Effects of interaction symmetry on delocalization and energy transport in one-dimensional disordered lattices

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We study effects of interaction symmetry in one-dimensional, momentum-conserving disordered lattices. It is found that asymmetric and symmetric interparticle interactions may result in significant difference: localized modes can be delocalized by very weak asymmetric interactions but survive much stronger symmetric interactions. Moreover, in the delocalization regime, asymmetric and symmetric interactions also have qualitatively different effects on transport: the former (the latter) may lead to a fast decaying (slow power-law decaying) heat current correlation function and in turn a convergent (divergent) heat conductivity. A method for detecting delocalization in systems at a nonzero temperature is proposed as well.

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It is well known that the Anderson localization problem [1] becomes much more complicated if particle interactions have to be taken into account [2,3]. Whether the localized modes survive weak enough anharmonic interactions, how to identify the delocalization energy threshold induced by interactions if it exists, and what transport properties may emerge beyond the delocalization threshold are some of the fundamental issues. In the case of electrons, in 1980 Fleishman and Anderson showed that at a low enough temperature electron-electron interactions cannot destroy localization [4], while another group found that electron-electron interactions may destroy the constructive interference and lead to a finite electric conductance [2]. Based on these results, Basko *et al.* further suggested that there is a metal-insulator transition at some intermediate temperatures induced by interactions [5].

However, as to phonons in one-dimensional (1D) disorder lattices, a counterpart picture has not been established yet. For disordered harmonic (DH) lattices, it has been proved that the normal modes of high frequencies are localized while those of low frequencies are extended [6]. The boundary between the two, i.e., the mobility edge, is related to the particle number N (or the system size) as $\sim N^{-1/2}$. This result leads to that, when a 1D DH lattice is attached to two heat bathes of different temperatures, the stationary energy current along the lattice (or heat current equivalently [7]) depends on the system size as $\sim N^{-1/2}$ for free boundary conditions but $\sim N^{-3/2}$ for fixed boundary conditions [8–11], which in turn implies that in the thermodynamic limit, the thermal conductivity diverges in the former but vanishes instead in the latter case.

The next question is whether and how anharmonic interactions may influence these results. To this question, numerical studies [12] have revealed that in the regime of high temperature and strong anharmonic interactions, the thermal conductivity (denoted by κ) diverges as $\kappa \sim N^{\delta}$ with $\delta = 2/5$ in the disordered Fermi-Pasta-Ulam-β (DFPU-β) chain, the same as in the homogenous Fermi-Pasta-Ulam-β (FPU-β) chain [13–15]. In the low-temperature regime, the thermal conductivity was observed to tend to converge as the system size is increased [12], but Dhar and Saito argued that to increase the system size further, the thermal conductivity may turn to increase again, and they speculated that it will diverge with the same exponent of $\delta = 2/5$ as well [16]. Other studies also support this speculation [17]. In general, the present understanding to the 1D disordered and momentum-conserving lattices is that anharmonic interactions may bring in some significant changes compared with DH chains, but heat conduction is still anomalous; i.e., the heat conductivity diverges in the thermodynamic limit.

Nevertheless, this understanding is based on the DFPU-β model where the interactions are symmetric. Recently, in studies of 1D homogenous systems, it has been found that interaction symmetry may play a crucial role in transport: In systems with asymmetric interactions, heat current correlation may decay fast enough to result in a size-independent (or effectively size-independent [18]) thermal conductivity [19–21]. The studied models are various, including the exponential-harmonic model [19], the piecewise harmonic model [20], the Lennard-Jones model [21,22], and even the Fermi-Pasta-Ulam-α-β (FPU-α-β) model with proper parameters [21]. Note that some researchers have argued that the observed size-independent thermal conductivity in these studies may be a finite-size effect [23,24], and this could be true in particular for the FPU-α-β model in the thermodynamic limit. But in spite of this, a significant difference between symmetric and asymmetric interactions has been clearly evidenced in all these studies [19–24]. For example, in Ref. [23] the authors have found that in the low-temperature regime the thermal conductivity of the FPU-α-β model converges, while in the high-temperature regime there is a platform in the dependence of κ on the system size N. These properties are in clear contrast to those of the systems of symmetric interactions. Moreover, these properties may have deep significance; e.g., the platform in the κ-N curve has also been found in the integrability limit [25], and it could be wide enough to involve macroscopic systems [18].

In view of their important effects in homogeneous systems, it is necessary to scrutinize the effects of asymmetric interactions in disordered systems as well. In addition, recall that fundamental problems related to anharmonic interactions, such as whether the localized modes can survive low enough temperatures and in what way the anharmonic interactions

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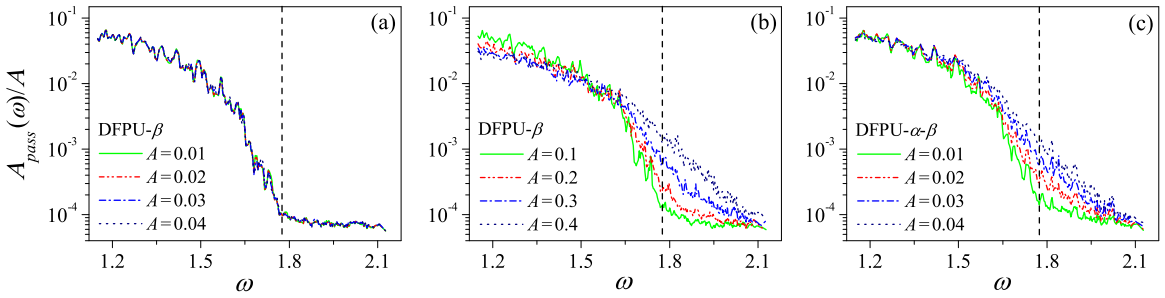

FIG. 1. (Color online) The amplitude of the wave passing through the lattice of size $N = 512$. Panels (a) and (b) are for the DFPU-β model and (c) is for the DFPU-α-β model. As comparison, the vertical dashed line in each panel indicates the mobility edge of the DH system.

may affect the mobility edge, are still open. Some related aspects of these problems have been investigated in the literature [12,16,17,26,27]; e.g., it has been shown that in disordered pinned anharmonic chains, the energy transport properties may be changed drastically by very weak on-site anharmonic interactions [27]. But, despite these efforts, understanding momentum-conserving disordered chains is still lacking.

In this work we address these problems by identifying the qualitative difference induced by interaction symmetry. The Hamiltonian for a 1D lattice system with the nearest neighboring interactions can be written as

$$H = \sum_i \left[\frac{p_i^2}{2m_i} + V(x_i - x_{i-1} - a) \right], \tag{1}$$

where p_i, m_i, and x_i denote, respectively, the mass, the momentum, and the displacement of the ith particle, and the lattice constant, a, is fixed to be unity. We consider mass disordered chains with $m_i = 1 + R_i$, where R_i is a random number distributed uniformly in the range of $-0.1 < R_i < 0.1$. The potential V between two neighboring particles is

$$V(x) = \frac{1}{2}x^2 - \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4; \tag{2}$$

it gives the disordered Fermi-Pasta-Ulam-α-β (DFPU-α-β) model with asymmetric interactions for $\alpha \neq 0$ and $\beta \neq 0$, the DFPU-β model with symmetric interactions only for $\alpha = 0$ and $\beta \neq 0$, and the DH model for $\alpha = 0$ and $\beta = 0$. For both the DFPU-β and DFPU-α-β model we fix $\beta = 1$ for the sake of comparison with previous studies in the literature and $\alpha = 2$ for the DFPU-α-β model to make interactions highly asymmetric [21]. We will mainly consider the temperature range of $10^{-4} < T < 0.1$ (the Boltzmann constant k_B is set to be unity throughout this paper), in which the averaged distance a particle moves around its equilibrium position is from about 0.01 to about 0.33. Notice that a solid will be melting if the vibration amplitude of its atoms exceeds 10%–20% of the lattice constant according to the Lindemann melting law [28]; hence, this temperature range not only ensures that the normal modes are meaningful to our study but also are relevant physically. With these settings, the dynamics of the lattice can be simulated directly with conventional integration algorithms.

We first study the effects of anharmonic interactions on the localized modes. For this aim we investigate the influence of anharmonic interactions on the mobility edge that plays a key role in determining the properties of a disordered system [29–31]. One usual method is to check and analyze the waves that pass through the lattice [30,31], by which we first prepare a disordered lattice with the fixed boundary conditions $x_0 = 0$ and $x_{N+1} = N + 1$ and drive the first particle sinusoidally with a given frequency ω and a given amplitude A; next, after a time $t = N/v_s$ (v_s is the sound speed whose value is about one with the adopted system parameters), we begin to measure the motion signals of the Nth particle. Finally, the recorded signals (time series) are analyzed with the fast Fourier transform, and the amplitude of the vibration component of frequency ω, denoted by $A_{\text{pass}}(\omega)$, is evaluated. Its ratio to the driving amplitude A is taken as a measure of the passing rate, or the extension rate of the mode of ω. In our simulations, the first particle is driven for a time of 20 periods, and in order to suppress the fluctuations in the results, 60 random realizations are performed for taking the ensemble average.

Figure 1(a) shows the results for the DFPU-β model with $0.01 \leqslant A \leqslant 0.04$, representing the case of weak and symmetric anharmonic interactions. It can be seen that all curves collapse onto one perfectly. Moreover, there is a transition frequency above which the passing rate is close to a negligible constant value. This frequency can therefore be regarded as the critical frequency that separates extended modes and localized modes and by definition is exactly the mobility edge [6]. On the other hand, the mobility edge of the corresponding DH chain can be calculated by using the Thouless criterion [32]; it can be seen that this theoretical result (indicated by the dashed line) agrees with the transition frequency very well. Therefore, in the DFPU-β model, weak anharmonic interactions ($A < 0.04$) cannot break the localized modes and affect the mobility edge. Indeed, we find delocalization does not happen until $A > 0.08$ [results for $0.1 \leqslant A \leqslant 0.4$ are shown in Fig. 1(b)]. For $A < 0.08$, the mobility edge always exists and its position does not shift; but when A is increased up to about 0.08, the mobility edge disappears suddenly, suggesting that all the localized modes get delocalized when the symmetric anharmonic interaction exceed a certain threshold. In clear contrast to the DFPU-β model, we find delocalization may occur in the DFPU-α-β model even when A is as small as about 10^{-3}. As a comparison, the results of the DFPU-α-β model for $0.01 \leqslant A \leqslant 0.04$ are shown in Fig. 1(c). It suggests that asymmetric anharmonic interactions may break the localized modes much more efficiently.

These observations, however, may not necessarily represent the properties of the studied systems at a nonzero, finite

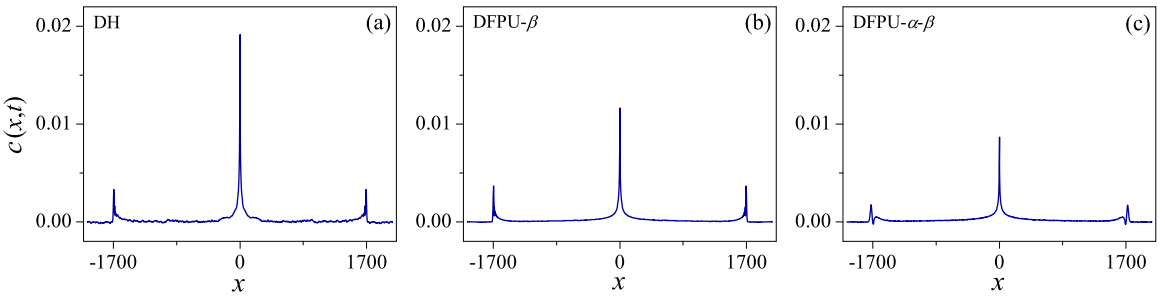

FIG. 2. (Color online) The snapshot of the spatial-temporal correlation function of the energy density fluctuations for (a) the DH model, (b) the DFPU-β model, and (c) the DFPU-α-β model at time $t = 1700$. The system size is $N = 4096$ and the temperature is $T = 10^{-3}$.

temperature. In the following we will show that, when a system is at the equilibrium state of temperature $T > 0$, the localization and delocalization properties can be revealed by the spatial-temporal correlation function of the energy density fluctuations, which can be calculated as [33,34]

$$c(x,t) = \frac{\langle \delta e(x,t)\delta e(0,0)\rangle}{\langle \delta e(0,0)\delta e(0,0)\rangle} + \frac{1}{N-1}, \tag{3}$$

where $\delta e(x,t) = e(x,t) - \langle e(x,t)\rangle$ represents the fluctuations of the energy density $e(x,t)$ to the ensemble averaged energy density $\langle e(x,t)\rangle$. We adopt the microcanonical ensemble, and for each sample system, the periodic boundary conditions and a zero total momentum is imposed. To calculate the energy density, we divide the chain into N unit bins, which, together with the momentum conservation condition, results in the $1/(N-1)$ correction term in the right-hand side of Eq. (3) to the conventionally defined spatial-temporal correlation function [34].

The snapshot of $c(x,t)$ at a certain time for the studied systems at temperature $T = 10^{-3}$ are presented in Fig. 2. One can see that in all the cases $c(x,t)$ is featured by a still center peak and two moving side peaks, whose physical meanings can be understood by studying the DH model. In the DH model, it is clear that any configuration is a superposition of the normal modes; in particular, $\delta e(x,t)$ can be decomposed into two parts, which are the superposition of, respectively, all the localized modes and all the extended modes. The former should keep localized in space, corresponding to the center peak, while the latter should move ballistically, corresponding to the two side peaks. These speculations are well verified by our simulations: For the DH model [Fig. 2(a)], we have checked and verified that the speed of the two moving side peaks is exactly the sound speed of the system, and meanwhile the center peak will keep its height after a short transient time. (See Fig. 3 where the height of the center peak as a function of time is presented.)

The DH model does not contain anharmonic interactions, but it provides a useful reference for understanding the effects of the latter. In Fig. 2(b) the effects of the symmetric FPU-β interactions are studied. We find that at a low temperature (e.g., $T = 10^{-3}$), the properties of $c(x,t)$ are qualitatively the same as those of the DH model; i.e., the side peaks move ballistically at the sound speed and the height of the center peak converges to a constant (see Fig. 3), suggesting that delocalization does not occur. But in clear contrast again, the asymmetric FPU-α-β interactions can induce delocalization. In this case, though the main features of $c(x,t)$ [see Fig. 2(c)] look similar, the center peak remains to relax and its height keeps decreasing continuously (see Fig. 3). In other words, the localized modes continuously lose the energy they carry due to the anharmonic interactions.

Increasing the temperature, delocalization can be observed also in the DFPU-β model; e.g., for $T = 5 \times 10^{-3}$, the height of the center peak begins to decay continuously as shown in Fig. 3. As a comparison, the temperature for delocalization in the DFPU-α-β model could be much lower, at least for $T = 10^{-4}$, the lowest temperature accessible to our simulations (see Fig. 3). It shows that at a nonzero, finite temperature, asymmetric anharmonic interactions are still much more efficient in resulting in delocalization.

Now let us turn to the energy transport problem. According to the Green-Kubo formula [35,36], i.e., $\kappa = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{Nk_BT^2}\int_0^\tau C(t)\,dt$, the heat conductivity can be obtained by calculating the energy current correlation function $C(t) = \langle J(t)J(0)\rangle$, where the energy flux $J(t)$ is defined [37] by $J = \sum_i \dot{x}_i \partial V(x_{i+1} - x_i)/\partial x_i$. How $C(t)$ decays thus determines the energy transport properties. We first check decay of $C(t)$ in the DFPU-β model when delocalization does not happen. In Fig. 4(a), the results of the DFPU-β model at a low temperature $T = 10^{-3}$ are compared with those of the DH model. It can be seen that the two curves almost overlap with each other as expected, and decay in a power-law manner with the exponent approximates to -0.5. This

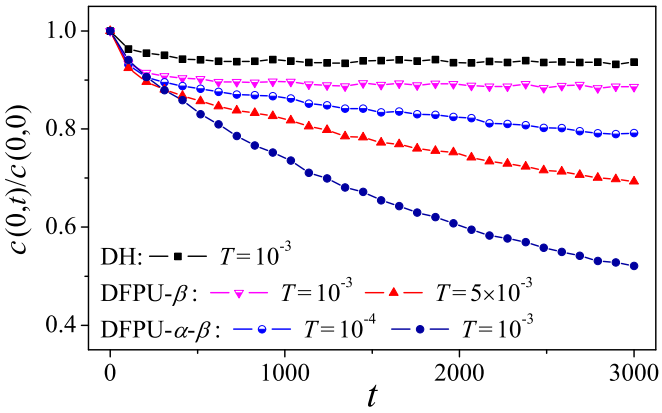

FIG. 3. (Color online) The height of the center peak in the spatial-temporal correlation function of the energy density fluctuations (see Fig. 2) as a function of time.

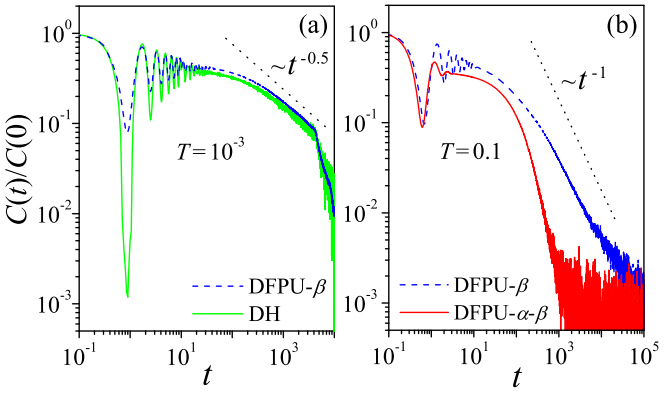

FIG. 4. (Color online) The correlation function of the energy current. (a) $T = 10^{-3}$, which is below the delocalization threshold for the DFPU-β model; (b) $T = 0.1$, delocalization occurs in both the DFPU-β model and the DFPU-α-β model. The black dotted lines indicating scaling $\sim t^{-0.5}$ (a) and $\sim t^{-1}$ (b), respectively, are for reference.

is analogous with the theoretical prediction for DH chains with the free boundary conditions. [In calculating $C(t)$ the periodic boundary conditions have been adopted.] Therefore, below the delocalization threshold the symmetric anharmonic interactions do not change the decay behavior of $C(t)$ that characterizes the DH chains. (Note that the abrupt drop of $C(t)$ curves around $t \approx N/v_s$ is a finite-size effect induced by sound mode collision [38,39].)

Increasing the temperature to exceed the delocalization threshold of the DFPU-β model, one may expect $C(t)$ curves for both the DFPU-β model and the DFPU-α-β model would separate from that of the DH model [see Fig. 4(b)]; but intriguingly, how they decay is qualitatively different: in the DFPU-β model $C(t)$ tends to decay in a power-law manner after a transient stage, which is consistent with the conclusion of previous studies [16], i.e., heat transport is anomalous in the DFPU-β model, the same as in the homogeneous FPU-β model. But in the DFPU-α-β model, $C(t)$ decays much faster than $\sim 1/t$ and the faster decaying stage lasts for at least three orders. Following the Green-Kubo formula, faster decay of $C(t)$ implies a size-independent thermal conductivity or normal heat conduction governs by the Fourier law.

In summary, symmetric and asymmetric anharmonic interactions can result in significantly different properties in disordered systems. Asymmetric anharmonic interactions, even weak, can break the localized modes, making the energy current correlation function decay faster than $\sim 1/t$ and the thermal conductivity converge. But symmetric anharmonic interactions, if weak enough, would not affect the properties of the DH chains qualitatively. Only when the temperature is above the delocalization threshold occurs delocalization, but thermal conductivity still diverges.

As asymmetric interactions and disorder are common in real materials, our study also has practical significance: It implies that the normal heat conductive behavior may be common in low-dimensional materials. Our study also shows that the spatial-temporal correlation function of energy density fluctuations can be applied to explore delocalization in systems at a nonzero temperature; this makes it more advantageous than the conventional method for measuring the mobility edge performed in a zero temperature background.

Finally, as a numerical study, our results are obtained with systems of a finite size. Whether they can be "extrapolated" to the thermodynamic limit needs further studies. For the DFPU-α-β model, simulation accuracy allow us to be confident that the energy current correlation function decays faster than $\sim 1/t$ for at least three orders, and this fact can guarantee that the thermal conductivity unchanged as the system size even up to a macroscopic scale even though the faster decaying stage is followed by a power-law tail [18]. This result has important practical significance, but for theoretical understanding, if the power-law tail really follows should be clarified by large-scale simulations. Similarly, for the DFPU-β model, large-scale simulations are also needed to obtain the accurate power-law exponent with which $C(t)$ decays.

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