Dynamics of Solitary Wave Scattering in the Fermi-Pasta-Ulam Model

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In this Letter, we study the scattering dynamics of a pair of solitary waves in the Fermi-Pasta-Ulam model with interaction potential $V(x) = \alpha x^2/2 + x^4/4$ and establish a quantitative connection between the scattering property and the energy transport behavior. The energy and momentum conservation laws are obtained and the scattering rates of solitary waves are calculated. Our studies suggest that the anharmonic limit model with $\alpha = 0$ can be taken as a paradigm model for studying lattice solitary waves.

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Solitary waves may occur in a variety of systems[1] such as solids, hydrodynamics, biological molecules, optical systems, etc. Insights into the dynamical and thermodynamical properties of these systems require the detailed knowledge of scattering behaviors of solitary waves. In an integrable system it is clear that solitary waves do not exchange energy when they collide with each other and thus get the name of "soliton". The scattering of solitons are elastic [1,2], even in the dissipative environment[2]. In a nonintegrable system, energy exchange may take place when two solitary waves collide with each other. Different scenarios of solitary wave interaction have been observed in various nonintegrable systems [1,3,4], however, quantitative studies on solitary wave scattering are still insufficient.

Recently, heat conduction behaviors in lattice models have attracted more and more attention[5–9]. It has been found that certain lattices show anomalous heat conduction behavior, i.e., the thermal conductivity κ computed according to the Fourier law of heat conduction $J = -\kappa dT/dx$ behaves as $\kappa \sim N^{\gamma}$, where J is the heat flux and dT/dx is the temperature gradient. The value of the exponent γ is crucial on determining the transport property of the lattices, i.e., $\gamma = 0$ represents normal transport behavior that obeys the Fourier law, while a nonvanishing value of γ indicates anomalous transport behavior and is related to the anomalous diffusion [9]. The value of γ reported in previous researches is different in different models, and even is different for a specific model in different works, e.g., in the Fermi-Pasta-Ulam model it ranges from about 0.37 to 0.45 [5,6,8]. Several groups have worked out in the theoretical frameworks that γ should be constant in momentum conservative systems (i.e., model independent and temperature independent), however, its value is controversial [10]. Thus, what determines γ and whether its value differs in different cases are unclear.

The purpose of this Letter is to establish the conservation laws of momentum and energy that govern the scattering process, and then to calculate the scattering rates of solitary waves that determine the scattering. To show that the quantitative knowledge of solitary waves is of importance in establishing the connections between the dynamical property and the statistical behaviors, we will link the scattering rates and the exponent γ.

The model adopted in our research is the Fermi-Pasta-Ulam model which is given by the Hamiltonian

$$H = \sum_{i}^{N} H_i, \qquad H_i = \frac{p_i^2}{2} + V(x_{i+1} - x_i) \tag{1}$$

with $V(x) = \alpha x^2/2 + x^4/4$. In our investigations, special attention will be focused on the anharmonic limit case of $\alpha = 0$. For convenience, we will call the model in this particular case as the "pure quartic model", and the model with $\alpha = 1$ the "quadratic-quartic model". The excitation and propagation properties of a single solitary wave for both $\alpha = 1$ and $\alpha = 0$ have been studied in Refs. [11–13]. The interaction of solitary waves in the quadratic-quartic model has been studied qualitatively in Ref. [4], and quantitatively in Ref. [6]. In Ref. [6], it has been shown that a big solitary wave may transfer momentum to a small one on average. To our best knowledge, this is the first work on the line of quantitative studies of solitary waves interaction.

To study the collision of solitary waves, we apply a kick $p_1 = c_1$ at $t = 0$ on the first lattice and a kick $p_N = c_N$ at $t = \delta$ on the last lattice to excite two solitary waves under the free boundary condition. The kick $p_1 = c_1$ excites a solitary wave travels towards the right, while the kick $p_N = c_N$ excites a solitary wave travels towards the left. Before the collision, each solitary wave maintains both shape and velocity, as shown in Fig. 1(a) and 1(b). After the collision, both the shape and the velocity of each solitary wave will be changed and an extra wave pocket is excited, as shown in Fig. 1(c) and 1(d). The parameters applied here are $c_1 = 6$, $c_N = 7$, and $\delta = 0$. The scattering process can thus be interpreted as

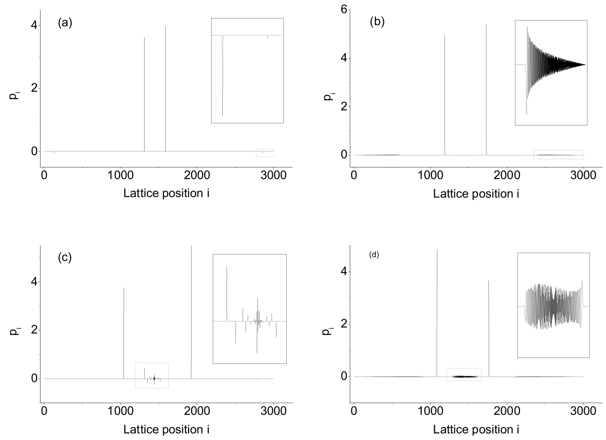

FIG. 1. A pair of solitary waves before collision, (a) and (b), and after collision, (c) and (d), for the pure quartic model and the quadratic-quartic model, respectively. The corresponding insets enlarge the regions indicated by the dotline rectangles.

$$\begin{aligned}&\text{Solitary wave } a + \text{solitary wave } b\\ &\quad\Rightarrow \text{Solitary wave } a' + \text{solitary wave } b'\\ &\qquad + \text{excited waves}\end{aligned} \tag{2}$$

for both models. However, the details are different. The insets in Fig. 1 enlarge the tails of the solitary waves and the excited wave pockets for the two models correspondingly. In the case of the pure quartic model, the tail involves only several small solitary waves, and the excited wave pocket is also composed of small solitary waves, i.e., no linear modes or phonons are excited in this model. In the case of the quadratic-quartic model, on the contrary, both the tail and excited wave pocket appear as a wave pocket of linear waves.

To establish the conservation laws of momentum and energy by imitating free particle collision, we need to endow momentum and energy to a single solitary wave first. Because of the localization, we define

$$P = \sum_{|p_i|>10^{-10}} p_i, \text{(3a)}$$
$$E = \sum_{|p_i|>10^{-10}} H_i \text{(3b)}$$

as the momentum and the energy of a solitary wave, where the sum is performed only over those lattices with significant momentum around the peak. Furthermore, since the excited wave pockets in both models have distinct boundaries, we can thus calculate their total momentum ΔP and total energy ΔE in the same way of calculating P and E. Let P_a, P_b, P'_a, and P'_b, and E_a, E_b, E'_a, and E'_b represent the momentum and the energy of the solitary waves a, b, a', and b', respectively. We can examine numerically that the conservation laws of momentum and energy are kept correctly with errors below 10^{-7}. In other words, the solitary wave scattering is also governed by the conservation laws

$$P_a + P_b = P'_a + P'_b + \Delta P, \text{(4a)}$$
$$E_a + E_b = E'_a + E'_b + \Delta E, \text{(4b)}$$

as in the case of free particles collision. Note that in the free particle case ΔP and ΔE represent the total momentum and energy of the particles, involving photons, excited by the collision.

To solve the equations, one usually needs to know the relationship of P and E, e.g., in the case of a classical free particle, we have $E = P^2/(2m)$, while in the case of a high-energy particle we have $E = c\sqrt{P^2 + m_0c^2}$, where m and m_0 are the mass and the rest mass, respectively, and c is the light velocity. To obtain the similar relationship for a solitary wave, let us first analyze the pure quartic model. This model has a well-defined scaling property: Applying a scaling transformation of $x = \lambda\tilde{x}$ and $t = \tilde{t}/\lambda$ (thus $p = \dot{x} = \lambda^2\tilde{p}$) to the Hamiltonian (1) in the case of $\alpha = 0$ one obtains $H(x(t), p(t)) = \lambda^4\tilde{H}(\tilde{x}(t), \tilde{p}(\tilde{t}))$, where λ is a scaling constant. As a result of the scaling property the equations of motion of the systems with H and $\tilde{H}$ are identical, and two solitary waves related by a scaling transformation are dynamically indistinguishable. Under the scaling transformation, a solitary wave with P and E in the system H is transformed to a solitary wave with $\tilde{P}$ and $\tilde{E}$ in the system $\tilde{H}$, and it has $P = \lambda^2\tilde{P}$ and $E = \lambda^4\tilde{E}$. Therefore, to keep the relationship function of E and P unchanged under the scaling transformation, P and E must be related by $E = a_1P^2$. Similar discussions can be applied to obtain the relationships among the momentum P, the velocity v, and the amplitude h of x_i of a solitary wave, which gives $P = a_2v^2$ and $v = a_3h$ correspondingly. To determine the constant a_1, a_2, and a_3 one has to employ numerical simulations. In Fig. 2(a) and 2(b) we plot E against P and P against v in log-log scale, respectively. The best fit gives $E = 0.48877P^2$ and $P = \sqrt{3}v^2$. Similarly, we can obtain $v = h/\sqrt{3}$ numerically, which consists to the result reported in Ref. [13] qualitatively.

The corresponding relationship functions for the quadratic-quartic model are more complex and need to be determined numerically. In Fig. 2(a) and 2(b) we also show the corresponding relationship curves for the quadratic-quartic model, where one can realize that the relationship functions approach those of the pure quartic model only when $|P| \to \infty$. The relationship function of E and P in the quadratic-quartic model can be also obtained by using the best fit, which gives $E = 0.487P^2 - 0.134P - 0.358$.

Though the conservation laws are the same, the solutions for free particles and solitary waves may be different qualitatively. For elastic scattering with ΔP, $\Delta E = 0$, $P'_a = P_a$, and $P'_b = P_b$ is a trivial set of solution for free particles, while it is a practical set of solution for solitary waves as solitary waves can pass through each other.

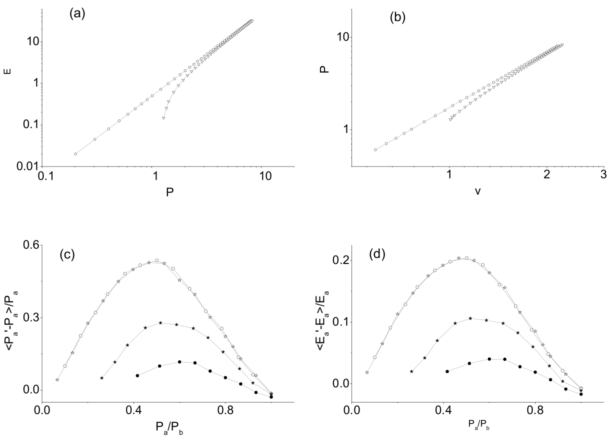

FIG. 2. (a) shows the log-log plot of $E - P$ and (b) shows the log-log plot of $P - v$ for a single solitary wave (open dots for the pure quartic model and up triangles for the quadratic-quartic model). (c) plots the average scattering rate of the momentum and (d) plots that of the energy of the solitary wave a against $\frac{P_a}{P_b}$ for the pure quartic model (open dots for $P_b = 3.034$ and open stars for $P_b = 7.08$) and the quadratic-quartic model (solid dots for $P_b = 3.277$ and solid stars for $P_b = 7.288$).

Another set of elastic scattering solution is $P'_a = P_b$ and $P'_b = P_a$ for both models. This set of solution is just the elastic collision solution of free particles with equal mass, but we do not know whether it is also a practical solution in the solitary wave case.

In the case of nonelastic scattering with nonvanishing ΔP and ΔE, it is difficult to obtain exact solutions for both free particles and solitary waves. In this situation, the scattering rates of momentum and energy of solitary waves (or free particles) should be the most important parameters to describe the scattering behavior. Thus we next calculate the scattering rates of a pair of solitary waves. It has shown in Ref. [6] that the scattering of solitary waves depends not only on the initial momentum P_a and P_b, but also on the time delay δ. It can be easily found that this property originates from the discrete nature of lattices. For practical application, however, statistical properties have more significance than the prompt values. Thus we average Eq. (4) against δ and investigate the average scattering rates of the momentum and energy, $\frac{<P'_a - P_a>}{P_a}$, $\frac{<P'_b - P_b>}{P_b}$, $\frac{<E'_a - E_a>}{E_a}$, $\frac{<E'_b - E_b>}{E_a}$, as well as the rates of the momentum and energy "loss", $\frac{<\Delta P>}{(P_a + P_b)}$, $\frac{<\Delta E>}{E_a + E_b}$. In general, these quantities are functions of P_a and P_b. However, in the case of the pure quartic model we find that they are universal functions of ratio $\frac{P_a}{P_b}$ only. In Fig. 2(c) and 2(d), we demonstrate $\frac{<P'_a - P_a>}{P_a}$ and $\frac{<E'_a - E_a>}{E_a}$ against $\frac{P_a}{P_b}$ as examples. Without loss of generality, in our calculations we fix P_b and vary P_a under the restriction of $P_a \leq P_b$. The open dots in the plots are the results obtained by fixing $P_b = 3.034$ (excited by $c_N = 3$), while the open stars are obtained by fixing $P_b = 7.08$ (excited by $c_N = 7$). It is clear that the two curves in each plot collapse into a universal curve, which means that two pairs of solitary waves with the same ratio $\frac{P_a}{P_b}$ have the same scattering rates. This effect can be easily understood by relating it to the scaling property of the model. If two pairs of solitary waves with (P_a, P_b) and $(\tilde{P}_a, \tilde{P}_b)$ satisfy $\frac{P_a}{P_b} = \frac{\tilde{P}_a}{\tilde{P}_b}$ then one can apply a scaling transformation to one pair to obtain the other pair, and the two pairs must have the same scattering rates since their equations of motion are identical. In the case of the quadratic-quartic model, on the other hand, the corresponding scattering curves obtained by fixing $P_b = 3.277$ (excited by $c_N = 3$) and those obtained by fixing $P_b = 7.288$ (excited by $c_N = 7$) are separated, see Fig. 2(c) and 2(d). The results in the figure show that the corresponding scattering rates of the model for a fixed ratio $\frac{P_a}{P_b}$ will increase with the increase of P_b, and one can deduce accordingly that when $P_b \rightarrow \infty$ the scattering rates will approach those of the pure quartic model.

The scattering rates of solitary waves must be closely related to the transport behavior of systems in which solitary waves are the dominant excitations. In molecular dynamics simulations, the temperature at position i is defined as $T_i = <p_i^2>/2$ and the role of a thermostat can be interpreted as a series of kicks on the ends of the lattice chain. The distribution of the solitary waves excited at a thermostat is then determined by the temperature of the thermostat. Let T_+ and T_- represent the temperature of the high-temperature and low-temperature thermostats, respectively. For the sake of simplicity, assume roughly the momenta of the solitary waves excited at T_+ are P_b and at T_- are P_a, respectively. Then $\frac{P_a}{P_b}$ is determined by $\frac{T_-}{T_+}$ since $T \sim P^2$. In the case of soliton scattering, the scattering rates vanish and the heat flux J is size independent, which leads to $\kappa \sim JN/(T_+ - T_-) \sim N^\gamma$ with $\gamma = 1$. In the case of nonelastic scattering, the heat flux will decrease with the increase of the system size N because of the scattering effect, and it is reasonable to suppose that the larger the scattering rates are, the faster J decreases. In other words, the exponent γ should decrease with the increase of the scattering rates. If this is the case, one can predict that γ should keep as a constant in the pure quartic model for arbitrary temperature when $\frac{T_-}{T_+}$ is fixed. The reason is that for fixed $\frac{T_-}{T_+}$, the ratio $\frac{P_a}{P_b}$ is fixed, and for fixed $\frac{P_a}{P_b}$ the scattering rates are identical as has been illustrated in Fig. 2. In the quadratic-quartic model, with the same condition of fixed $\frac{T_-}{T_+}$ and thus fixed $\frac{P_a}{P_b}$, one can deduce that γ must decrease with the increase of the temperature since Fig. 2 reveals that the scattering rates will increase with the increase of P_b. Moreover, since the scattering rates of the quadratic-quartic model tend to approach those of the pure quartic model when $P_b \rightarrow \infty$, one can also predict that the value of γ of the former will approach

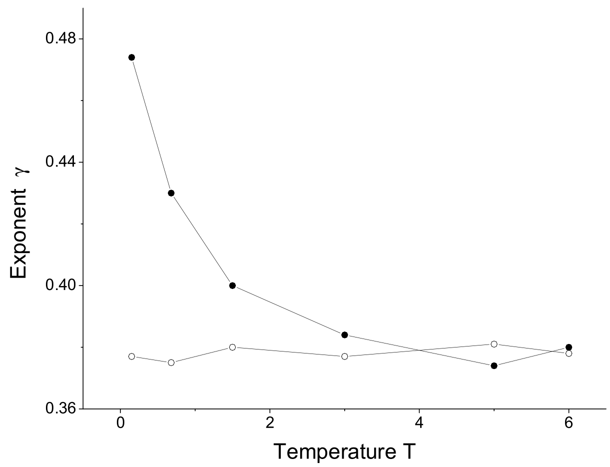

FIG. 3. The exponent γ of the thermal conductivity against the temperature T for the pure quartic model (open dots) and the quadratic-quartic model (solid dots).

that of the latter in the high-temperature limit. To test these ideas, we have studied the heat conduction of the two models using the common method introduced in previous works [5,6] to capture the exponent γ of the thermal conductivity. In our calculations we fix $\frac{T_-}{T_+} = \frac{2}{3}$ and limit N to $N > 400$ to avoid the boundary jump effect [8]. In Fig. 3, we plot γ against the average temperature $T = (T_+ - T_-)/2$ in an interval $(0.01, 6)$. One can find that γ keeps almost as a constant around $\gamma \sim 0.38$ for the pure quartic model, while it decreases with the increase of T and approaches 0.38 when T is high enough in the quadratic-quartic model. These results support our guess and confirm that γ is determined by the scattering rates of solitary waves, and explain why in the previous research of the quadratic-quartic model the smallest value of γ (~ 0.37) was observed in the high-temperature limit of $T_+ = 152$ and $T_- = 24$ [5] and the relatively big values of γ were obtained in the temperature region of $T < 1$ [6].

In summary, the scattering of solitary waves and free particles obeys the same forms of conservation laws of momentum and energy, and therefore the scattering problem of solitary waves can be treated by imitating free particles. The scattering rates of a pair of solitary waves are functions of the initial momenta of the two solitary waves in general, but they are merely determined by the ratio of the initial momenta in the anharmonic limit. It is shown that the exponent γ of the thermal conductivity of lattices depends on the scattering rates of solitary waves. Since the scattering rates are generally model dependent and temperature dependent, γ should be model dependent and temperature dependent as well, which explains the results reported in previous works regarding the value of γ. Though it is widely believed that solitary waves play an important role in determining the energy transport properties of the anharmonic systems, we emphasize that the connection between the scattering rates and the exponent γ established in this Letter is the first direct evidence supporting such a view.

The pure quartic model can be taken as a paradigm model for studying solitary wave dynamics. Because of the scaling property, the dynamics of the system is relatively simple and certain results can be obtained in the theoretical framework. Furthermore, due to the absence of phonons, the observed effects in this system can be assigned to solitary waves unambiguously.

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