Effects of interplay between disorder and anharmonicity on heat conduction

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Heat conduction through a disordered Fermi-Pasta-Ulam-β (DFPU-β) chain is studied. The presence of disorder makes the heat current behave significantly different from that of the ordered Fermi-Pasta-Ulam-β (FPU-β) chain. Thanks to the interplay between disorder and anharmonicity, a nonmonotonic-monotonic transition occurs when the disorder strength increases. That is, a peak for the heat current emerges for weak disorder; however, monotonic increasing of the heat current shows up for strong disorder. This can be understood based on the competition between two effects of anharmonicity on phonons, namely, delocalization and phonon-phonon scattering, which is shown by the spectral decomposition of heat current.

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I. INTRODUCTION

Since the pioneering study of Anderson [1], localization has been a fundamental concept in condensed-matter physics [2,3]. For electronic systems, it is well known that localization has the strongest effect in one dimension; that is, under broad conditions, all quantum states are localized in the thermodynamic limit [4,5]. Since only the electrons near the Fermi level contribute to transport, the electrical current decays exponentially with the system size.

Similar but different conclusions exist in phononic systems. In fact, as early as in 1970, Matsuda and Ishii [6] have already proven that for one-dimensional isotopically disordered harmonic chain of N atoms with the average mass $m = \langle m_l \rangle$, the variance $\sigma_m^2 = \langle (m_l - m)^2 \rangle$ and spring constant k, the effective mobility edge is given by

$$\omega_d = 4\sqrt{\frac{km}{N\sigma_m^2}}. \tag{1}$$

The normal modes of $\omega \ll \omega_d$ are extended, whereas the normal modes of $\omega \gg \omega_d$ are localized. Contrary to electronic systems, since low-frequency extended phonons can contribute to energy transport, the dependence of heat conductivity κ on the system size shows a power-law behavior $\kappa \sim N^\alpha$ for phononic systems without onsite potential. In the context of heat conduction in a disordered harmonic chain, a longstanding puzzle is that there are two different exponents, namely, $\alpha = 1/2$ for free boundaries [7,8], and $\alpha = -1/2$ for fixed boundaries [9]. This puzzle clarified with the finding that the spectral properties of heat baths and boundary conditions of the system have a strong effect on phonon transmission in disordered harmonic chains using the Langevin equations and Green's function (LEGF) method [10].

When anharmonicity is concerned, generally speaking, chaos [11,12] plays a role in heat conduction through the interaction of phonon modes, and the coexistence of anharmonicity and disorder makes the issue more complicated. In a study of disordered Fermi-Pasta-Ulam-β (DFPU-β) chains, Li *et al.* [13] found that the heat conductivity diverges as $\kappa \sim N^{2/5}$ at high temperature like the ordered Fermi-Pasta-Ulam-β (FPU-β) chain [14], whereas a nonvanishing convergent heat conductivity, i.e., normal heat conduction, is observed at low temperature. Nevertheless, Dhar and Saito [15] found that heat conductivity still diverges in the same way as the ordered FPU-β chain even at low temperature when a stochastic heat bath is used. The results in Ref. [16] also support this conclusion. Therefore, the disorder-induced change in the behavior of heat conduction seems only quantitative but not qualitative.

In addition, it has been shown that, in the disordered pinned anharmonic chain, heat conduction is normal [17], which is the same as its ordered counterpart. It is worth noting that the spreading of localized energy wave packets in isolated disordered pinned anharmonic chain shows subdiffusion [18–23] or partial localization [21–24]. However, the diffusion at finite temperature is significantly different from that at zero temperature. As pointed out in Ref. [25], the spatiotemporal correlation of energy density fluctuation is necessary to understand the equilibrium energy diffusion at finite temperature. The study in Ref. [26] shows that the equilibrium energy diffusion in disordered ϕ^4 chains is still normal diffusion, consistent with the results of heat conduction [17]. Once again, disorder is irrelevant to the behavior of heat conduction in anharmonic chains. However, if looking closely at the result corresponding to $N = 1024$ shown in Fig. 1 of Ref. [17], one can find that, as anharmonicity increases, the heat current in the disordered ϕ^4 chain first increases and then decreases, different from that for the ordered ϕ^4 chain where the heat current decreases monotonically with increasing anharmonicity. A similar observation can also be found in Ref. [27]. As a matter of fact, in a pioneering numerical study of heat conduction in disordered systems, Payton *et al.* [28] discovered that a small amount of anharmonicity enhances heat conductivity, which, as they argued, comes from energy transfer of localized phonons to extended phonons. However, as we see below, it

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lies in the contribution of localized phonons themselves to heat conduction increases due to the delocalization effect.

In the present paper, effects of the interplay between disorder and anharmonicity on heat conduction is revisited by studying the heat current as a function of the strength of anharmonicity in the DFPU-β chain. It is found that, with the increase of disorder, the heat current undergoes a transition from nonmonotonic variation to monotonic variation. A physical interpretation for this transition is given and verified by the spectral heat current. The paper is organized as follows. The model studied and numerical methods are introduced in Sec. II. The simulation results are discussed in Sec. III. Finally, a brief summary is given in Sec. IV.

II. MODEL AND NUMERICAL METHODS

The Hamiltonian of the model considered in this paper is given by

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=0}^{N} \left[k\frac{(x_l - x_{l+1})^2}{2} + \beta\frac{(x_l - x_{l+1})^4}{4} \right], \quad (2)$$

where p_l and x_l denote the momentum and the displacement from its equilibrium position of the lth particle with mass m_l, respectively. k is the coefficient of the harmonic spring. β represents the strength of anharmonicity. We consider the mass disordered chain only, in which $\{m_l\}$ are chosen independently from a uniform distribution in the interval $(1 - \Delta m, 1 + \Delta m)$, where Δm denotes the strength of disorder. The chain is connected, at its ends, to two Langevin heat baths at temperature T_L and T_R. The equations of motion of the chain are then given by

$$m_l\ddot{x}_l = k(x_{l-1} - 2x_l + x_{l+1}) + \beta[(x_{l-1} - x_l)^3 + (x_{l+1} - x_l)^3] - \lambda_l\dot{x}_l + \xi_l, \quad (3)$$

where $\lambda_l = \lambda(\delta_{l,1} + \delta_{l,N})$ and $\xi_l = \xi_L\delta_{l,1} + \xi_R\delta_{l,N}$. The noise term is related to the dissipation coefficient λ by the fluctuation-dissipation relation $\langle\xi_L(t)\xi_L(t')\rangle = 2\lambda k_B T_L \delta(t - t')$ where k_B is the Boltzmann constant, and a similar relation for the heat bath at the right end of the chain also exists. Throughout the paper, we use fixed boundary conditions only, i.e., $x_0 = x_{N+1} = 0$, and the parameters for two heat baths are set to $T_L = 1.2$, $T_R = 0.8$, $\lambda = 0.8$. Unless otherwise noted, the system size and the coefficient of the harmonic spring are set to $N = 1024$ and $k = 1$, respectively.

In our simulation, the velocity-Verlet algorithm with a time step of 0.005 is used to integrate the equations of motion. To study heat conduction in the nonequilibrium steady state, we compute the heat current by averaging over 2×10^9 steps after a relaxation process of 2×10^8 steps. The heat current is given according to the usual definition [29,30] $j = \sum_{l=2}^{N}\langle v_l f_{l,l-1}\rangle/(N - 1)$, where $f_{l,l-1}$ is the force acting on the lth particle from the $(l - 1)$st particle and $\langle\cdots\rangle$ denotes a steady-state average. Due to the nature of disordered systems, we also take disorder averaging over 100 different realizations, and the resulting heat current is denoted by J.

For the purpose of understanding the effect of disorder and anharmonicity on heat conduction in depth, we also compute, using the method proposed by Sääskilahti *et al.* [31,32], the spectral heat current defined by

$$q_{l\to l+1}(\omega) \approx \frac{1}{t_c}\mathrm{Re}\langle\widetilde{f}_{l+1,l}(\omega)[\widetilde{v}_l(\omega) + \widetilde{v}_{l+1}(\omega)]^*\rangle, \quad (4)$$

where $\widetilde{f}_{l+1,l}(\omega)$ and $\widetilde{v}_l(\omega)$ are the discrete Fourier transforms of force $f_{l+1,l}(t)$ and velocity $v_l(t)$ trajectories obtained from molecular-dynamics simulations, and t_c is the cutoff time used in the discrete Fourier transforms. Because of the identity $j_{l\to l+1} = \int_0^{+\infty}(d\omega/2\pi)q_{l\to l+1}(\omega)$ where $j_{l\to l+1}$ denotes the heat current from the lth particle to the $(l + 1)$st particle, $q_{l\to l+1}(\omega)$ can be interpreted as the contribution of phonons at frequency ω to heat current. In the whole paper, only the spectral heat current of two middlemost particles ($l = N/2$) is considered, and hereafter the subscript of $q_{l\to l+1}(\omega)$ is omitted for brevity. It is worth mentioning that, using the Wiener-Khinchin theorem, one can find that, in harmonic systems, the spectral heat current can be reduced to the transmission defined in the LEGF method with only a constant multiplier difference at most (see Appendix for details).

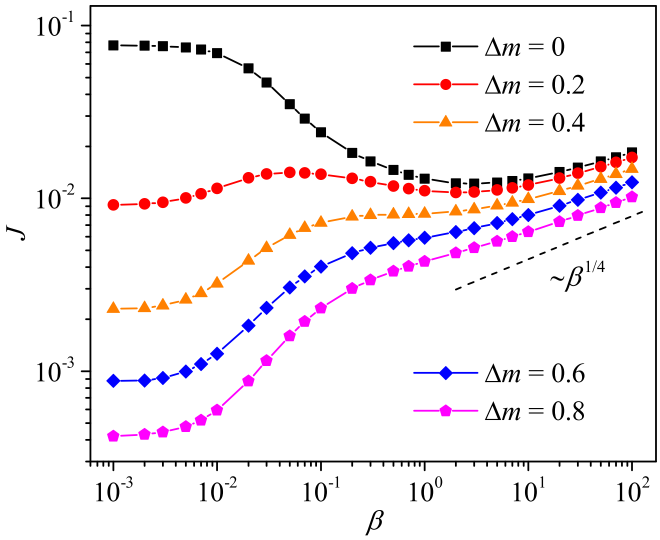

FIG. 1. Heat current J as a function of the strength of anharmonicity β for different values of the strength of disorder Δm. The error bars coming from both numerical errors and disorder averaging are smaller than the symbols. The dashed line is drawn as a reference for the power-law behavior $\beta^{1/4}$. The solid lines are drawn to guide the eyes.

III. RESULTS AND DISCUSSIONS

To show the interplay between anharmonicity and disorder clearly, we compare simulation results of the β dependence of heat current J for different Δm, as depicted in Fig. 1. For $\Delta m = 0$, i.e., the ordered FPU-β chain, the heat current first falls significantly to a minimum and then increases slowly with increasing β. However, when Δm increases to 0.2, the behavior of heat current changes qualitatively; that is, with increasing β, the heat current first climbs towards the peak at $\beta \approx 0.05$, and then drops very gently to the bottom at $\beta \approx 2$ before the final slight increasing. When disorder is strong enough, e.g., $\Delta m = 0.6$, the heat current becomes a monotonically increasing function of β. Therefore, as Δm

increases from 0 to 0.8, the behavior of the heat current as a function of β has a transition from nonmonotonic to monotonic, during which a more complicated situation, namely, $\Delta m = 0.2$, exists.

To understand this transition, let us first consider the ordered FPU-β chain. Based on kinetic theory, the nonmonotonic dependence of the heat current on β has been understood [33]. In the regime of weak anharmonicity, phonon-phonon scattering shown by the mean-free path that decreases with increasing β dominates the behavior of heat conduction. But when anharmonicity is strong, the main contribution to heat conduction comes from the phonon velocity which increases with increasing β due to phonon renormalization. This physical picture can be manifested more clearly in the spectral heat current.

Because anharmonicity makes not only phonon renormalization resulting in β dependent phonon velocity but also frequency broadening indicating phonon-phonon scattering, the renormalized phonon frequency depends on the strength of anharmonicity β. Hence, in order to compare the results of the spectral heat current between different β, we use a rough method of linearly rescaling the spectral heat current $q(\omega)$ by the upper frequency bound of the corresponding ordered system ω_c. Hereafter, ω_c is numerically extracted from the spectral heat current corresponding to the ordered FPU-β chain with $N = 32$, and we have numerically verified that ω_c is basically independent of N when $N \geqslant 32$. The scaled spectral heat current $q(\omega)\omega_c$ as a function of the scaled frequency ω/ω_c is shown in Fig. 2. In the regime of weak anharmonicity, the contribution of the high-frequency phonons of $\omega/\omega_c \gtrsim 0.3$ to heat current gradually decreases with the increase of β due to phonon-phonon scattering, as shown in Fig. 2(a). In the regime of strong anharmonicity, the phonon velocity which increases with increasing β plays a critical role in heat conduction. Because low-frequency phonons are less affected by phonon-phonon scattering, the effect of phonon velocity on heat conduction is first reflected in the low-frequency region. However, when anharmonicity is so strong that the mean-free path is saturated at a lattice spacing, in terms of the kinetic theory, the contribution of high-frequency phonons to heat conduction will also be enhanced by the β-dependent phonon velocity. This can be seen when one looks at Fig. 2(b) in detail. Comparing the two curves corresponding to $\beta = 2$ and $\beta = 10$, one can find that, when $\omega/\omega_c \gtrsim 0.1$, the two curves are almost the same. But, when β increases to 50, the part of $0.1 \lesssim \omega/\omega_c \lesssim 0.2$ starts to rise. It is worth mentioning that the reason why $q(\omega) \to 0$ as $\omega \to 0$ is that the low-frequency phonons are very sensitive to the onsite potentials, which appear at two ends of the chain due to fixed boundary conditions used in the present paper. This phenomenon also exists in the transmission of the harmonic chain [34].

In the DFPU-β chain, when anharmonicity is not very strong, the existence of anharmonicity leads to two effects, namely, delocalization and phonon-phonon scattering. Delocalization enhances heat conduction, while the phonon-phonon scattering effect hinders heat conduction.

When disorder is weak, e.g., $\Delta m = 0.2$, the existence of a peak for heat current comes from the competition between delocalization and phonon-phonon scattering. The

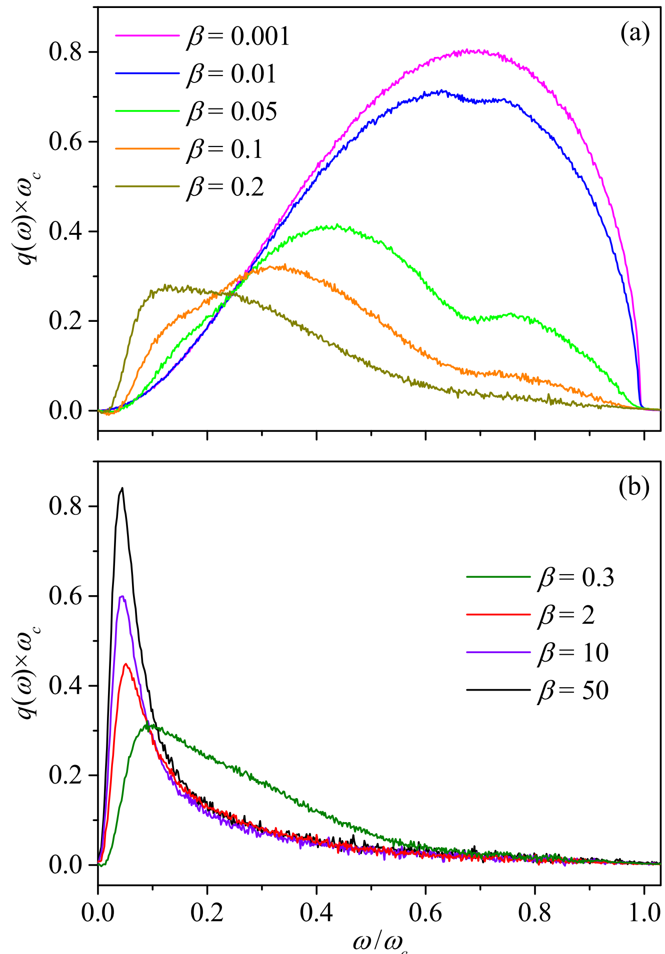

FIG. 2. Scaled spectral heat current $q(\omega)\omega_c$ as a function of the scaled frequency ω/ω_c for the FPU-β chain. (a) The weak anharmonicity regime. The curves, from top to bottom on the right part of the plot, correspond to different values of the strength of anharmonicity $\beta = 0.001$, 0.01, 0.05, 0.1 and 0.2, respectively. (b) The strong anharmonicity regime. The curves, from top to bottom on the left part of the plot, correspond to different values of the strength of anharmonicity $\beta = 50$, 10, 2, and 0.3, respectively.

delocalization effect makes the dominant contribution when anharmonicity is extremely weak. This can be seen from Fig. 3(a). For comparison, the scaled spectral heat current corresponding to the harmonic system ($\beta = 0$) is also given by the LEGF method [30]. Since the scattering effect of disorder on low-frequency phonons is so weak that the characteristic peaks of low-frequency phonons remain, the curve corresponding to $\beta = 0$ fluctuates violently in the low-frequency region of $\omega/\omega_c \lesssim 0.3$. The near coincidence between the curves corresponding to $\beta = 0$ and $\beta = 0.001$ implies that the anharmonicity is too weak to delocalize high-frequency phonons. This is consistent with the results in Ref. [35]. When β increases to 0.01, it can be seen that the contribution of the localized phonons of $\omega/\omega_c \gtrsim 0.7$ to heat current is enhanced by delocalization effect. However, as anharmonicity increases further, phonon-phonon scattering increases and comes to overwhelm the effect of delocalization. It is shown in Fig. 3(b) that the scaled spectral heat current for the high-frequency

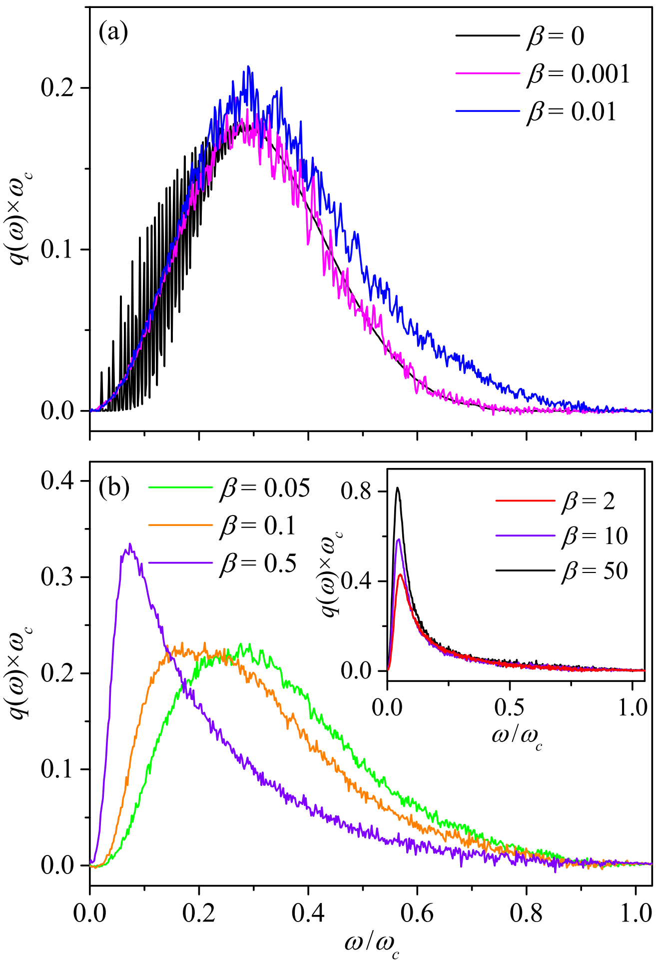

FIG. 3. Scaled spectral heat current $q(\omega)\omega_c$ as a function of the scaled frequency ω/ω_c in the DFPU-β chain of $\Delta m = 0.2$. (a) The extremely weak anharmonicity regime. The curve that fluctuates violently on the left part corresponds to $\beta = 0$ and is computed by the LEGF method [30]. The other two curves, from top to bottom, correspond to different values of the strength of anharmonicity $\beta = 0.01$ and 0.001, respectively. (b) The moderately weak anharmonicity regime. The curves, from top to bottom on the middle part of the plot, correspond to different values of the strength of anharmonicity $\beta = 0.05$, 0.1, and 0.5, respectively. The inset shows the strong anharmonicity regime. The curves, from top to bottom on the left part of the plot, correspond to different values of the strength of anharmonicity $\beta = 50$, 10, and 2, respectively.

phonons of $\omega/\omega_c \gtrapprox 0.3$ decreases with increasing β, similar to the situation in the FPU-β chain, see Fig. 2(a). When anharmonicity is strong enough, disorder is irrelevant due to sufficient delocalization effect. In this case, heat conduction behaves like a ordered system; this is why on the right portion of Fig. 1, those different curves have similar behavior. In the FPU-β chain, when anharmonicity is strong, the heat conduction is dominated by the phonon velocity proportional to $\beta^{1/4}$ [33]; in consequence, $J \sim \beta^{1/4}$. This scaling relation should also apply to the DFPU-β chain according to the statement above. It can be seen from Fig. 1 that the growth of heat current is slightly slower than $\beta^{1/4}$, which may be due to the phonon-phonon scattering. We expect that, if anharmonicity increases further, the heat current will obey the scaling relation $J \sim \beta^{1/4}$. In addition, as depicted in the inset of Fig. 3(b), the scaled spectral heat current for $\beta \geqslant 2$ shows almost the same behavior as Fig. 2(b), which again suggests that the effect of disorder becomes irrelevant for strong anharmonicity.

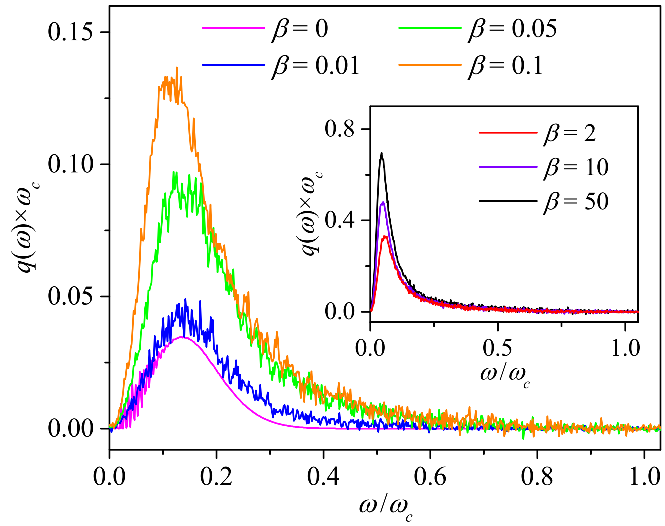

FIG. 4. Scaled spectral heat current $q(\omega)\omega_c$ as a function of the scaled frequency ω/ω_c in the DFPU-β chain of $\Delta m = 0.6$ in the weak anharmonicity regime. The curves, from top to bottom, correspond to different values of the strength of anharmonicity $\beta = 0.1$, 0.05, 0.01, and 0, respectively. The curve corresponding to $\beta = 0$ is computed by the LEGF method [30]. The inset shows the strong anharmonicity regime. The curves, from top to bottom in the left part of the plot, correspond to different values of the strength of anharmonicity: $\beta = 50$, 10, and 2, respectively.

To some extent, delocalization means that the phonon packet broadens and hence the localization length becomes longer, or in other words, the localization length increases with increasing β. However, on the other hand, the mean-free path suggesting phonon-phonon scattering decreases with increasing β. For weak disorder, the presence of anharmonicity first leads to delocalization of the high-frequency phonons; when the localization length increases to near the mean-free path, phonon-phonon scattering comes to play. This leads to the occurrence of a peak of the heat current in the weak-anharmonicity regime. However, for the case of strong disorder, which suggests strong localization, the strength of anharmonicity required to make the localization length exceed the mean-free path is so large that the β-dependent phonon velocity becomes relevant. Consequently, as long as disorder is strong enough, the scaled spectral heat current at any given scaled frequency will be a monotonically increasing function of β. In the case of $\Delta m = 0.6$, it can be seen from Fig. 4 that, in the weak anharmonicity regime, the scaled spectral heat current for the high-frequency phonons of $\omega/\omega_c \gtrapprox 0.3$ is always enhanced by the delocalization effect. It is worth noting that $\omega/\omega_c \gtrapprox 0.3$ is exactly the region where phonon-phonon scattering acts in the FPU-β chain, see Fig. 2(a). In the inset of Fig. 4, again, the results for strong anharmonicity ($\beta \geqslant 2$), give almost the same behavior as Fig. 2(b). Therefore, the reason why heat current increases monotonically with the strength of anharmonicity is that the delocalization

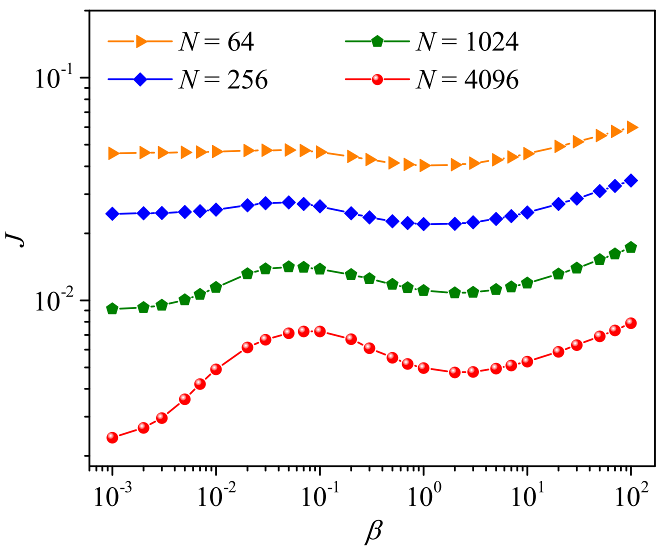

FIG. 5. Heat current J as a function of the strength of anharmonicity β for the system size $N = 64$, 256, 1024, and 4096, respectively. Here $\Delta m = 0.2$. The current is obtained by averaging over 20 disorder realizations for $N = 4096$ and 100 disorder realizations for others. The error bars coming from both numerical errors and disorder averaging are smaller than the symbols. The solid lines are drawn to guide the eyes.

effect dominates heat conduction in the regime of weak anharmonicity.

Finally, the size effect of the heat current as a function of β is also studied. According to the size-dependent mobility edge, see Eq. (1), the larger the system size, the larger the proportion of localized phonons, and then the more significant the delocalization effect. Therefore, as illustrated in Fig. 5, the peak for heat current becomes more and more pronounced as the system size increases.

IV. SUMMARY

In summary, we studied heat conduction through the DFPU-β chain. We found that variation of heat current with anharmonicity undergoes a change of monotonicity when disorder increases. For weak disorder, a peak for heat current emerges due to the competition between delocalization and phonon-phonon scattering. When disorder is strong, the delocalization effect dominates heat conduction in weak anharmonicity regime, and then heat current increases monotonically with the strength of anharmonicity. This physical interpretation is corroborated further by the results of spectral heat current.

In addition, we expect that the nonmonotonic-monotonic transition observed in this paper may be generalized to higher-dimensional disordered systems, especially the effect of delocalization on heat transport. In fact, it has been found in an earlier study [28] that a small amount of anharmonicity enhances heat conductivity in a two-dimensional disordered system. Furthermore, in a recent study of disordered one-dimensional FPU-α-β chains [36], it was found that the increase of nonlinearity strength did not lead to a monotonic route to thermalization. And it has been shown that the interaction symmetry does have effects on delocalization and energy transport [35]. Overall, it is worth paying attention to further clarify the effects of interaction symmetry on localization.

As noted in Ref. [17], the heat current in the DFPU-β chain satisfies the scaling relation $J(sT_L, sT_R, \beta) = sJ(T_L, T_R, s\beta)$, s being an arbitrary positive real number. Therefore, at a fixed value of β, the thermal conductance $G = J/(T_L - T_R)$ as a function of average temperature $T = (T_L + T_R)/2$ which is easier to measure in experiments, will also exhibit the same behavior as in Fig. 1. We expect that similar behavior can also be observed numerically [37,38] or even experimentally [39–43] in realistic materials, e.g., superlattices, considering the current techniques for material manufacturing and experimental measurement.

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APPENDIX: THE SPECTRAL HEAT CURRENT IN ONE-DIMENSIONAL CLASSIC HARMONIC CHAINS

In this Appendix, using LEGF method [30,44], we calculate the spectral heat current in 1D classic nearest-neighbor interacting harmonic chains with the Hamiltonian

$$H = \tfrac{1}{2}\dot{X}^T M \dot{X} + \tfrac{1}{2} X^T \Phi X, \tag{A1}$$

where $M_{l,n} = m_l \delta_{l,n}$, $\Phi_{l,n} = (2k + k_o)\delta_{l,n} - k(\delta_{l,n-1} + \delta_{l,n+1}) + (k' - k)\delta_{l,n}(\delta_{l,1} + \delta_{l,N})$, and $X = \{x_1, x_2, \dots, x_N\}^T$.

The Green's function is as follows:

$$G^{\pm}(\omega) = \frac{1}{-\omega^2 M + \Phi - \Sigma_L^{\pm}(\omega) - \Sigma_R^{\pm}(\omega)}, \tag{A2}$$

where $\Sigma_{L,R}^{\pm}$ is the self-energy of the heat baths. For the Langevin heat baths considered in this paper, the only nonzero elements of $\Sigma_{L,R}^{\pm}$ are respectively $[\Sigma_L^{\pm}]_{1,1} = \Sigma = i\lambda\omega$ and $[\Sigma_R^{\pm}]_{N,N} = \Sigma = i\lambda\omega$, where λ is the coupling strength between the end particles and the heat baths.

In terms of the Green's function $G^{\pm}$, the Fourier transformation of the cross-correlation function between x_l and v_n is as follows:

$$\widetilde{C}_{x_l,v_n} = 2ik_B\Gamma(\omega)(T_L G_{l,1}^{+} G_{n,1}^{-} + T_R G_{l,N}^{+} G_{n,N}^{-}), \tag{A3}$$

with $\Gamma(\omega) = \mathrm{Im}[\Sigma(\omega)]$.

In the one-dimensional (1D) harmonic chain, Eq. (4) can be expressed as

$$q_{l\to l+1}(\omega) = \frac{k}{2\pi}\mathrm{Re}\big[\widetilde{C}_{x_l,v_l} + \widetilde{C}_{x_l,v_{l+1}} - \widetilde{C}_{x_{l+1},v_l} - \widetilde{C}_{x_{l+1},v_{l+1}}\big]. \tag{A4}$$

Substituting Eq. (A3) into Eq. (A4), after some algebraic calculation, one gets

$$q_{l\to l+1}(\omega) = \frac{2k_B(T_L - T_R)}{\pi}\frac{\Gamma^2(\omega)}{k^2|\mathrm{Det}Z|^2}, \tag{A5}$$

with $G^+ = Z^{-1}/k$.

It is easy to see from Eq. (A5) that in 1D classical nearest-neighbor interacting harmonic chains, the spectral heat current between particles is the same as that between heat bath and system and is independent of the position l.

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