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Phonon scattering by localized equilibria of nonlinear nearest-neighbor chains

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We study scattering of phonons by localized equilibria, for example, localized defects on nonlinear chains. We show that *perfect* transmission occurs at $k=0$ at the threshold for creation of localized modes and there exists a characteristic transition involving perfect transmission of long-wavelength phonons near the threshold. The theory is illustrated for the stationary case of a discrete kink on a translationally invariant Hamiltonian nearest neighbor chain, which is then generalized to any symmetric localized defects. The implications for discrete breathers are also discussed. [S1063-651X(97)50811-7]

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Recently, there has been an upsurge of research activities on localized dynamics on nonlinear lattices, in particular, for a class of spatially discrete, nonintegrable, translationally invariant systems on lattices [1]. It has been shown that in suitable circumstances they have spatially localized time-periodic solutions, known as ''discrete breathers (DB)'' [2], the discrete analogue of breathers in continuous systems.

Recently it was numerically found [3] that some of the Floquet modes of the linearized problem about a discrete breather are also spatially localized, which are *localized modes on localized modes* (LMs). The spectral study of the LMs and their creation thresholds provides a systematic way to study some important aspects of DB dynamics such as quasi-periodiclike dynamics after finite energy perturbations to a DB [4,5], and the pinning mode and movability of a DB [6], etc.

In this Rapid Communication, we study consequences of LMs for the scattering of phonons by *discrete* localized objects by focusing on a simpler problem of a stationary defect and discussing its implications for DB scattering. We show that the existence of the thresholds for creation of LMs is manifested in the phonon scattering with localized objects as a *perfect* transmission at $k=0$ at the LM thresholds and a dramatic change from a ''reflecting'' state to a perfectly transmitting state for long-wavelength phonons as the threshold is crossed. The DB-phonon scattering has been previously studied numerically to yield strong wave-vector dependence [4] and the existence of perfect transmission [7], which together with our results provides strong implications for heat flux in long molecules, for example, a mechanism for energy trapping between two localized objects or prevention of the heat flux penetration into certain areas of the chain [4,8]. The theory is illustrated with numerics for localized equilibria on a translationally invariant nearest neighbor chain with a (discrete) kink in the uncoupled limit, where properties of LMs and their consequences for scattering can be perturbatively analyzed for a wide range of potentials with the help of a natural tuning parameter. However, it can be naturally extended to any localized objects that are symmetric under spatial reflection and a DB with time-periodic dynamics by considering truncation of Fourier modes.

Consider a Hamiltonian for the translationally invariant, discrete Klein-Gordon chain with one degree-of-freedom per site and nearest neighbor coupling

$$H(x)=\sum_n \left[\frac{1}{2}\dot{x}_n^2+V(x_n)+\varepsilon u(x_{n+1}-x_n)\right], \qquad (1)$$

where V has at least two nondegenerate local minima, x_*, with $V''(x_*)=\omega_0^2>0$, and $u'(0)=1, u''(0)=1$. For example, we take $u(x)=\frac{1}{2}x^2$ and study either the ϕ^4 Klein-Gordon model with the double well potential, $V(x)=x^4/4-x^2/2$, with minima at $x_*=\pm 1$, or the sine-Gordon model with the cosine potential, $V(x)=1-\cos(x)$, with minima $x_*=2\pi n$, where n is an integer.

We start with a stationary solution of

$$\ddot{x}_n+V'(x_n)=\varepsilon[x_{n+1}-2x_n+x_{n-1}], \qquad (2)$$

which is translation invariant except for a localized defect, for example, a *(discrete) kink* defined in the uncoupled limit ($\varepsilon=0$) by $x_n=-1 (n\leqslant 0), x_n=+1 (n\geqslant 1)$ for the double well potential and $x_n=2\pi n (n\leqslant 0), x_n=2\pi(n+1) (n\geqslant 1)$ for the cosine potential. By the implicit function theorem, such an equilibrium has a unique continuation $x(\varepsilon)$ for small ε, called a *localized equilibrium (LE)*, which is exponentially localized in space.

The linearized equation around the LE is given by

$$\ddot{\xi}=-L\xi, \quad (L\xi)_n=A_n\xi_n-\varepsilon(\xi_{n+1}-2\xi_n+\xi_{n-1}), \qquad (3)$$

where $A_n=V''(x_n)$ is time independent. Among eigenmodes of L we are interested in localized modes of the form $\xi_n=\lambda^n e^{i\omega t}$ ($|\lambda|<1$) with a frequency ω and a decay exponent λ satisfying

$$\omega_0^2-\omega^2=\varepsilon(\lambda-2+1/\lambda). \qquad (4)$$

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The frequency of the LM, which lies outside the phonon band, is determined by a matching condition for a bounded solution.

In the case of the kink, perturbative calculations for equilibria for small ε show that x_0 and x_1 move by $O(\varepsilon)$ and the rest by at most $O(\varepsilon^2)$ with an exponential decay as $|n|\to\infty$. Therefore, the simplest LM is given by an *idealized kink*, a first order approximation of the kink without exponential tails; $A_n=\omega_0^2(n\neq 0,1)$, and $A_1=A_0=\omega_0^2-K\varepsilon$, where $K>0$ is called the *detuning parameter*. The frequencies and decay exponents for the symmetric and asymmetric modes are given by [9]

$$\omega_S^2=\omega_0^2-\frac{K^2}{1+K}\varepsilon, \quad \lambda_S=\frac{1}{K+1}, \tag{5}$$

$$\omega_A^2=\omega_0^2-\frac{(K-2)^2}{K-1}\varepsilon, \quad \lambda_A=\frac{1}{K-1}.$$

For localization, $|\lambda_{S,A}|<1$, which gives two thresholds for creation of LMs out of the bottom edge of the phonon band; $K=0$ for the symmetric LM and $K=2$ for the antisymmetric LM. Therefore, if $0\leqslant K\leqslant 2$, there is a symmetric LM and no antisymmetric LM. For $K>2$, there exists both a symmetric LM and an antisymmetric LM. Similarly for $K<0$, we get LMs emerging from the top edge of the phonon band.

For a kink for the double well potential, $K\sim 6+O(\varepsilon)$, and, therefore, both a symmetric and an antisymmetric LM exist in the uncoupled limit. These LMs persist under continuation for the full problem since the correction to the spectrum is at most $O(\varepsilon^2)$, which is confirmed by numerical continuation of the spectrum of L in ε. In the case of the cosine potential, however, $V'''=0$ at the potential minima and $K\sim 2\pi^2\varepsilon$, and, therefore, for small ε only a symmetric LM exists, which also persists for the full problem. The fact that $K\sim\varepsilon$ for the cosine potential allows a natural control of the detuning parameter by tuning the coupling strength ε. Numerical calculations of the spectrum for the cosine potential chain with 64 sites in fact shows that an antisymmetric LM is created at a critical value of $\varepsilon\approx 0.26-0.27$, far away from the perturbative regime.

The existence of creation thresholds for LMs leads to significant consequences for scattering properties of phonons. Consider a scattering setup with a phonon incident on a stationary localized object. Suppose that asymptotic solutions at either end of the chain are of the form

$$\xi_n\sim_{n\to-\infty}e^{ikn}+re^{-ikn}, \quad \xi_n\sim_{n\to\infty}te^{ikn}, \tag{6}$$

where t and r are transmission and reflection amplitudes, respectively. Then after some algebra with transfer matrices [10], we get

$$\mathcal{T}=|t|^2=4\ \sin^2 k/D(k), \tag{7}$$

where

$$D(k)=[(\mathcal{M}_{11}-\mathcal{M}_{22})\cos k+\mathcal{M}_{12}-\mathcal{M}_{21}]^2 + (\mathcal{M}_{11}+\mathcal{M}_{22})^2\sin^2 k. \tag{8}$$

Here $\mathcal{M}_{i,j}$, $i,j=1,2$ are matrix elements of

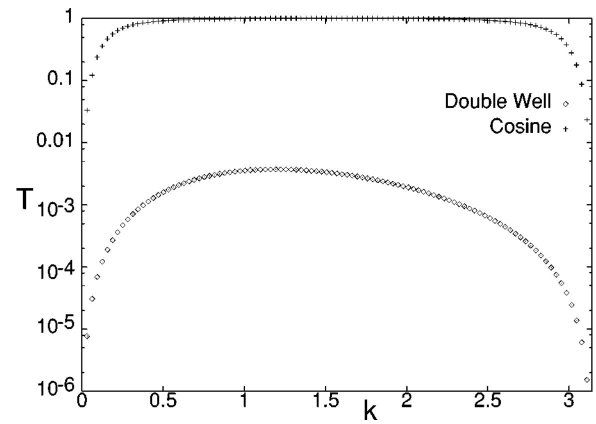

FIG. 1. Transmission coefficient as a function of k for a kink for the double well potential and the cosine potential with $\varepsilon=0.01$.

$$\mathcal{M}=\prod_{\infty}^{\infty}\mathcal{M}_n, \quad \mathcal{M}_n=\begin{bmatrix}0 & 1\\ -1 & E_n\end{bmatrix}, \tag{9}$$

where $E_n=(A_n-\omega^2)/\varepsilon=2\cos k-K_n$ and detuning parameters $K_n=(\omega_0^2-A_n)/\varepsilon$. Note that unless $D=0$, $\mathcal{T}$ vanishes quadratically in k in the limit $k\to 0,\pi$, as in the case of one static diagonal defect [11]. The numerical implementation of our scheme for a finite chain involves only determination of the LE by Newton-Raphson method and repeated matrix multiplications that can be performed very fast and efficiently.

As the simplest example, consider scattering of phonons by an idealized kink, where $E_0=E_1=E=2\cos k-K$ and $E_{n\neq 0,1}=2\cos k$. Then we get

$$D(k)\equiv D_K(k) =(K-2\ \cos k)^2(2\ \sin^2 k+K\ \cos k)^2 +[(2\ \cos k-K)^2-2]^2\sin^2 k. \tag{10}$$

A simple calculation yields that the maximum of $\mathcal{T}$ for a double well potential with $K\sim 6$ is about 0.0035, so that the kink is almost opaque to phonons for the entire range of k for a double well potential. On the other hand, for the cosine potential with $K\sim\varepsilon$, a straighforward perturbative estimate shows that in the uncoupled limit the kink is almost perfectly transmitting ($|1-\mathcal{T}|<\varepsilon$) for phonons except in the small neighborhood of $k=0,\pi$ of size $\sqrt{\varepsilon}$, which is confirmed by numerical computation of transmission coefficients as a function of k, as in Fig. 1 for a kink (with exponential tails) of the double well potential and the cosine potential with $\varepsilon=0.01$.

When $D(k)$ is zero, there is a possibility of nonzero transmission at $k=0$ or $k=\pi$. We consider the $k=0$ limit only since the other case with $k=\pi$ can be analyzed similarly for LMs on the top of the phonon bands. For an idealized kink $D_K(k)$ vanishes at $K=0$ and $K=2$, which are, in fact, thresholds for creation of symmetric and antisymmetric LMs, respectively. Moreover, simple algebra shows that at the threshold $K=2$ the transmission at $k=0$ becomes *perfect*, a dramatic deviation from typical scattering behaviors of static diagonal defects. Moreover if $K<2$ there exists a perfect transmission ($\mathcal{T}=1$) at $k_p=\cos^{-1}(K/2)$ and if $K>2$

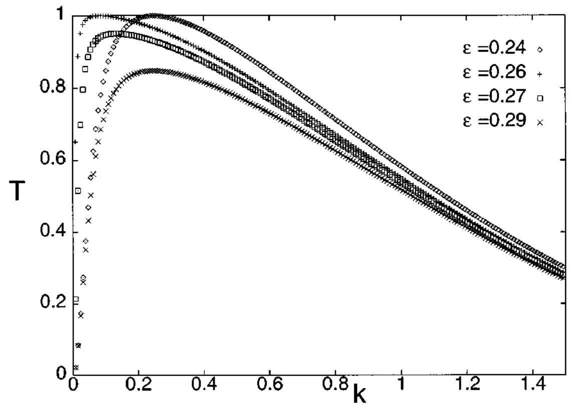

FIG. 2. Characteristic change in transmission near the LM threshold for a kink for the cosine potential.

there is no perfect transmission but a maximum $T_{max}=4/[4+(K^2-4)K^2]$ at $k_m=\cos^{-1}(2/K)$, which decreases from 1 as K moves away from the threshold. This characteristic change in transmission near the LM threshold is in fact observed for a kink (with exponential tails) for the cosine potential near the antisymmetric LM threshold of $\varepsilon\approx 0.26-0.27$ as in Fig. 2.

Our approach is very general and can be extended to the neighborhood of any LM threshold of any localized defects which is *symmetric* under spatial reflection. First, a necessary condition for nonzero transmission at $k=0$ is that $D(0)=0$, which leads to

$$\delta\equiv[\mathcal{M}_{11}-\mathcal{M}_{22}+\mathcal{M}_{12}-\mathcal{M}_{21}]_{k=0}=0. \tag{11}$$

At the LM thresholds, the band-edge solution at the bottom of the phonon band, $\xi_n^0\equiv\xi_n(k=0)$, with boundary condition $\xi_{n\geqslant N}^0=1$ for some large N is given by $\xi_n^0=\alpha_0 n+\beta_0$ for $n\leqslant N$. This band-edge solution must be bounded, so that the slope $\alpha_0=\xi_{-N}^0-\xi_{-N-1}^0=\delta$ must vanish. Therefore only at the LM threshold, we get nonzero transmission at $k=0$.

In fact, at the threshold, the transmission at $k=0$ becomes *perfect* and we get the characteristic change in transmission discussed before for a kink. For localized objects with symmetry under spatial reflection, $\mathcal{M}$ is antisymmetric, that is, $\mathcal{M}_{12}+\mathcal{M}_{21}=0$. This together with $\det\mathcal{M}=1$ yields after some algebra a simplified form for $\mathcal{T}$ for the symmetric localized objects:

$$\mathcal{T}=\frac{1}{1+F(k)}, \tag{12}$$

where

$$F(k)=\frac{(\mathcal{M}_{11}-\mathcal{M}_{22}+2\mathcal{M}_{12}\cos k)^2}{4\sin^2 k}. \tag{13}$$

We get *perfect* transmission when $F(k)=0$; that is, if

$$\mathcal{M}_{11}-\mathcal{M}_{22}+2\mathcal{M}_{12}\cos k=0 \tag{14}$$

has a solution for k. Note that the parameter δ in Eq. (11) measures deviation from the LM threshold. Since $\mathcal{M}$ is even in k, for small k and δ Eq. (14) becomes $\delta+ck^2\approx 0$, where

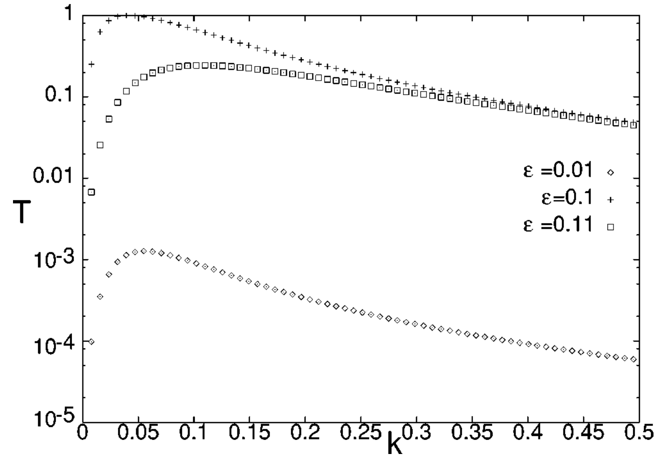

FIG. 3. Transmission coefficient as a function of k for a discrete breather of a Klein-Gordon chain with double well potential for various values of ε.

$c=[(\partial^2/\partial k^2)(\mathcal{M}_{11}-\mathcal{M}_{22}+\mathcal{M}_{12}-\mathcal{M}_{21})-\mathcal{M}_{12}]_{k=0}$ ($c\neq 0$ in general). If $c\delta<0$, there is a perfect transmission at $k_p\approx\sqrt{-\delta/c}$. Note that the breaking of spatial symmetry in localized objects leads to nonperfect transmission. If $c\delta>0$, we solve for the maximum transmission and obtain a peak in transmission at $k_m\approx\sqrt{\delta/c}$ with a maximum $\mathcal{T}_{k=k_m}\approx 1-|c|\delta$. For an idealized kink near the antisymmetric LM threshold, $K=2$, $c\approx-2<0$ and $\delta\approx 2(K-2)$, which leads to predictions consistent with previous analysis of the idealized kink and numerical computations for a kink.

We emphasize that thresholding behavior of LMs has also been found in a DB for a one-dimensional nearest neighbor chain with the double well potential, for example, with a frequency $\omega_b=0.8\omega_0$ [9], where in the uncoupled limit no LMs exist and a symmetric LM and an asymmetric LM are created at finite coupling, $\varepsilon_S\approx 0.07$ and $\varepsilon_A\approx 0.1$, respectively. Our analysis of scattering can be naturally extended to the DB with time-periodic functions with an appropriate enlargement of the dimension of transfer matrices to account for truncated Fourier modes. Preliminary numerical evidence for a DB with $\omega_b=0.8\omega_0$ shows that in the case of elastic scattering the DB is almost opaque for weak coupling but its transmission is dramatically enhanced near the LM thresholds showing a characteristic change in transmission similar to the case of the LE (see Fig. 3). This explains why perfect transmission of phonons through a DB was observed for a very small wave vector for $\omega_b=0.8323$ and $\varepsilon=0.1$ by Cretegny *et al.* [7].

In conclusion, we have studied thresholds of LMs for a class of symmetric localized defects, in particular, a discrete kink on a Klein-Gordon chain and their connection with phonon scattering. We found that the transmission at $k=0$ becomes perfect at the LM threshold with characteristic change involving perfect transmission for long-wavelength phonons in the neighborhood of the threshold. The explicit connection between creation thresholds for LMs and phonon scattering provides ways to investigate properties of LMs through scattering experiments. For example, by studying the phase shifts in $\mathcal{T}$, the total number of LMs could be enumerated as in Levinson's theorem [7,12,13]. It would be interesting to solve inelastic scattering problems in connection with experiments on LMs. The results on phonon-scattering may also present clues to understand and control heat flux in long molecules, for example, energy trapping and heat penetration prevention into some areas of chain [8,4].

Our approach can be extended to a wide class of localized defects, static or time periodic, on a chain. Much of our results on scattering is expected to hold for a broad class of Hamiltonian chains outside the realm of applications of the transfer matrix method and the discrete Sturm-Liouville theory. It would be interesting to understand LMs of time-periodic DBs and their connection to DB-phonon scattering with in the discrete nonlinear Schrödinger equation on one-dimension and the Fermi-Pasta-Ulam chain. The detailed analysis of DB-phonon scattering will be the subject of on-going investigations.

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