Fano resonances in translationally invariant nonlinear chains

Sang Wook Kim and Seunghwan Kim
Nonlinear and Complex Systems Laboratory, Department of Physics, Pohang University of Science and Technology, Pohang, Korea 790-784

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We show that the Fano resonance, which has been actively studied in the context of mesoscopic transport in systems with impurities or defects, also occurs in *translationally invariant* nonlinear chains. We find that the phonon scattering with the intrinsic nonlinear localized excitation, called the discrete breather, in this system produces a rich resonance structure involving the typical signatures of Fano resonance with both perfect transmission and perfect reflection, and the anomalous resonance structures. Our system can serve as a simple paradigm for understanding rich Fano-related phenomena in a wide class of nonlinear lattices, based on the global structure of the localized modes and the perfect reflection.

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When a discrete energy level interferes with a continuum of states, a Fano resonance occurs leading to asymmetric excitation spectra.[1] After its first observation in the autoionization of atomic physics, it has been found in many other physical problems including the asymmetric spectra of the Kondo resonance line shape in the tunneling experiment into a single magnetic impurity on a metallic substrate[2,3] and other mesoscopic transport problems.[4,5] The electronic transport in a ultrasmall semiconductor structure resembles wave propagation in wave guides, where the transmission amplitude exhibits a rich structure related to resonance phenomena. In particular, quasibound states in resonantly coupled cavities, called the stubs, give rise to the asymmetric transmission which has been discussed in the context of the Fano resonance. In the systems studied so far, one must introduce impurities or attached stubs[4,5] to obtain the Fano resonance, which generate quasibound states that break the translational invariance.

In this report, we propose another scheme to produce the Fano resonance *without* a breakup of translational invariance which is based on the discrete breathers, the time-periodic and spatially localized excitations on the nonlinear lattice.[6,7] They are intrinsic modes of the nonlinear lattice with translational invariance, not imposed impurities, which require practically no activation energy in one dimension and thus bridges the gap between the highly nonlinear modes and the linear phonon modes.[8] Recently Schwarz *et al.*[9] reported experimental observation of intrinsic localized spin-wave modes in the anisotropic antiferromagnet, which may serve as an experimental realization of the discrete breather in a lattice of atomic dimension.

The discrete breathers can affect the energy transport by scattering phonons, playing the role of the scattering center similar to the intrinsic impurity in mesoscopic transport problems. The time dependence of the discrete breather can lead to rich phenomena associated with the phonon transport including the Fano resonance. For example, electron transport through a point barrier oscillating at frequency ω was shown to yield the transmission resonances including the Fano resonance, similar to those found in other multiple quantum channel scattering problems such as the transmission through a donor impurity in a quasi-one-dimensional (1D) wire.[10]

The scattering properties of the localized structures are related to the structure of the internal modes of the localized structure itself.[11] In particular, it was shown that the perfect transmission occurs at the localized mode threshold, which has been extended to a wide class of the nonlinear systems with time-dependent localized structures such as discrete breathers.[12,13] In the case of the phonon scattering with the static localized mode for the nearest-neighbor chain, the perfect reflection cannot be found since it involves only one scattering channel, whereas discrete breathers can admit infinitely many scattering channels displaying a rich transmission structure involving perfect reflections.

In our study of the Fano resonance, we focus on the one-dimensional nonlinear Klein-Gordon chain in translationally invariant lattices. This system proves to be a much simpler paradigm for studying rich Fano resonance related phenomena than typical mesoscopic transport problems extending the existing studies on the global structure of the localized modes of the discrete breather. Our results can be generalized to a wide class of translationally invariant nonlinear chains supporting discrete breathers.

Let us consider a Klein-Gordon chain with on-site potential and nearest-neighbor harmonic spring coupling with the Hamiltonian

$$H=\sum_{n=-\infty}^{\infty}\left[\frac{p_n^2}{2}+V(x_n)+\frac{1}{2}\epsilon(x_n-x_{n-1})^2\right], \tag{1}$$

where x_n, p_n are the coordinate and the momentum at the site n, respectively, and ϵ is the spring constant. The equation of motion for the system in Eq. (1) is given by

$$\ddot{x}_n(t)=-V'[x_n(t)]+\epsilon(x_{n+1}-2x_n+x_{n-1}). \tag{2}$$

Let $x_n^0(t)$ be a discrete breather solution which is time periodic with period T_b. The linearized equation of Eq. (2) near the discrete breather for $\xi_n(t)=x_n(t)-x_n^0(t)$ is given by

$$\ddot{\xi}_n(t)=A_n(t)\xi_n(t)+\epsilon[\xi_{n+1}(t)-2\xi_n(t)+\xi_{n-1}(t)], \tag{3}$$

where $A_n(t)=-V''[x_n^0(t)]$. By Floquet theorem, the solution for the linearized equation in Eq. (3) can be put into $\xi_n(t)$

$=\overline{\xi_n}(t)e^{-i\omega t}$, where $\overline{\xi_n}(t+T_b)=\overline{\xi_n}(t)$. Since $\overline{\xi_n}(t)$ and $A_n(t)$ are time periodic with period $T_b=2\pi/\omega_b$, they can be expanded in terms of Fourier series using the rotating wave approximation,

$$\overline{\xi_n}(t)=\sum_{m=-M}^{M} b_{n,m}e^{-im\omega_b t}, \quad A_n(t)=\sum_{m=-M}^{M} a_{n,m}e^{-im\omega_b t}, \tag{4}$$

where $a_{n,m}$ and $b_{n,m}$ are Fourier coefficients, and M is the cutoff. Then the linearized equation can be expressed as the linear relations between Fourier coefficients:

$$\left(2-\frac{(\omega+m\omega_b)^2}{\epsilon}\right)b_{n,m}-\frac{1}{\epsilon}\sum_{k=-M+m}^{M-m} b_{n,k}a_{m,-k}-b_{n+1,m} = b_{n-1,m}, \tag{5}$$

which can be put into a transfer matrix form for $\vec{b}_n =(b_{n,-M},b_{n,-M+1},\ldots,b_{n,M})^T$:

$$\begin{pmatrix}\vec{b}_n\\ \vec{b}_{n-1}\end{pmatrix}=M_n\begin{pmatrix}\vec{b}_{n+1}\\ \vec{b}_n\end{pmatrix}. \tag{6}$$

Note that M_n is the transfer matrix which maps the set of Fourier coefficients at site $n+1$ to one at site n.

We consider the scattering setup with the discrete breather at the center of the chain. Since the superposition of the traveling phonons and the decaying solutions of the linearized equation in the absence of the discrete breather is the solution of the linearized equation with the discrete breather at sites far from the center, we require

$$b_{n,m}=\alpha_m^-\lambda_m^n+\alpha_m^+\lambda_m^{-n} \quad \text{as } n\to-\infty,$$

$$b_{n,m}=\beta_m^+\lambda_m^n+\beta_m^-\lambda_m^{-n} \quad \text{as } n\to\infty, \tag{7}$$

where the decay exponents, λ_m, satisfy $\lambda_m+\lambda_m^{-1}-2+[(\omega+m\omega_b)^2-\Omega_0^2]/\epsilon=0$ $[\Omega_0=\sqrt{V''(0)}]$ and $|\lambda_m|<1$ for $m\neq m^*$ (m^* is the scattering channel). Considering the nonlinear lattice with $2N+1$ sites with the asymptotic boundary conditions in Eq. (7), we get

$$\begin{pmatrix}\vec{b}_{-N}\\ \vec{b}_{-N-1}\end{pmatrix} = M\begin{pmatrix}\vec{b}_{N+1}\\ \vec{b}_N\end{pmatrix}, \tag{8}$$

where $M=M_{-N}\cdot M_{-N+1}\cdots M_N$.

In the case of one channel scattering, the frequency $\omega_m=\omega+m\omega_b$ for $m\neq m^*$ does not belong to the phonon band of the scattering channel m^*, for example, defined by $[\Omega_0,\sqrt{\Omega_0^2+4\epsilon}]$ for $m^*=0$. In this case, $\lambda_0=e^{ik}$ with the real wave vector k, $\alpha_0^-=r(k)$, the reflection coefficient, and $\beta_0^+=t(k)$, the transmission coefficient, fixing $\alpha_0^+=1$. To satisfy the boundary condition, the solution on one side should be obtained after repeatedly multiplying transfer matrices to the solution on the other side, which leads to the solution matching condition. In the case of the localized modes, $|\lambda_m|<1$ for all m, where the solutions can be simply found by solving the secular Eq. (8).

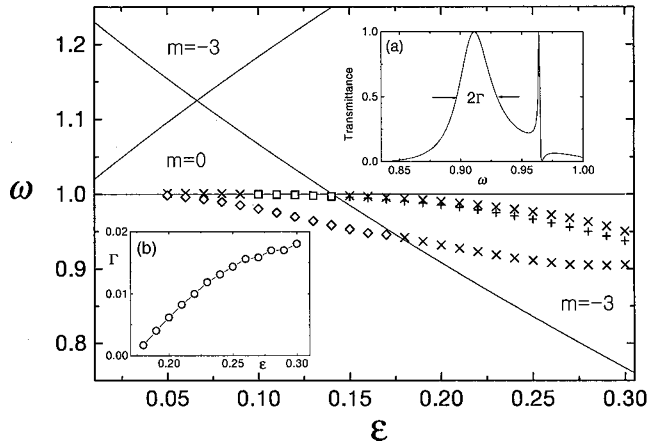

FIG. 1. Two phonon bands for $m=0$ and $m=-3$ are shown in the parameter space of the input phonon frequency ω and the coupling strength ϵ in the nearest-neighbor Klein-Gordon chain with cubic on-site potential for $\omega_b=0.75$. The perfect transmissions, the perfect reflections, and the localized modes are denoted by $\times$, $+$, $\diamond$ (symmetric mode), and $\Box$ (antisymmetric mode), respectively. Inset (a): one channel phonon transmission through the discrete breather for $\epsilon=0.25$. Inset (b): the linewidth Γ of the Fano peak due to the symmetric localized mode versus ϵ.

Now we consider the phonon scattering by the discrete breather with $\omega_b=0.75$ for the nearest-neighbor Klein-Gordon chain with a cubic on-site potential, $V(x)=x^2/2-x^3/3$. Figure 1 shows the locus of the localized modes, the perfect transmission, and the perfect reflection in the parameter space of the frequency ω, and the coupling strength ϵ. It is now well established that the perfect transmission occurs at the threshold for the symmetric localized mode, $\epsilon\approx0.05$ and terminates at the threshold for the antisymmetric localized mode, $\epsilon\approx0.1$ for $m=0$ channel scattering. Note that in Fig. 1 the branch of the localized mode penetrates the phonon band with $m=-3$, producing the perfect transmission. This phenomenon has been previously studied and interpreted as the true breather instability which is not connected with the finite-size effect.[14,15] In the following, we provide an explanation of these perfect transmissions in the context of Fano resonance.

We show in inset (a) of Fig. 1 the transmittance of the $m=-3$ scattering channel versus the input phonon frequency for the coupling strength $\epsilon=0.25$, where a clear asymmetric Fano resonance is visible at $\omega\approx0.96$. It is due to the interplay between $m=-3$ phonon band, i.e., the continuum of states, and the antisymmetric localized mode, i.e., a quasibound state in the phonon band, which originates from the $m=0$ scattering channel. Another Fano resonance due to the symmetric localized mode at $\omega\approx0.91$ has a different resonance structure with a broader line width and no perfect reflection. In the mesoscopic transport problem, the linewidth Γ corresponds to the imaginary part of a pole of the transmission amplitude in the complex energy plane, and is related to the life time of a quasibound state. It also corresponds to the instability exponent in the dynamical sense. The instability of the discrete breather caused by the collision between the localized mode and the phonon band has

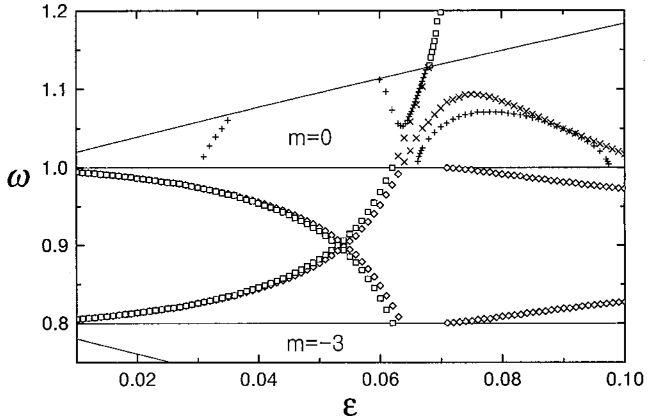

FIG. 2. The same as in Fig. 1 for the Morse on-site potential for $\omega_b = 0.6$.

been extensively studied by Marin *et al.*[15] Inset (b) of Fig. 1 shows the width of the Fano peak corresponding to the symmetric localized mode as a function of ϵ. This is in agreement with the behavior of the modulus of the eigenvalues in Fig. 3 of Ref. 15, in which the modulus of one of the eigenvalues starts to considerably deviate from one at the location of the collision between the symmetric localized mode and the phonon band, $C \approx 0.18$. In general, Fano resonances show the asymmetric line shape including the perfect transmission and the perfect reflection. In the case of the Fano peak corresponding to the symmetric localized mode the perfect reflection accompanies the perfect transmission in most two-channel scattering regions. Note that the anomalous resonances without either the perfect transmission or the perfect reflection may occur in a very small parameter range.

We show in Fig. 2 another example of Fano resonances in phonon scattering by the discrete breather for the nearest-neighbor Klein-Gordon chain with an on-site Morse potential, $V(x) = [1 - \exp(-x)]/2$ with $\omega_b = 0.6$. It displays a more complex structure, but still the Fano resonances are easily identified from the perfect transmissions and the neighboring perfect reflections. Figure 3 for $\epsilon = 0.067$ represents clear asymmetric resonance line shapes in transmittance. At a rather smaller value of ϵ below the coupling strength of the band-band crossing, the Fano resonance occurs, which depends on the characteristic of the nonlinear on-site potentials considered. In Fig. 3 the phase shifts of the outgoing wave are also shown. Note that at the perfect reflection the phase jumps sharply by the amount of π, while at the perfect transmission the phase drops monotonically by the amount of π. This phenomenon can be clearly understood by using a symmetry argument only.[16] It must be noted that in some regions only the perfect transmission is found, while in other regions only the perfect reflection is found. For example, in Fig. 2, the region with $0.060 \leqslant \epsilon \leqslant 0.062$ exhibits only the perfect reflection, while the regions with $0.064 \leqslant \epsilon \leqslant 0.066$ and $0.097 \leqslant \epsilon$, only the perfect transmission. These *anomalous* Fano resonances occur due to the existence of the forbidden regions of the phonon transport in the phonon band structure arising from the discrete translational symmetry. Note that the perfect reflection in the region with $0.031 \leqslant \epsilon \leqslant 0.035$ has nothing to do with Fano resonance.

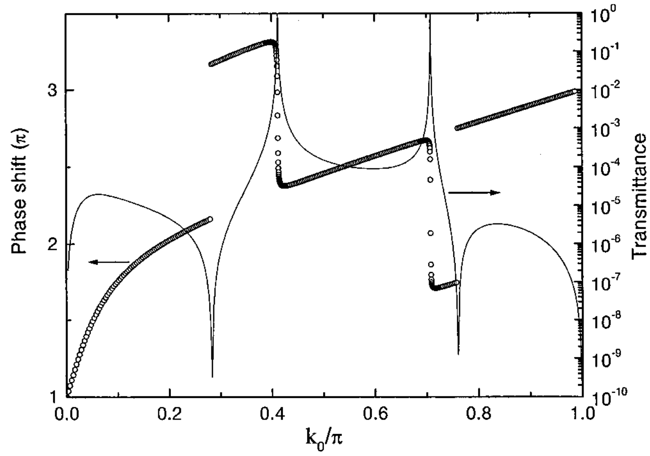

FIG. 3. The phonon transmission (units on the right y axis) through the discrete breather as in Fig. 2 for $\epsilon = 0.067$ (units on the right y axis) and the phase shift of the outgoing phonon (units on the left y axis).

Based on the zero-pole pair nature of Fano resonances, the transmission amplitude in the vicinity of each quasibound state can be written by $t \sim (z - E_0)/[z - (E_P - i\Gamma)]$, where z, E_0, and E_P are the complex energy, the positions of the perfect reflection and the pole, respectively.[17] The lifetime of the quasibound state is given by $\tau = \hbar/(2\Gamma)$. From this it can be shown that the transmission probability is given by

$$T(E) = \frac{\Gamma^2}{(E_P - E_0)^2 + \Gamma^2} \frac{(E - E_0)^2}{(E - E_P)^2 + \Gamma^2}. \tag{9}$$

With the known energies for the perfect reflection E_0 and perfect transmission E_1, we can derive the energy of the pole as $E_P = (E_0 + E_1)/2 \pm \sqrt{(E_0 - E_1)^2 - 4\Gamma^2}/2$. When Γ is much smaller than the difference between E_0 and E_1, E_P can be

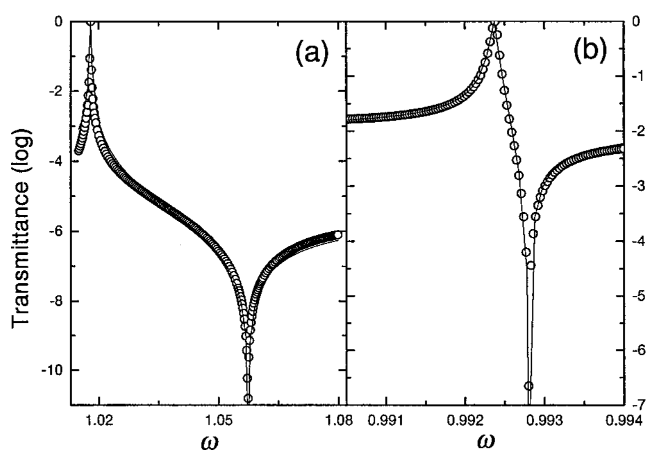

FIG. 4. Fitted line shapes of the Fano resonance: (a) the same as in Fig. 1 with $\epsilon = 0.063$ and (b) the same as in Fig. 2 with $\epsilon = 0.17$. The fitted values using the formula (9) are shown in solid lines, and the data from numerical computation of the phonon scattering with the discrete breather in circles.

simply approximated as E_1. Using this and Eq. (9) transmittance curves can be fitted with a single fitting parameter Γ very well. Figure 4 shows the fitted line shapes of the Fano resonance with the sharp peak in the case of small Γ, which is in excellent agreements with one from the formula (9) for small Γ.

To gain more physical intuition on the existence of Fano resonance in translationally invariant nonlinear chains, we rewrite Eq. (5) as a discrete Schrödinger equation of coupled channels for one-dimensional electron transport:

$$(-\epsilon\nabla_n^2+U_{n,m})b_{n,m}=\sum_{k=-M+m}^{M-m} a_{m,-k}b_{n,k}, \qquad (10)$$

where ∇_n^2 is the discrete Laplacian, $\nabla_n^2 b_{n,m}\equiv b_{n-1,m}+b_{n+1,m}-2b_{n,m}$ and $U_{n,m}$ is the effective potential energy, $U_{n,m}\equiv-(\omega+m\omega_b)^2$. Each channel m (originally Fourier index) has the kinetic energy, $-\epsilon\nabla_n^2$ and the effective potential energy $U_{n,m}$, and the terms on the right-hand side denotes the coupling. In the case of one channel scattering, the electron state in the propagating channel is extended over the entire sites, while the electron states in other channels are strongly localized. Thus this situation is essentially identical to a one-dimensional wave guide coupled with multiple stubs in a typical mesoscopic transport problem, which has been studied actively in the context of the Fano resonance.

In summary, we find the Fano resonance in phonon transmission through the discrete breather in a translationally invariant nonlinear chain, which is explained based on the global structure of the localized modes and perfect reflections. In addition, our system reveals more complex resonance behavior involving anomalous Fano resonances without either perfect transmission or perfect reflection. The observed Fano resonance in nonlinear chains is closely related to one in the quasi-1D mesoscopic transport problem with impurities or stubs. Our results can be generalized to a wide class of nonlinear lattices that support discrete breathers. Our system should serve as a simple paradigm for studying rich Fano resonance related phenomena.

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