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Rapid Communications

Delocalization of phonons and energy spectrum in disordered nonlinear systems

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We study phonon delocalization in disordered media in the presence of nonlinearity. By considering the Fermi-Pasta-Ulam β-model, we show that regardless of whether the initial state of the linear system is localized or not, the final state will be an extended mode after turning on the nonlinear term. We report on the results of an extensive dynamical simulation of a disordered nonlinear system, which show that, independent of the initial mode frequency, in the final state the energy spectrum is excited according to the Kolmogorov spectrum $E(\omega) \sim \omega^{-5/3}$. Finally, we show that disorder will not cause delocalization of intrinsic localized modes.

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Introduction. According to Bloch's theorem, eigenstates or modes of a pure periodic system are extended [1]. In general, disorder induces *wave localization*, therefore degrading the transport properties of a medium, an effect which is largely pronounced in lower dimensions. The propagation of waves in heterogeneous materials [2] has been studied for several decades [3]. Many rigorous results have been derived. For example, it has been shown rigorously that in one-dimensional disordered media with diagonal disorder and short-range correlations, even infinitesimally small disorder is sufficient to localize the wave function, irrespective of the energy [4–6]. In that case, the envelope of the wave function $\psi(r)$ decays exponentially at large distances r from the domain's center, i.e., $\psi(r) \sim \exp\{-\frac{r}{\xi(E)}\}$, with $\xi(E)$ being the localization length at energy level E. The known exact results are limited mostly to low-dimensional and linear media [7–16]. Under the assumption of long-range correlated off-diagonal disorder, it was shown that localized states in a linear one-dimensional (1D) system can become delocalized [17]. In this Rapid Communication, we study the dynamics of elastic waves (phonons) in a disordered medium and in the presence of nonlinearity. We investigate whether the nonlinearity enhances the localization or extends the localized modes, and finally present the energy spectrum in these systems.

Model and methods. To study the propagation of phonon waves in a disordered medium in the presence of a nonlinear effect, we consider the one-dimensional Fermi-Pasta-Ulam (FPU) β-model [18]. The system consists of spring-coupled masses, where the value of the masses at each site fluctuates around a positive mean, and the springs have cubic nonlinearity. The equation of motion for the amplitude x_n of the nth mass is given by

$$m_n\ddot{x}_n = -\alpha_n(2x_n - x_{n+1} - x_{n-1}) - \beta_n(x_n - x_{n+1})^3 - \beta_n(x_n - x_{n-1})^3, \qquad (1)$$

where the linear coupling coefficients for the nth site are denoted by α_n (we set them to be constant) and the magnitude of cubic nonlinearity is represented by β_n. We assume the mass to be a random variable taken from a uniform distribution (see below). At first, let us study the linear system by considering the case $\beta_n = 0$. In this case, using the transfer matrix (TM) method, we estimate the localization length of the phonon waves [11–16]. The localization length of each vibrational mode is taken as the inverse of the Lyapunov exponent γ defined by

$$\gamma = \lim_{N\to\infty}\left\langle \frac{1}{N}\log\frac{|Q_N\, c(0)|}{|c(0)|}\right\rangle, \qquad (2)$$

where $c(0) = \binom{x_1}{x_0}$ is a generic initial amplitude of the first two sites, and N is the length of the chain. We set $x_0 = x_1 = 1/\sqrt{2}$. The sign $\langle\cdots\rangle$ denotes an ensemble average over different realizations of masses. Here, $Q_N = \prod_{n=1}^{N} T_n$, and the transfer matrix T_n is given by $T_n = \begin{pmatrix} 2-m_n\omega^2a^2 & -1 \\ 1 & 0 \end{pmatrix}$, where a is the lattice constant (here, $\alpha_n = 1/a^2$). In Fig. 1, the localization length $\xi(\omega)$ is depicted as a function of frequency ω for a lattice with size $N = 10^5$ sites, where we set $a = 1$. The masses are taken from a uniform distribution $[\bar{m} - W, \bar{m} + W]$, in which $\bar{m}$ and W are 2 and 0.9, respectively. The plot is derived by ensemble averaging over 100 realizations of the disorder. According to Fig. 1, for this system one finds localized and extended regions, separated by a "mobility edge" at $\omega_c \simeq 0.15$ for this lattice size [the criterion being $\xi(\omega_c) \simeq N$].

Next, we study the effect of nonlinearity on localized and extended modes using a dynamical method [11–16,19]. We consider the transmission of two modes, one from the localized region ($\omega = 1$) and the other from the extended

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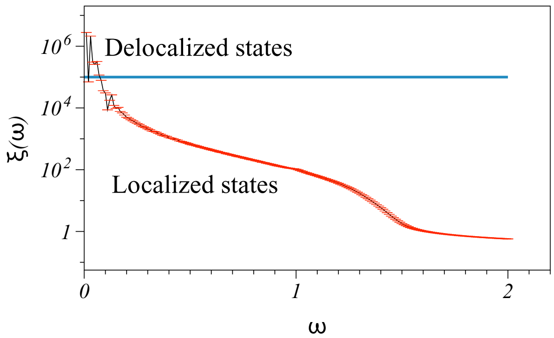

FIG. 1. The localization length as a function of frequency ω for a lattice with $N = 10^5$ sites. There are localized and extended regions, separated by a "mobility edge" at $\omega_c \simeq 0.15$. The masses are taken from a uniform distribution $[\bar{m} - W, \bar{m} + W]$, in which $\bar{m}$ and W are 2 and 0.9, respectively.

region ($\omega = 0.1$). Using the dynamical method, we find that both localized and extended modes become "extended" when the nonlinear term is added. In this case, a system of spring-coupled masses with a length of 500 is considered. We note that the angular frequencies $\omega = 1$ and $\omega = 0.1$ are also localized and extended modes, respectively, for length $N = 500$. Similar to the linear case in Fig. 1, masses are taken from a uniform distribution $[\bar{m} - W, \bar{m} + W]$, in which $\bar{m} = 2$ and $W = 0.9$. We solve the dynamical equation using a fourth-order Runge-Kutta method with a time step $dt = 0.01$, and consider the following boundary conditions at the two ends: $x_1(t) = A\sin(\omega t)$ and $x_{n+1} = x_n$. This means that the first site is subjected to a sinusoidal function with frequency ω and with amplitude $A = 1$ and the last site is free (open). This type of boundary condition in the last site prevents reflections from the boundary.

We have chosen the values of the nonlinearity coupling β_n to be constant and considered $\beta_n = 0.001$, 1, and 10. In Figs. 2–4, we plot the time variations of the wave amplitude at different distances from the source for frequency $\omega = 1$, where the linear system was initially strongly localized. As shown in these figures, for $\beta_n = 1$ and 10, at long timescales, the wave amplitudes at distances $n = 1$, 300, and 500 increase and become delocalized due to the presence of large nonlinearity. However, as depicted in Fig. 2(a), the nonlinearity with coupling $\beta = 0.001$ is not able to propagate and its amplitude decreases as the distance from the origin gets larger. The positional dependence of amplitude for the sine wave subjected to frequency 1 at the origin is plotted also in Fig. 2(b) and shows localization for the coupling $\beta = 0.001$.

As shown in Figs. 3 and 4, for high values of nonlinear coupling β, low-frequency modes are activated in the system (see below, and Fig. 5). Here, nonlinearity has enhanced the exchange of energy between modes since we keep injecting energy into the system and increase the relative importance of anharmonicity to harmonic frequencies. It should be noted that the unexpected result originally obtained by FPU was due to nonresonant frequencies in the 1D harmonic system and insufficient nonlinearity or energy present in the system, as well as a short simulation time and system length. Later studies have shown that equipartition can be reached if enough energy, or equivalently, enough anharmonicity, is

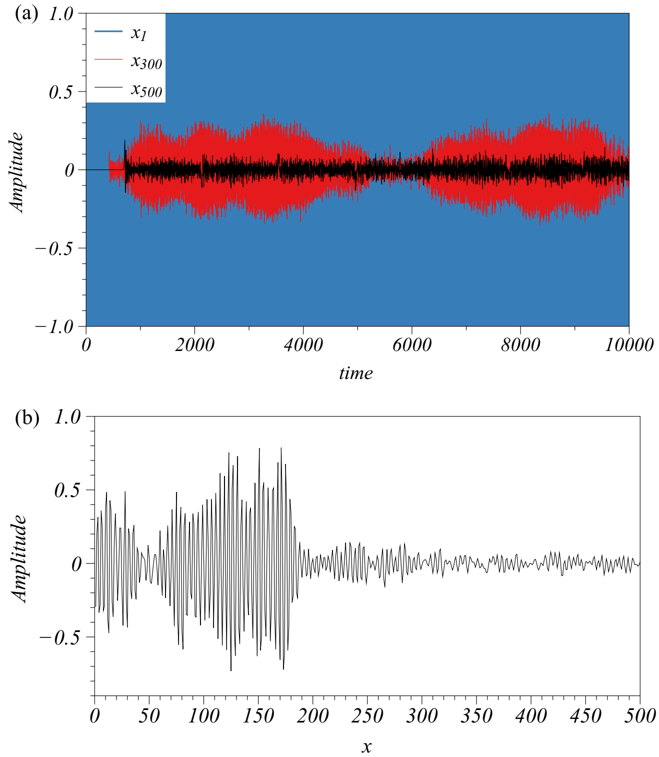

FIG. 2. (a) Amplitude change of sine wave at distances $n = 1$, 300, and 500, vs time, and in the presence of both disorder and nonlinearity ($\beta = 0.001$). The initial sine wave has frequency 1 (a localized mode in the linear system) imposed directly at the first site. Note that amplitudes decay from 1 as one gets further from the site 1. (b) Positional dependence of the vibrational amplitudes for the exciting sine wave of frequency 1. Nonlinearity with coupling $\beta = 0.001$ is not able to delocalize this localized mode.

present in the system, and the simulation is run for long enough times [20,21] and long enough systems [22]. If the system is excited with a frequency in the delocalized region of the harmonic spectrum, for instance, $\omega = 0.1$, we find similar results, namely, large amplitudes far from the source point, a signature of delocalized states, and excitation of lower-frequency modes. These forms are reminiscent of solitons proposed by Zabusky and Kruskal [23–26]. As we will later point out, however, the addition of nonlinearity will

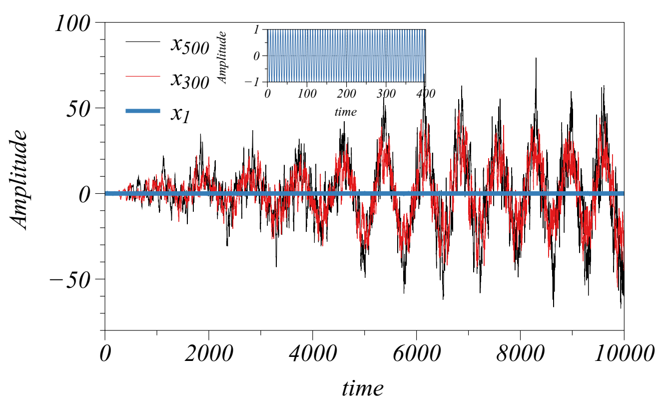

FIG. 3. Same as Fig. 2(a), but for $\beta = 1$.

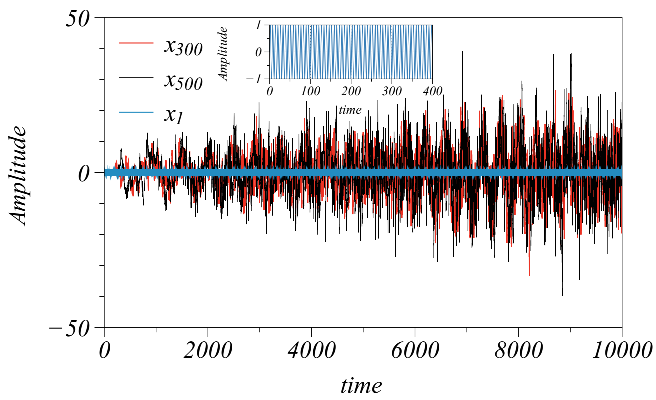

FIG. 4. Same as Fig. 2(a), but for $\beta = 10$.

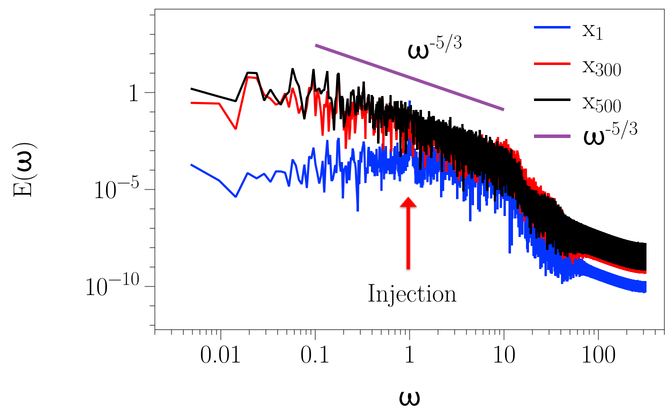

FIG. 6. Log-log plot of the Fourier transforms of energy $E_n(t)$ at different distances from the source in the presence of disorder and nonlinearity ($\beta = 10$), for frequency $\omega = 1$. The blue, red, and black are for sites $n = 1$, $n = 300$, and $n = 500$, respectively. Regardless of the initial excitation frequency, the energy is distributed between different modes in a power law, extended over about two decades in ω with exponent $\simeq -5/3$, i.e., the Kolmogorov exponent. The energy is injected with frequency $\omega = 1$ and the system shows cascades of energy to high- and low-frequency modes.

also create localized excitations known as intrinsic localized modes or ILMs even in the absence of disorder.

To look at the energy distribution among modes, we study the amplitude spectrum of long-time states of the *disordered* nonlinear Fermi-Pasta-Ulam system. To this end, we calculate the spectral density $|\psi_n(\omega)|^2$, where $\psi_n(\omega)$ is the Fourier transform of $x_n(t)$ at distance n measured from the source. In Fig. 5, the spectrum of incident waves with $\omega = 1$ and $\omega = 0.1$ as well as the spectrum of amplitudes at distances $n = 300$ and 500 are displayed. The nonlinear coefficient is fixed to $\beta_n = 10$ for all simulations. It turns out that for high values of nonlinear coupling β, small-frequency modes below the excitation frequency are activated in the system, and are robust with respect to ensemble averaging over different realizations of disorder. A peak slightly above $\omega \simeq 0.01$ can be observed corresponding to the quasiperiods in Fig. 4 which we attribute to the excitation of soliton modes.

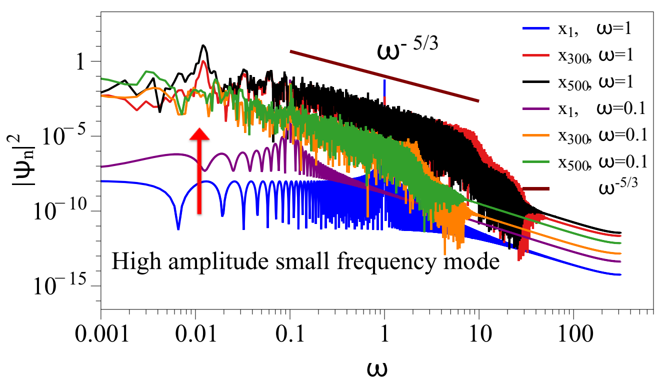

FIG. 5. Log-log plot of the Fourier transforms of a sine wave with initial frequencies 0.1 (purple) and 1 (blue) at different distances from the source in the presence of disorder and nonlinearity ($\beta = 10$). The blue, red, and black curves are for $\omega = 1$ at sites $n = 1$, $n = 300$, and $n = 500$, respectively. The spectra in purple, green, and orange colors are for $\omega = 0.1$ at sites $n = 1$, $n = 300$, and $n = 500$, respectively. Independent of initial frequency, the amplitude power is distributed between different modes in a power law, extended over about two decades in ω with exponent $\simeq -5/3$, i.e., the Kolmogorov exponent. The masses are taken from a uniform distribution with mean $\bar{m} = 2$ and fluctuation amplitude $W = 0.9$.

Next, we ask whether or not the final steady state is a thermalized state. As we said, original studies of the FPU problem did not show thermalization until the initial input energy was large enough and simulations were run for long enough times. We now study the energy spectrum of long-time states of a *disordered* nonlinear Fermi-Pasta-Ulam system. To address this question, we calculate the energy spectral density $E_n(\omega)$, which is the Fourier transform of energy $E_n(t)$ at time t on site n measured from the source. This energy is given by

$$E_n(t) = \frac{1}{2}m_n\dot{x}_n^2 + \frac{\alpha}{4}[(x_n - x_{n-1})^2 + (x_{n+1} - x_n)^2] + \frac{\beta}{8}[(x_n - x_{n-1})^4 + (x_{n+1} - x_n)^4].$$

In Fig. 6, the energy spectrum at distances $n = 1$, 300, and 500 are displayed as a function of ω. The nonlinear coefficient is fixed to $\beta_n = 10$ for all simulations. Instead of obtaining thermalization, where $E_n(\omega)$ would become constant, we find that irrespective of the initial frequency, the energy of the modes is distributed in a power law extended over about two decades with exponent $\simeq -5/3$, i.e., Kolmogorov exponent obtained in the case of fully developed turbulence [27]. For instance, for an initial localized mode with $\omega = 1$, turning on the nonlinearity causes energy exchange between different modes and there is an energy transfer to small and large frequency modes as shown in Fig. 6. It is interesting that the aforementioned activated small-frequency modes are absent in the energy spectrum, which means that they have almost the same power as the neighbor frequencies. The numerical observation of power-law behavior of an energy spectrum with a Kolmogorov exponent is the main result of this Rapid Communication. We must emphasize that, in contrast to molecular dynamics simulations of a FPU system with periodic boundary conditions sampled from a microcanonical or canonical ensemble, our results have been obtained for an *open system*

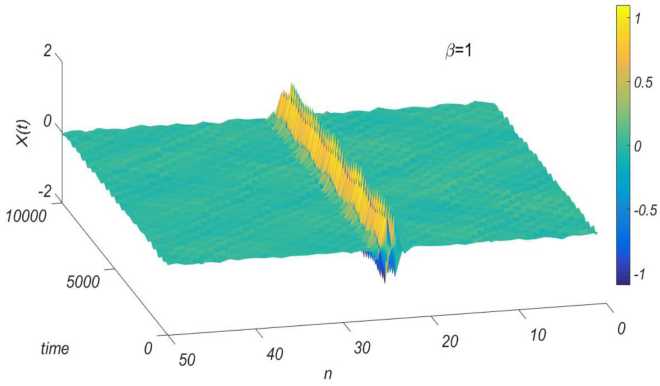

FIG. 7. Dynamics of an intrinsic localized mode in the disordered Fermi-Pasta-Ulam β-model. The masses are taken from a uniform distribution with mean $\bar{m} = 2$ and fluctuation amplitude $W = 0.9$. The mode remains localized around the center $n = 25$. The nonlinearity coupling β_n is set to unity.

which does not have a state of thermal equilibrium. Our result shows the spectral spreading of the energy spectrum under injection of energy at a single frequency ω and the presence of an energy cascade to high- and low-frequency modes.

Finally, we are interested in the behavior of intrinsic localized modes (ILMs) which are excitations of a nonlinear ordered lattice. This is in contrast to localized modes of a linear but disordered lattice. We showed that the latter become delocalized as the springs become nonlinear. To find out the fate of ILMs in the presence of disorder, we next consider a lattice with N sites with periodic boundary conditions. We start the dynamical simulation with the initial condition corresponding to an ILM at site $j_c = N/2$ where the amplitudes are given by $x_j(0) = (-1)^j \operatorname{sech}[k(j - j_c)]$ with $k = 1$. We consider randomness in the mass according to the previously mentioned distribution. The result of the dynamical simulations of the ILM state in a disordered medium is shown in Fig. 7. As can be seen in this figure, this mode remains stable and will not propagate. It will instead oscillate around the center, implying that mass disorder will not cause delocalization of ILMs.

Conclusions. We studied the interplay between nonlinearity and disorder in the context of wave transmission through a discrete periodic structure under nonequilibrium conditions. We found that the nonlinearity led to the delocalization phenomenon, by which enhanced wave transmission occurs within the localized region of the spectrum of a linear system when the value of coupling β exceeds a certain threshold (here, $\beta \gtrapprox 0.001$). By investigating the energy spectral density in the presence of nonlinearity, it was found that energy spreads to both low- and high-frequency modes regardless of the initial spectral content. Most interestingly, similar to the results in turbulence, the energy spectrum showed the Kolmogorov $\omega^{-5/3}$ distribution. Finally, it was observed that disorder had no effect on the stability of ILMs.

We believe that our results are relevant to a deeper understanding of thermal transport in quasi-one-dimensional systems. Examples are the localization-delocalization of phonons in nanowires displaying a diffusive to ballistic transition as their length is decreased [28–35]. Localization can reduce the contribution of diffusive modes and disorder can convert some of the ballistically propagating modes to diffusive ones, thereby strongly reducing the thermal conductance of a nanowire. Another example is the effect of roughness on the thermal conductivity of nanowires. It would be interesting to map the physics of nanowires with rough boundaries in a low Knudsen number (high Reynolds number) to the problem of nonlinear fluctuating hydrodynamics for anharmonic chains with disorder [36]. In addition, our numerically obtained Kolmogorov exponent provides hints for a possible connection of hydrodynamics for anharmonic chains to the recent phonon hydrodynamics models such as those proposed to describe materials such as graphene [37–39].

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