Scattering of lattice solitons and decay of heat-current correlation in the Fermi-Pasta-Ulam-α-β model

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As is well known, solitons can be excited in nonlinear lattice systems; however, whether, and if so, how, this kind of nonlinear excitation can affect the energy transport behavior is not yet fully understood. Here we study both the scattering dynamics of solitons and heat transport properties in the Fermi-Pasta-Ulam-α-β model with an asymmetric interparticle interaction. By varying the asymmetry degree of the interaction (characterized by α), we find that (i) for each α there exists a momentum threshold for exciting solitons from which one may infer an α-dependent feature of probability of presentation of solitons at a finite-temperature equilibrium state and (ii) the scattering rate of solitons is sensitively dependent on α. Based on these findings, we conjecture that the scattering between solitons will cause the nonmonotonic α-dependent feature of heat conduction. Fortunately, such a conjecture is indeed verified by our detailed examination of the time decay behavior of the heat current correlation function, but it is only valid for an early time stage. Thus, this result may suggest that solitons can have only a relatively short survival time when exposed in a thermal environment, eventually affecting the heat transport in a short time.

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I. INTRODUCTION

Since Debye's pioneering work, it has been recognized that the lattice heat conduction can be described by lattice vibrations, which are rephrased as various collective excitations. Among them, one of the well-known energy carriers is the phonon [1]. Within this framework, the energy transport behavior can be understood by the interplay of these excitations, determined by a key factor, i.e., the focused system's type of interparticle interaction (IPIA), if other effects, such as the external potential [2,3], defect [4], and boundary [5], are ignored.

To use the above picture to model real systems' heat conduction, a nonlinear IPIA is crucial [6]. That is because, if the IPIA is linear type, there is no interaction between phonons and as a consequence the energy transport follows a ballistic way, with the feature of heat conductivity proportional to the system size [6]. Viewing this fact, Peierls [7] first took the nonlinearity of the IPIA into account and suggested that it can induce phonon-phonon interaction and thus the heat transport in an anharmonic lattice can be understood by the picture of gases of interacting phonons. Such a viewpoint certainly signifies great progress; however, we should note that, triggered by a later work of Fermi, Pasta, and Ulam [8], it was further realized that in addition to phonons, other nonlinear excitations, such as solitons [9], are ubiquitous in the lattice system after including the nonlinear IPIA. Therefore, a complete picture to understand heat transport should also involve soliton-soliton interaction. At present, however, few contributions have been presented on this issue.

In this respect, some earlier results conjectured that solitons play a key role in anomalous heat conduction of one-dimensional Fermi-Pasta-Ulam-β (FPU-β) lattice systems [10,11], while in the same systems, others found [12] that the energy carriers may be the effective phonons but not the solitons and this argument remains valid for even high-temperature regions. This disagreement may result from the fact that both viewpoints are based on the particular FPU-β model whose IPIA is of the symmetric type. Such special collective dynamics of a nonlinear system at finite temperature can be understood through a renormalized phonon theory [13], which implies that researchers did not thoroughly take the role of solitons in heat conduction into consideration.

Recently, there has been an increasing interest in the study of heat transport in nonlinear lattices with asymmetric IPIA. This is because the asymmetry feature of IPIA is also crucial in modeling real systems. The relevant theoretical studies revealed that, compared to the systems with symmetric IPIA, the heat conductivity in a system with asymmetric IPIA will diverge with system size in a quite different way [14–17]. This distinctive divergent behavior has been predicted by the theory of nonlinear fluctuating hydrodynamics [15], which proposed a relevant noisy Burgers equation [16] for the heat modes and used the mode-coupling theory [17] to solve it. Such a difference has also been carefully considered in several numerical studies [18] (see also the detailed discussion in Sec. 7 of Ref. [15]). Now in the context of collective excitations, different properties of heat transport would suggest that different excitations dynamics would be shown in the system. Thus, it would be interesting to explore what roles the nonlinear excitations, such as solitons, will play in heat transport in this kind of system.

In this paper we therefore attempt to study the effects of the scattering dynamics of solitons on heat conduction in the FPU-α-β model with an asymmetric IPIA. For this purpose, we first examine the exciting threshold for solitons. Then, with this information, the scattering rate of solitons is carefully investigated. Finally, together with a conjecture of the probability of solitons in thermalized states, we try to relate the observed microscopic dynamics to the heat transport property.

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II. MODEL AND METHOD

The dimensionless Hamiltonian of the FPU-α-β model with N particles can be represented by

$$H = \sum_{i=1}^{N} H_i, \quad H_i = \frac{p_i^2}{2} + V(r_i), \tag{1}$$

where p_i and x_i are the momentum and position of the ith particle, respectively, and we set $r_i \equiv x_{i+1} - x_i - 1$. Both the particle's mass and lattice constant are set unity. The IPIA of this system is usually described as

$$V(r_i) = \frac{1}{2}r_i^2 + \frac{\alpha}{3}r_i^3 + \frac{\beta}{4}r_i^4. \tag{2}$$

For the convenience of analysis, we set $\beta = 1$ and thus the symmetry degree of the IPIA is controlled by α. To be specific, with the increase of the absolute value of α, this kind of symmetry degree will increase as well. In particular, for $\alpha = 0$, the IPIA is symmetric and the system reduces to the FPU-β model, as mentioned above.

There are two types of solitons that can be excited in the FPU-type systems. The first one is kink shaped, usually called a kink for brevity, moving in the same direction as particles. The other one is antikink shaped (called an antikink), moving, however, in the opposite direction to the associated particles. To study the soliton scattering dynamics, usually one can produce a pair of solitons in the focused lattice, labeled a and b, in the following way. Initially (at time $t = 0$), all the particles are located at their equilibrium position and with zero momentum and we apply a kick on the first particle with a momentum p_a. Then, at time $t = \delta$, we apply another kick on the last particle with momentum p_b. Note that applying the kick will excite a soliton followed by a wave packet if the kicking momentum is strong enough, but with the evolution of the system, the soliton will be separated from the wave packet because of their different velocities. Our focus now will be mainly limited to the solitons, when they are completely separated. Finally, as t increases, the two solitons, a and b, will collide with each other, which then enables us to study their scattering dynamics.

To evolve the system, the Runge-Kutta-Nystrom algorithm of order 8(6) is adopted, which has been verified to be sufficient to obtain good accuracy [19]. With this algorithm, we then are able to derive information on all the particles' positions and momenta. This information is used to measure the properties of soliton and wave packets. In addition, we consider a relative large system with long size, which is to ensure that the excited solitons could be separated from the wave packets.

In practice, through controlling the sign of p_a and p_b, one can obtain three different types of collisions, i.e., (i) positive values for both p_a and p_b gives a kink-antikink collision; (ii) one positive value (for example, p_a) and the other negative (p_b) is called an antikink-antikink collision; and (iii) negative values for both p_a and p_b produces a kink-kink collision. Such results are well known from previous studies of the FPU-β model [3,10,20].

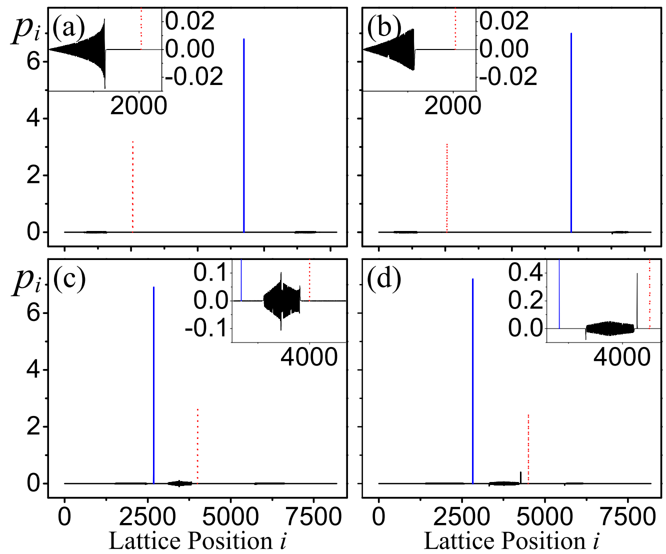

FIG. 1. Snapshots of two solitons (a) and (b) before scattering and (c) and (d) after scattering for (a) and (c) $\alpha = 0.0$ and (b) and (d) for $\alpha = -0.7$. The red dotted line is the kink soliton moving to the right and the blue solid line is the antikink soliton moving to the left. The insets are used to further identify the wave packets.

III. SOLITON BEHAVIOR

With the above technique, we conclude the following two qualitative points: (i) For a specific system, the soliton can be excited only if the kicking momentum exceeds a certain value p_c, i.e., there is a threshold of momentum for exciting the soliton, and (ii) the scattering of two pairs of solitons will result in some extra wave packets. Motivated by this, in Fig. 1 we show a typical snapshot of the kink- and antikink-type solitons, before [see Figs. 1(a) and 1(b)] and after [see Figs. 1(c) and 1(d)] collisions, in the FPU-α-β system with two different α values. The kicking momenta are fixed at $p_a = 4$ and $p_b = 8$, respectively. In order to identify the extra wave packets, we also provide further details in the corresponding insets. From Fig. 1 one may find the following unusual properties compared to the traditional FPU-β system with $\alpha = 0$. (i) For the fixed kicking momentum, the maximum momentum of the associated particle of the soliton is different for the two focused values of $\alpha = 0$ and $\alpha = -0.7$. This may suggest that for different α, the threshold for exciting the soliton is different. (ii) There is an extra soliton emerging for $\alpha = -0.7$, but this is not the case for $\alpha = 0$, which of course indicates the different scattering dynamics for the system with different α.

With the above evidence in mind, in the following we propose a numerical method to estimate the threshold of the kicking momentum for the excitation of the kink and antikink for different α values. This method is actually based on the following fact. The soliton in lattices is a type of topological soliton, for which the associated particles have two equilibrium positions [21], whereas for the wave packet in lattices, its associated particles only have a single equilibrium position. This difference results in the following: If a soliton travels through two particles, e.g., the ith and $(i + l)$th ones, these particles change from one of the equilibrium positions to the other, without losing energy. As a consequence, one may

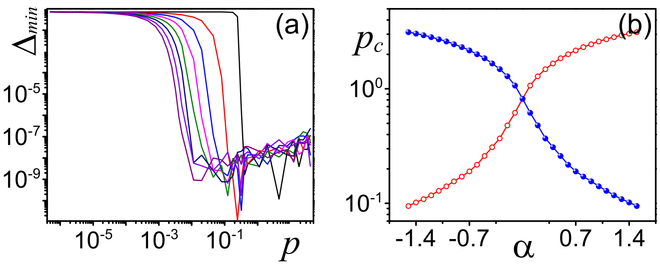

FIG. 2. (a) Minimum loss of momentum $\Delta_{\min}$ versus the kicking momentum p for, from right to left, $\alpha = 0.0$, -0.2, -0.4, -0.6, -0.8, -1.0, -1.2, and -1.4. (b) Measured threshold of momentum for kink $p_c^k(\alpha)$ (red open circles) and antikink $p_c^a(\alpha)$ (blue closed circles) versus α. These results are obtained from the system size $N = 8192$ and the parameter l is $l = 1024$.

expect that the maximum momenta between these particles, denoted by $p_i^{\max}$ and $p_{i+l}^{\max}$, are almost the same. However, since all particles are around their equilibrium positions, when a wave packet travels through two particles, it will dissipate energy and finally one should find that $p_i^{\max}$ is much larger than $p_{i+l}^{\max}$. Based on this difference, we then proceed to measure the minimum loss $\Delta_{\min}$ of momentum of the particles with maximum momentum when a certain kick is applied, i.e.,

$$\Delta_{\min} = \min\left\{\frac{\left|p_i^{\max} - p_{i+l}^{\max}\right|}{\left|p_i^{\max}\right|};\ i = \frac{N}{2},\ldots,N-l\right\}. \quad (3)$$

Obviously, under this definition, a vanished $\Delta_{\min}$ corresponds to the fact that a soliton is excited.

The result of $\Delta_{\min}$ versus the different kicking momentum p is shown in Fig. 2(a). Several α values from $\alpha = 0.0$ to $\alpha = -1.4$ are compared. As can be seen, for each α, with the increase of p, a sharp crossover from a nonvanishing to vanishing value of $\Delta_{\min}$ can be clearly identified. Interestingly, the crossover point p_c indicates that the exciting threshold is different for different α. In particular, a larger absolute value of α suggests a smaller p_c.

Figure 2(b) plots the result of p_c versus α for two different kinds of solitons, i.e., kink and antikink. We denote them by p_c^k and p_c^a, respectively. Now from Fig. 2(b) one may understand that there is a big difference between the properties of the kink and antikink, i.e., with the increase of α, p_c^k increases, whereas p_c^a decreases. However, regardless of this difference, all the curves of Fig. 2(b) show the property of symmetry for $\alpha < 0$ and $\alpha > 0$. Thus, in our following analysis, we only need to study the case of $\alpha \leqslant 0$.

Next we study the scattering dynamics of solitons. To do this, one can usually measure the scattering rate for the collision of two solitons. This scattering rate is usually defined by

$$\widetilde{\Gamma} = \frac{|E - E'|}{E}, \quad (4)$$

which characterizes the rate of energy change of solitons before and after scattering. Here $E = \sum_{\{i\}} H_i$ and $E' = \sum_{\{i\}}' H_i$ are the energies for the same soliton before and after scattering; $\sum_{\{i\}}$ means that the summation is performed only over those associated particles having significant momenta ($|p_i| > 10^{-10}$) [10]. We have verified that the numerically measured $\widetilde{\Gamma}$ not only is dependent on the kicking momentum of the focused two solitons, but also depends on the time delay δ to excite them. Considering this fact, for energy transport, we need statistical properties. In the following we will investigate the averaged scattering rate over δ, i.e., $\Gamma \equiv \langle\widetilde{\Gamma}\rangle_\delta$.

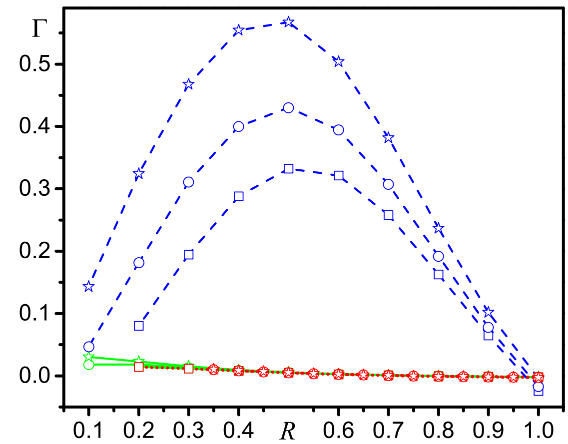

FIG. 3. Averaged scattering rate $\Gamma \equiv \langle\widetilde{\Gamma}\rangle_\delta$ for kink-antikink (blue dashed line), kink-kink (green solid line), and antikink-antikink (red dotted line) collisions vs the ratio of the kicking momentum $R \equiv |\frac{p_a}{p_b}|$. Here $\alpha = 0.0$ (squares), $\alpha = -0.7$ (circles), and $\alpha = -1.4$ (stars).

Figure 3 shows the result of Γ as a function of the ratio $R \equiv |\frac{p_a}{p_b}|$. Here, for convenience, we set $|p_b| = 8$ to explore different types of two-soliton scattering. It is easy to find that for both antikink-antikink and kink-kink collisions, there are no changes of Γ for different R, but this is not the case for the kink-antikink collision; here, with the increase of the absolute value of α, Γ increases remarkably. Since it has always been believed that the scattering behavior of energy carriers or, in other words, the nonlinear excitations will certainly change the heat conduction, the result here seems to suggest that if the collisions of solitons do play roles in heat conduction, only kink-antikink-type scattering plays a major role.

All of the above results are from simulations performed at zero temperature. To further figure out the effects of the kink-antikink collision on heat conduction, we need to estimate the soliton-soliton scattering probability rate at the nonzero finite-temperature equilibrium state, which is still a very challenging issue. Viewing this situation, based on the above results, it is reasonable to assume that a kink (antikink) could be excited at position x_i only when $|p_i| \geqslant |p_c^k|$ ($|p_c^a|$). Then, for the finite-temperature equilibrium state, using the assumption of a Maxwell distribution, one can infer that the probability to present a kink (antikink) soliton is proportional to $\frac{2}{\sqrt{2\pi\kappa_B T}}\int_{p_c^k}^{\infty} e^{-(p^k)^2/2\kappa_B T} dp^k$ ($\frac{2}{\sqrt{2\pi\kappa_B T}}\int_{p_c^a}^{\infty} e^{-(p^a)^2/2\kappa_B T} dp^a$). Here T is the focused temperature and κ_B is the Boltzmann constant. Thus, there is a joint probability to present both kink and antikink solitons, i.e.,

$$P_{ka} = \frac{4}{2\pi\kappa_B T}\int_{p_c^k}^{\infty}\int_{p_c^a}^{\infty} \exp\left(-\frac{(p^k)^2 + (p^a)^2}{2\kappa_B T}\right) dp^k dp^a. \quad (5)$$

Finally, the scattering probability of the kink-antikink collision should certainly be proportional to P_{ka}. Given this understanding, and knowing from Fig. 2(b) that with the increase of α, p_c^k decreases and p_c^a increases, one may expect that P_{ka} will decrease with α. We should note that although the P_{ka}

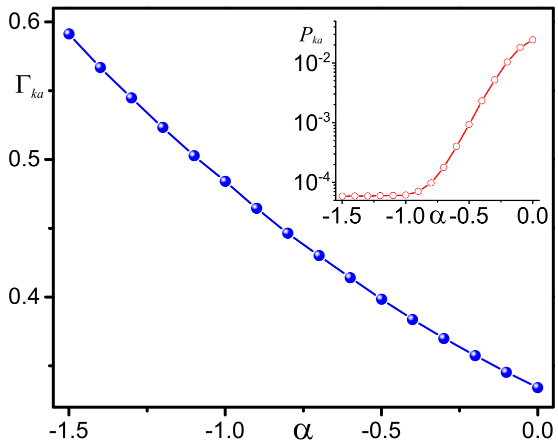

FIG. 4. Scattering rate Γ_{ka} of the kink-antikink solitons collision vs α for $R = 0.5$. The inset shows their scattering probability $P_{ka}(\alpha)$ for $T = 0.3$.

estimated in the above way will be quantitatively different from reality, the qualitative conclusion should be the same, i.e., the scattering probability decreases with the increase of α.

So far, we have clarified that for kink-antikink soliton collisions, with the increase of α, the scattering rate Γ_{ka} increases and the scattering probability P_{ka} decreases. To further address this point, in Fig. 4 we show the results of both Γ_{ka} versus α for $R = 0.5$ and P_{ka} versus α for $T = 0.3$. As can be seen, this is indeed the case. In fact, we have carefully checked that such properties are valid for any T and R. In the following, we attempt to use these properties to understand heat conduction. Our idea is that with the increase of α, the increase of the scattering rate together with the decrease of the scattering probability should naturally lead to a nonmonotonic dependent behavior of heat conduction on α. Thus, in what follows, we try to capture this idea.

IV. HEAT CONDUCTIVITY

To study the heat conduction behavior, one can usually employ the heat current correlation function

$$C(t) = \langle J(0)J(t)\rangle. \quad (6)$$

With this and applying the Green-Kubo formula $\kappa = \lim_{N\to\infty} \int_0^\infty C(t)dt$ [22], one then obtains the heat conductivity κ. Here $J(t) = \sum_{i=1}^N j(t)$, with $j(t) = \frac{dx_i}{dt}\frac{\partial V(r_i)}{\partial r_i}$ the instantaneous heat current at time t. Angular brackets are used to denote the equilibrium thermodynamic average. For finite system size N, one can only derive the finite-time heat conductivity, i.e.,

$$\kappa_\tau = \int_0^\tau C(t)dt, \quad (7)$$

where the integration is cut off by a finite time τ. Therefore, for a FPU-α-β system with finite system size, κ_τ is a function of both α and τ. Thus, to verify the nonmonotonic heat conduction property caused by kink-antikink scattering, our strategy is to calculate κ_τ by fixing τ and varying α. It would also be worthwhile to note that κ_τ measured in this way only reveals the finite-time decay behavior of the heat current correlation, which is naturally related to the dynamics of energy carriers.

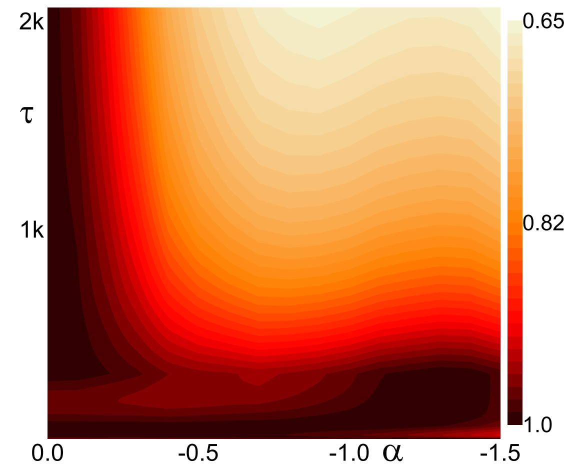

FIG. 5. Counterplot showing the result of $\kappa_\tau^* = \frac{\kappa_\tau}{\kappa_\tau^m}$ versus both α and τ. Here the temperature is fixed at $T = 0.3$ and the system size is $N = 4096$.

In order to easily present the result of $\kappa_\tau(\alpha,\tau)$, we first rescale κ_τ as $\kappa_\tau^* = \frac{\kappa_\tau}{\kappa_\tau^m}$, with κ_τ^m the maximum value of κ_τ for a certain α during the considered time τ. Figure 5 shows the results of κ_τ^* for different τ and α. The results are obtained from a system with a periodic boundary and using the formula (7). The simulation details to obtain the heat current correlation function can be found in many works; see, e.g., [6]. From Fig. 5 one can see that the expected nonmonotonic behavior of κ_τ^* does appear, but only for small τ, and gradually disappears as τ increases. This means that only the early stage of decay of the heat current correlation follows the nonmonotonic behavior. Since in the equilibrium state the early decay of the current is obviously related to the local carrier propagation, this result is consistent with our argument induced from the scattering dynamics of solitons. This is because solitons in a thermalized environment might frequently suffer many types of scattering and eventually decay very rapidly.

V. SUMMARY AND DISCUSSION

In summary, our study here suggests that solitons in the nonlinear FPU-α-β lattice can only have a relatively short survival time and thus they can only affect the heat conduction behavior in a short time. This argument has been supported by the following evidence. There is a momentum threshold to excite the soliton and this threshold strongly depends on the symmetry degree of the interparticle interaction (characterized by α). The scattering dynamics of solitons here is mainly induced by the kink-antikink soliton collision and the scattering rate of this type of collision increases remarkably as α increases. From this property, we proposed a method to qualitatively measure the scattering probability of the kink-antikink soliton collision and thus suggested a nonmonotonic α-dependent property of heat conduction behavior. Fortunately, our simulation results of the heat current correlation function nicely verify this nonmonotonic behavior for a short time. Thus, we may conclude that if the scattering of solitons does play a role in heat conduction in nonlinear lattices, it can only do so at an early time stage.

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