation correlation function  $\rho_P(i, t)$  defined in Eq. (2). The spatial profiles of momentum fluctuation correlation function  $\rho_P$  for different times with varying lattice width for the purely quartic lattices and the FPU- $\beta$  lattices are depicted in Fig. 7. It is interesting to investigate the dimensional-crossover features of momentum diffusion from 1D to 2D system. It can be seen from the figure that two side peaks of the sound mode move ballistically outward with a constant sound velocity c. We numerically fitted the sound speed from the profiles of  $\rho_P(i, t)$  at different correlation times, obtaining c = 0.914, 0.861 for the purely quartic lattices with  $N_y = 1$ , 1024 and c = 1.22, 1.16 for the FPU- $\beta$  lattices with  $N_y = 1$ , 1024, respectively. A small decrease of sound speed can be observed with the increase of lattice width. This decrease of sound speed may originate from the reduction of phonon group velocity because the phonon dispersion relations will change with the increase of lattice width.

To further investigate the momentum diffusion, we also calculated the decay of the peak height of the momentum fluctuation correlation function. The decay of the peak height of the momentum fluctuation correlation function as a function of time is depicted in Fig. 8 for the 2D purely quartic lattice and the FPU- $\beta$  lattice, respectively. It can be seen from the figure that the decay of momentum height can be fitted to a power-law distribution  $H_c^P \sim t^{-\mu}$ , which is similar to that of energy. A normal diffusion of momentum is characterized by the value of the decay exponent  $\mu = 0.5$ . For the 1D system, both the purely quartic lattice and the FPU- $\beta$  lattice demonstrate a superdiffusion of momentum, with a decay exponent  $\mu = 0.616 \pm 0.001, 0.611 \pm 0.003$ correspondingly. Here our result for the 1D nonlinear lattices is consistent with the previous hypothesis [27] that anomalous heat transport in 1D momentum-conserved Hamiltonian lattice systems is corroborated by the superdiffusive spreads of momentum excess density. However, when the lattice width increases, the momentum diffusion induces a crossover from superdiffusion in the 1D system to normal or subdiffusion in



FIG. 7. The spatial profiles of the momentum fluctuation correlation function  $\rho_P(i, t)$  for the purely quartic lattices and the FPU- $\beta$  lattices with the width  $N_y = 1$ , i.e., 1D lattices and  $N_y = 1024$ . The spatial profiles of  $\rho_P(i, t)$  at times t = 10, 50, 200 are labeled by the black solid, red dashed, and green dotted lines shown in the figure, respectively.

2D systems. For example, in the case of the purely quartic lattice, the decay exponent  $\mu$  changes from 0.616  $\pm$  0.001 for the 1D system ( $N_y = 1$ ) to 0.402  $\pm$  0.002 for the 2D system ( $N_y = 1024$ ). Similar behaviors can also be observed in the

FPU- $\beta$  lattices. Contrary to the hypothesis of the 1D system, we find that anomalous heat transport in the 2D momentumconserved Hamiltonian lattice systems is not accompanied by the superdiffusion of momentum any longer.



FIG. 8. The decay of the peak height  $H_c^P$  of the momentum fluctuation correlation function as a function of time (a) in the 2D purely quartic lattice and (b) in the FPU- $\beta$  lattices. The decay of height is fitted to a power-law distribution  $H_c^P \sim t^{-\mu}$  as shown in the figure.

# IV. CONCLUSION AND DISCUSSION

In summary, we successfully investigated energymomentum diffusions from one to two dimensions in three types of nonlinear lattices: the purely quartic lattice, the FPU- $\beta$  lattice, and the momentum-nonconserved  $\phi^4$ model. The apparent advantage of the approach of the fluctuation correlation function is that it circumvents the finite-size problem during the direct simulation of heat transport. Our simulation confirms that energy diffusion of the momentum-conserved 2D nonlinear lattices is anomalous and can be well fitted by the Lévy-stable distribution. As was expected, we find that nonlinear lattices with the  $\phi^4$  on-site potential exhibit normal energy diffusion, independent of its dimension. In addition, the simulations of momentum diffusion illustrate that two sound modes in the 2D nonlinear move ballistically outward with a constant sound velocity, similar to that of the 1D chain. Contrary to the hypothesis of the 1D system, we further clarify that anomalous energy

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diffusion in the 2D momentum-conserved system cannot be corroborated by the momentum superdiffusion any longer.

Our studies here confirm that energy diffusion in the momentum-conserved 2D nonlinear lattices is anomalous. The anomalous energy diffusion may suggest anomalous heat conduction in the 2D nonlinear lattices. How to relate energy diffusion to heat conduction will be an important and interesting problem. However, further investigations, both theoretical and numerical, are needed. We hope our results contribute to understanding heat transport in 2D nonlinear lattices.

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