Fano Resonances with Discrete Breathers

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A theoretical study of linear wave scattering by time-periodic spatially localized excitations (discrete breathers) is presented. A peculiar effect of *total reflection* occurs due to a Fano resonance when a localized state originating from closed channels resonates with the open channel. For the discrete nonlinear Schrödinger chain, we give an analytical result for the frequency dependence of the transmission coefficient, including the possibility of resonant reflection. We extend the analysis to chains of weakly coupled anharmonic oscillators and discuss the relevance of the effect for electronic transport spectroscopy of mesoscopic systems.

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It is a well established fact that various *nonlinear spatially discrete* systems can support time-periodic spatially localized excitations called *discrete breather* (DB) states [1]. These states originate from a peculiar interplay between the nonlinearity and the discreteness of the lattice rather than from a disorder. While the nonlinearity yields an amplitude-dependent tunability of frequencies of DBs Ω_b, the spatial discreteness of the system leads to finite upper bounds for the frequency spectrum of small amplitude plane waves ω_q. This tunability allows one to escape resonances of all multiples of the breather frequency Ω_b with the plane wave frequencies ω_q and, correspondingly, to stabilize the DB state. The frequency dependent localization length of DBs and their stability with respect to small amplitude perturbations have been widely studied [1]. DBs have been observed in experiments covering such diverse fields as interacting Josephson junctions [2], magnetic systems [3], and lattice dynamics of crystals [4].

For propagating linear waves, a DB acts as a time-periodic scattering potential, and the transmission coefficient T depends on both the wave vector q of the linear wave and the breather frequency Ω_b. The most peculiar effect, observed in many numerical studies of wave scattering by DBs, is the *total reflection* as $T = 0$ [5,6]. Note that the presence of a static potential cannot lead to such a total reflection in one-dimensional systems. Similar features are also discussed in other areas, such as electron transport through point contacts and quantum dots and wires [7,8]. The crucial condition allowing a total reflection in these systems is the presence of a few coupled channels connected with the transverse direction of motion. On the other hand, the wave propagation in the presence of a time-periodic scattering potential is characterized by *open and closed channels* emerging from the Floquet formalism [1,5,6]. The open channel guides the propagating waves, while the eigenfrequencies of closed channels do not match the spectrum of linear waves.

In this Letter, we show that the total reflection of linear waves in the open channel occurs when a *localized state* originating from one of the closed channels resonates with the open channel spectrum, a condition similar to the well-known Fano resonance [9]. We use this understanding to *predict* Fano resonance positions for wave scattering by breathers in weakly interacting anharmonic oscillator chains and to discuss the relevance of this effect for electronic transport spectroscopy.

We start our study of the wave scattering by DB with the discrete nonlinear Schrödinger system (DNLS), which has been used frequently to study breather properties due to its tractable form. Wave scattering by breathers in the DNLS was studied numerically in [10], where resonant total reflection was also observed. First, we provide an analytical solution for the DNLS scattering problem. The equations of motion for the DNLS are

$$i\dot{\Psi}_n = C(\Psi_{n+1} + \Psi_{n-1}) + |\Psi_n|^2\Psi_n, \tag{1}$$

where the integer n labels the lattice sites, Ψ_n is a complex scalar variable, and C describes the nearest neighbor interaction on the lattice. For small amplitude waves $\Psi_n(t) = \epsilon e^{i(\omega_q t - qn)}$ the dispersion relation is

$$\omega_q = -2C\cos q. \tag{2}$$

Breather solutions have the form

$$\hat{\Psi}_n(t) = \hat{A}_n e^{-i\Omega_b t}, \qquad \hat{A}_{|n|\to\infty} \to 0, \tag{3}$$

where the time-independent amplitude $\hat{A}_n$ can be taken real valued, and the breather frequency $\Omega_b \neq \omega_q$ is a function of the maximum amplitude $\hat{A}_0$. The spatial localization is given by an exponential law $\hat{A}_n \sim e^{-\lambda|n|}$, where $\cosh\lambda = |\Omega_b|/2C$ [11]. Thus, the breather can be

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approximated as a single-site excitation if $|\Omega_b| \gg C$. Then the relation between the single-site amplitude $\hat{A}_0$ and Ω_b becomes $\Omega_b = \hat{A}_0^2$. In the following, we neglect the breather amplitudes for $n \neq 0$, i.e., we assume $\hat{A}_{n\neq 0} \approx 0$, since $\hat{A}_{\pm 1} \approx (C/\Omega_b)\hat{A}_0 \ll \hat{A}_0$. We emphasize that in the limit of a nearly single-site localized breather solution in the DNLS the solution *is* linearly stable [11].

We add small perturbations to the breather solution

$$\Psi_n(t) = \hat{\Psi}_n(t) + \phi_n(t) \tag{4}$$

and linearize Eq. (1) with respect to $\phi_n(t)$:

$$i\dot{\phi}_n = C(\phi_{n+1} + \phi_{n-1}) + \Omega_b \delta_{n,0}(2\phi_0 + e^{-2i\Omega_b t}\phi_0^*), \tag{5}$$

with $\delta_{n,m}$ being the usual Kronecker symbol. The general solution to this problem is given by the sum of contributions due to two channels,

$$\phi_n(t) = X_n e^{i\omega t} + Y_n^* e^{-i(2\Omega_b + \omega)t}, \tag{6}$$

where X_n and Y_n are complex numbers satisfying the following algebraic equations:

$$-\omega X_n = C(X_{n+1} + X_{n-1}) + \Omega_b \delta_{n,0}(2X_0 + Y_0), \tag{7}$$

$$(2\Omega_b + \omega)Y_n = C(Y_{n+1} + Y_{n-1}) + \Omega_b \delta_{n,0}(2Y_0 + X_0). \tag{8}$$

Away from the breather center $n = 0$, Eq. (5) allows for the existence of plane waves with the spectrum ω_q. Keeping in mind the propagation of waves, we set $\omega \equiv \omega_q$ for some value of q. Thus, the X channel is an open one, while the Y channel is a closed one; i.e., its frequency $-(2\Omega_b + \omega_q)$ does not match the spectrum ω_q.

Instead of solving Eqs. (7) and (8), we consider a more general set of equations

$$-\omega_q X_n = C(X_{n+1} + X_{n-1}) - \delta_{n,0}(V_x X_0 + V_a Y_0), \tag{9}$$

$$(\Omega + \omega_q)Y_n = C(Y_{n+1} + Y_{n-1}) - \delta_{n,0}(V_y Y_0 + V_a X_0), \tag{10}$$

which is reduced to (7) and (8), if $\Omega = 2\Omega_b$ and $V_x = V_y = 2V_a = -2\Omega_b$. For a particular case $V_a = 0$, i.e., when the closed Y channel is decoupled from the open one, the former possesses exactly one localized eigenstate due to a nonzero value of V_y with the frequency

$$\omega_L^{(y)} = -\Omega + \sqrt{V_y^2 + 4C^2}. \tag{11}$$

To compute the transmission coefficient T, we use the transfer matrix method described, e.g., in Ref. [12]. The boundary conditions are $X_{N+1} = \tau e^{iq}$, $X_N = \tau$, $Y_{N+1} = D/\kappa$, $Y_N = D$ for the right end of the chain and $X_{-N-1} = 1 + \rho$, $X_{-N} = e^{iq} + \rho e^{-iq}$, $Y_{-N-1} = F$, $Y_{-N} = \kappa F$ for the left one. Here τ and ρ are the transmission and reflection amplitudes with $T = |\tau|^2 = 1 - |\rho|^2$. F and D describe the exponentially decaying amplitudes in the closed Y channel, where the degree of localization is described by the coefficient $\kappa \equiv e^{\lambda}$:

$$\kappa = \frac{1}{2C}[\Omega + \omega_q + \sqrt{(\Omega + \omega_q)^2 - 4C^2}]. \tag{12}$$

The 4×4 transfer matrix is defined by Eqs. (9) and (10) at $n = 0$. After finding the solutions of the corresponding four linear equations, we obtain

$$T = \frac{4\sin^2 q}{(2\cos q - a - \frac{d^2\kappa}{2 - b\kappa})^2 + 4\sin^2 q}, \tag{13}$$

$$a = \frac{-\omega_q + V_x}{C}, \qquad b = \frac{\Omega + \omega_q + V_y}{C}, \qquad d = \frac{V_a}{C}. \tag{14}$$

This is the central result of this Letter, which allows one to conclude that total reflection is obtained when the condition

$$2 - b\kappa = 0 \tag{15}$$

is realized. It is equivalent to the resonance condition

$$\omega_q = \omega_L^{(y)}, \tag{16}$$

which has a clear physical meaning: total reflection occurs when a local mode, originating from the closed Y channel, resonates with the plane wave spectrum ω_q of the open X channel. The only condition is that the coupling between the open and closed channels V_a is nonzero. Remarkably, the resonance position does not depend on the actual value of V_a; i.e., there is no renormalization. The existence of local modes, which originate from the X channel for nonzero V_x and possibly resonate with the closed Y channel, is evidently of no importance. Equation (13) also yields zero transmission for $q = 0, \pi$ due to a vanishing of the group velocity $d\omega_q/dq \sim \sin q$ for these q values; we do not focus on these trivial total reflections.

This resonant total reflection is very similar to the Fano resonance [9], since it is directly related to a local state resonating and interacting with the continuum of extended states. The fact that the resonance location is independent of the coupling V_a is due to the local, single-site, character of the coupling between the local mode (originating from the Y channel) and the open channel. If this coupling has a finite nonzero localization length, i.e., several neighboring sites are involved, then the total reflection happens at an energy which does not necessarily coincide with that of the local state (16) [13]. A more physical formulation for the condition of absence of significant renormalizations of the resonance location is that the wavelength of the propagating wave is large compared to the extension of the space region where the channel coupling occurs.

Returning to the case of a DNLS breather at weak coupling, we insert the values for Ω, V_x, V_y, and V_a into (13) and (14) and obtain the following expression for the transmission coefficient:

$$T = \frac{4\sin^2 q}{(\frac{2\Omega_b}{C} - \frac{\Omega_b^2}{2C^2}\frac{\kappa}{1+\kappa\cos q})^2 + 4\sin^2 q}. \tag{17}$$

The result is that any breather solution of the DNLS close to the anticontinuous limit (the interaction C goes to zero) provides us with a total reflection in close vicinity of $q = \pi/2$. Indeed, if we expand (17) in C/Ω_b, we obtain

$$T \approx \frac{4C^4}{\Omega_b^4}\sin^2 2q \tag{18}$$

in the lowest order, provided $C/2\Omega_b \ll |\cos q|$.

Figure 1 compares a numerically obtained q dependence of the transmission coefficient with (17) for $C = 0.01$ [14]. We obtain very good agreement, except for a small shift of the true total reflection position with respect to $q = \pi/2$. It is due to the small but nonzero *finite extension* of the scattering potential, which leads to a spread of the coupling between the local mode and the open channel.

Next, we consider the system of weakly interacting anharmonic oscillators:

$$\ddot{X}_n = -V'(X_n) + C(X_{n-1} + X_{n+1} - 2X_n), \tag{19}$$

where the oscillator potential V possesses one minimum, $V'(0) = 0$ and $V''(0) = 1$. The spectrum of small amplitude plane waves is given by $\omega_q^2 = 1 + 4C\sin^2(q/2)$ and discrete breather solutions are time-periodic spatially localized solutions of Eq. (19) with frequency $\Omega_b \neq \omega_q/m$ for any nonzero integer m. Here we again consider a weak interaction between the oscillators ($C \ll 1$) and

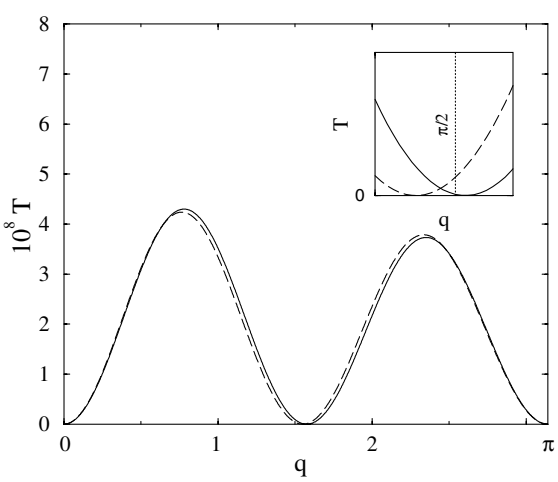

FIG. 1. Transmission coefficient T for DNLS breather with $C = 0.01$ and $\Omega_b = 1$ versus q. Dashed line: numerically exact result; solid line: analytical result (17). Inset: zoom around total reflection, where the dotted line marks $q = \pi/2$.

assume that the breather is essentially a single-site excitation $\hat{X}_0(t) = \hat{X}_0(t + 2\pi/\Omega_b) \neq 0$ and $\hat{X}_{n\neq 0}(t) \approx 0$. The equations for the linearized phase space flow around the breather solution are then given by [6]

$$\ddot{\epsilon}_n = -\epsilon_n + C(\epsilon_{n-1} + \epsilon_{n+1} - 2\epsilon_n) - \delta_{n,0}\{V''[\hat{X}_0(t)] - 1\}\epsilon_0. \tag{20}$$

For $C = 0$ we expand $V''[\hat{X}_0(t)] = \sum_k v_k e^{ik\Omega_b t}$ and use the Floquet representation $\epsilon_0(t) = \sum_k e_{0k} e^{i(\omega + k\Omega_b)t}$ to arrive at the set of equations

$$-(\omega + k\Omega_b)^2 e_{0k} = -\sum_{k'} v_{k-k'} e_{0k'}, \tag{21}$$

for the site $n = 0$, at which the breather is excited. This complete set of linear equations describes the coupling of the open channel (the corresponding amplitude of oscillations e_{00}) and many closed channels (the amplitudes of oscillations e_{0k} with $k \neq 0$).

To obtain the condition for total reflection, we apply a procedure which is similar to our analysis of the DNLS system. We "turn off" the coupling between the open channel and the closed channels; i.e., the amplitude e_{00} is set to zero in Eq. (21). The remaining homogeneous set of equations determines the local states ω_L of closed channels. The values of $\omega = \omega_L$ are those for which the corresponding determinant vanishes. Moreover, we are interested in the situation when $\omega_L^2 = 1$, which results in a resonance of a local mode of the system of closed channels with the open channel $\omega_q^2 \approx 1$. It is evident that such a situation is not necessarily realized for an arbitrary value of Ω_b. To find the proper value of Ω_b, we put $\omega = 1$ and scan Ω_b for a given potential V (note that the parameters v_k depend on Ω_b). As a result, we expect to find a discrete set of Ω_b values, for which the determinant of the reduced set of equations Eq. (21) zeros and a Fano resonance occurs.

Thus, at variance to the DNLS case, a Klein-Gordon chain in the anticontinuous limit will provide us with a total reflection of waves by breathers only for a selected discrete set of breather frequencies. Increasing the coupling C transforms each of these frequency values into frequency stripes on the real axis, which will continue to increase with C. This follows from the fact that the bandwidth of ω_q increases linearly with the coupling C, whereas the shift of the eigenvalues is proportional to C^2.

Note here that the Green function technique elaborated for the wave scattering by DBs in Ref. [6] leads to the same procedure described above in the limit of small v_k, allowing one to obtain the dependence of ω_L on the amplitude and frequency of the DB.

In order to demonstrate the validity of our constructive approach, we choose

$$V(x) = \tfrac{1}{2}x^2 + \tfrac{1}{3}x^3 + \tfrac{1}{4}x^4 \tag{22}$$

and carry out the above procedure. We obtain $\Omega_b \approx 1.38$.

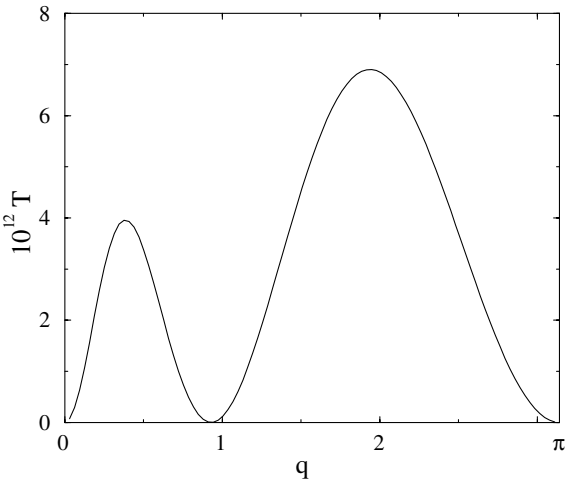

FIG. 2. Transmission coefficient versus q for a Klein-Gordon chain breather with $\Omega_b = 1.38$ and $C = 0.001$.

The prediction then is that for small C a breather with Ω_b close to this value yields a total reflection. The numerical result for the transmission is shown in Fig. 2 for $C = 0.001$ [14]. We indeed observe a total reflection around $q \approx 1$, as predicted. We also mention that similar Fano resonances have been observed numerically for the wave scattering by breathers in acoustic chains of oscillators with a nonlinear nearest neighbor interaction (for details, see [6]).

Our analysis can be directly used for the detection of Fano resonances in the propagation of linear waves in weakly dissipative Josephson junction arrays in the presence of discrete breathers [2,6]. Moreover, our results allow us to formulate optimal conditions for electronic transport spectroscopy of molecules, quantum dots, or optical cavities, coupled to a system of leads. Indeed, a one-dimensional electronic transport through the localized states in the presence of externally applied microwave radiation of frequency Ω will display a Fano resonance (and, correspondingly, zero conductivity) as the condition $E_F = \Omega \pm E_n$ is satisfied. Here E_F is the Fermi energy, and E_n are the localized levels. To establish this type of a spectroscopy leads should be quasi-one-dimensional such that only one transversal mode persists. Then we reduce the lead system to one open channel. The other important condition is to satisfy that the wavelength of excitations (e.g., at the Fermi energy for electronic transport) is *large* compared to the spatial extension of the coupling to the localized states. Additional optional spatial modulations, e.g., in the leads, may be used to generate artificial gaps in the electronic spectrum and, thus, to tune the wavelength. The power of microwave radiation has to be rather small to exclude the renormalization of E_n. The coupling between propagating states and localized states may be also provided by, e.g., spin-spin or spin-orbit interactions. In this case, zero conductance will be the consequence of a bare dot state passing the Fermi energy ($E_F = E_n$).

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[13] To find this result, we may look at the derivation of the renormalization of the Fano resonance in Ref. [8] for the case of electron scattering in quantum wires. The shift of the resonance is given there by the integral in the last line of Eq. (A11), which zeros if the coupling potential is δ-like. This analysis can be redone for discrete systems, which we consider here, and the same zero shift will be obtained for the single-site coupling (Kronecker symbol appears instead of the δ function). However, if the coupling involves several sites a finite shift of the total reflection with respect to the local mode due to the closed channel is obtained.
[14] For details concerning the numerical methods of obtaining high precision transmission data, we refer to [6].