DISCRETE BREATHERS CLOSE TO THE ANTICONTINUUM LIMIT: EXISTENCE AND WAVE SCATTERING

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The anticontinuum limit (i.e. the limit of weakly coupled oscillators) is used to obtain two surprising results. First we prove the continuation of discrete breathers of weakly interacting harmonic oscillators, provided a suitable coupling is chosen. Secondly we derive an analytical result for the wave transmission by a breather of the discrete nonlinear Schrödinger equation at weak coupling. We obtain a resonant full reflection due to a Fano resonance.

1. Introduction

The study of dynamical nontopological localization in nonlinear Hamiltonian lattices is a topic of widespread interest with results ranging from intensive theoretical studies[1] to experiments in such diverse areas as Josephson junction arrays[2], vibrational excitations in crystals[3] and localized excitations in antiferromagnets[4], to name a few. While basic theoretical investigations quickly spread into such directions as e.g. quantum theory and dissipative systems, there are still many interesting questions to be answered in the framework of classical Hamiltonian lattices.

One central class of systems is the model of a chain of interacting oscillators with the Hamiltonian

$$H = \sum_l \left(\frac{P_l^2}{2} + V(X_l) + \epsilon W(X_l - X_{l-1}) \right) \tag{1}$$

where P_l and X_l are pairs of canonically conjugated momenta and displacements of particles at lattice site l satisfying the equations $\dot{X}_l = \partial H / \partial P_l$ and $\dot{P}_l = -\partial H / \partial X_l$. The oscillator potential V and the nearest neighbour interaction W are assumed to be nonnegative functions with $V(0) = W(0) = V'(0) = W'(0) = 0$. The role of the positive constant ϵ is to control the strength of the interaction.

Another important system is the discrete nonlinear Schrödinger equation (DNLS)

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

where n is an integer labeling the lattice sites, Ψ_n is a complex scalar variable and C describes the nearest neighbour interaction (hopping) on the lattice. The last term in (2) provides with the requested nonlinearity.

2. Weakly interacting harmonic oscillators

According to a proof of existence by Aubry and MacKay[5] system (1) admits time-periodic and spatially localized solutions - discrete breathers - of the form

$$\hat{X}_l(t) = \hat{X}_l(t + \frac{2\pi}{\Omega_b}) \ , \ X_{|l| \to \infty} \to 0 \tag{3}$$

at suitably small coupling ϵ provided none of the multiples of the breather frequency Ω_b resonate with the spectrum of small-amplitude plane waves of (1) which for small coupling implies

$$k\Omega_b \neq \sqrt{V''(0)} \, . \tag{4}$$

In this limit of weak coupling $\epsilon \to 0$ the breather solution is typically assumed to be of a compact form, in the easiest case a single-site excitation $\hat{X}_0(t) \neq 0$ and $\hat{X}_{l \neq 0}(t) = 0$. Then the nonresonance condition (4) at the anticontinuum limit $\epsilon = 0$ can be satisfied only if the oscillator potential V is chosen to be nonisochronous, i.e. $d\Omega_b / dE \neq 0$ where E is the energy of a particle oscillating in V. This excludes from considerations all types of isochronous potentials, especially the well-known harmonic case $V(x) \sim x^2$. This lead to an expectation that for the case of harmonic potentials V there exist no breathers in weakly coupled systems. Below we will show that contrary to this expectation for suitable interaction functions W breathers exist and persist down to zero coupling even for harmonic potentials V.

To proceed we fix the potentials to

$$V(x) = \frac{1}{2}x^2 \ , \ W(x) = \frac{1}{4}x^4 \, . \tag{5}$$

The equations of motion read

$$\ddot{X}_l = -X_l - \epsilon(X_l - X_{l-1})^3 - \epsilon(X_l - X_{l+1})^3 \ . \tag{6}$$

Although the total potential of the system is not a homogeneous function of all coordinates, we may use the time-space separation ansatz[6]

$$X_l(t) = (-1)^l A_l G(t) \tag{7}$$

where A_l is a time-independent amplitude and $G(t)$ is a lattice site independent master function of time. The resulting equations are

$$A_l(\ddot{G} + G) = -G^3 \epsilon \left[(A_l + A_{l-1})^3 + A_l + A_{l+1})^3 \right] \tag{8}$$

which lead to a differential equation for G

$$\ddot{G} = -G - \kappa G^3 \tag{9}$$

and a difference equation for the amplitudes A_l

$$\frac{\kappa}{\epsilon} A_l = (A_l + A_{l-1})^3 + (A_l + A_{l+1})^3 \tag{10}$$

where $\kappa > 0$ is a separation constant of arbitrary choice. The differential equation (9) corresponds to the problem of an anharmonic oscillator with solutions being periodic in time. The difference equation (10) was studied by Flach[7], where it was proven that localized solutions of the type $A_{|l| \to \infty} \to 0$ do exist by considering (10) as a two-dimensional map and searching for homoclinic trajectories. Thus we arrive at a general existence proof of discrete breathers for the choice (5).

In particular we may choose $\kappa = \epsilon$. Then we easily may continue the system into the zero coupling limit $\epsilon \to 0$ and still keep the breather solution. The time dependence of the solution will correspond to the solution of a harmonic oscillator (cf. (9)). This concludes the proof that discrete breathers can be continued from the uncoupled limit of noninteracting harmonic oscillators by switching on a weak interaction. Note that the interaction has to be an anharmonic function of the coordinates, otherwise the only meaningful solutions would be delocalized plane waves. Note also that at the noninteracting limit the discrete breather solution is not a single site excitation, but is rather a spatially localized excitation of all oscillators. Details of the spatial decay are given by Dey et al[6].

By connecting the existence of breather solutions with tangent bifurcations of band edge plane waves[8], it is actually possible to extend the choice of interaction potentials to a much larger class of functions including also harmonic interaction parts, as well as to consider more general isochronous potentials[9].

3. Fano resonances

Another important issue concerning discrete breather properties is their scattering impact on small amplitude plane waves. While there exists some literature on that subject[10], there is an ongoing debate concerning the possibility of resonant total reflection of waves by discrete breathers[11], which has been observed numerically in many cases. Again we will use the anticontinuum limit to obtain analytical results. In the following we will consider the case of the DNLS (2). For small amplitude waves $\Psi_n(t) = \epsilon e^{i(\omega_q t - qn)}$ the equation (2) yields the dispersion relation

$$\omega_q = -2C \cos q \ . \tag{11}$$

Breather solutions have the form

$$\hat{\Psi}_n(t) = \hat{A}_n e^{i\Omega_b t} \ , \ \hat{A}_{|n| \to \infty} \to 0 \tag{12}$$

where the time-independent amplitude $\hat{A}_n$ can be taken real valued, and the breather frequency $\Omega_b \neq \omega_q$ is some 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 $\cosh \lambda = |\Omega_b|/2C$. Thus the breather can be approximated as a single-site excitation if $|\Omega_b| \gg C$. In this case the relation between the single-site amplitude $\hat{A}_0$ and Ω_b becomes $\Omega_b = -\hat{A}_0^2$. In the following we will neglect the breather amplitudes for $n \neq 0$, i.e. $\hat{A}_{n\neq 0} \approx 0$. In fact $\hat{A}_{\pm 1} \approx \frac{C}{\hat{A}_0} \ll 1$.

We add small perturbations to the breather solution

$$\Psi_n(t) = \hat{\Psi}_n(t) + \phi_n(t) \tag{13}$$

and linearize the equations for $\phi_n(t)$:

$$i\dot{\phi}_n = C(\phi_{n+1} + \phi_{n-1}) - \Omega_b \delta_{n,0}(2\phi_0 + e^{2i\Omega_b t}\phi_0^*) \tag{14}$$

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

$$\phi_n(t) = X_n e^{i\omega t} + Y_n^* e^{i(2\Omega_b - \omega)t} \tag{15}$$

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

$$-\omega X_n = C(X_{n+1} + X_{n-1}) - \Omega_b \delta_{n,0}(2X_0 + Y_0) \ , \tag{16}$$
$$-(2\Omega_b - \omega)Y_n = C(Y_{n+1} + Y_{n-1}) - \Omega_b \delta_{n,0}(2Y_0 + X_0) \ . \tag{17}$$

When treating (16,17) as an eigenvalue problem we note that the corresponding matrix is nonhermitian due to the nonzero coupling between the variables X_0 and Y_0. This is a consequence of the fact that the linearized phase space flow around a time-periodic orbit of a general Hamiltonian is characterized by a Floquet matrix which is symplectic. As a result the orbit may be either marginally stable or unstable, i.e. ω may be real or complex. In the following we will however focus on the transmission properties, leaving the issue of linear dynamical stability aside. We note however that in the considered limit of a nearly single-site localized breather solution in the DNLS it is well known that the solution *is* linearly stable[5].

Away from the breather center $n = 0$ Eq. (14) allows for the existence of plane waves with spectrum ω_q. This spectrum will be dense for an infinite chain. As we are interested in the propagation of waves, we will set $\omega \equiv \omega_q$ with some value of q. Then it follows that the X-channel is open and guides propagating waves, while the Y-channel is closed, i.e. its frequency $2\Omega_b - \omega_q$ does not match the spectrum ω_q itself.

Instead of solving (16,17) we will consider a slightly more general set of equations

$$-\omega_q X_n = C(X_{n+1} + X_{n-1}) - \delta_{n,0}(V_x X_0 + V_a Y_0) \ , \tag{18}$$
$$-(\Omega - \omega_q)Y_n = C(Y_{n+1} + Y_{n-1}) - \delta_{n,0}(V_y Y_0 + V_a X_0) \tag{19}$$

which is reduced to (16,17) for $\Omega = 2\Omega_b$ and $V_x = V_y = 2V_a = 2\Omega_b$. We note that for $V_a = 0$ the closed Y channel provides with exactly one localized eigenstate due to a nonzero value of V_y, located at

$$\omega_L^{(y)} = \Omega + \sqrt{V_y^2 + 4C^2} \ . \tag{20}$$

To compute the transmission coefficient we make use of the transfer matrix method described e.g. by Tong et al[12]. The boundary conditions are:

$$X_{N+1} = Te^{iq} \ , \ X_N = T \ , \ Y_{N+1} = D/\kappa \ , \ Y_N = D \ , \tag{21}$$
$$X_{-N-1} = 1 + R \ , \ X_{-N} = e^{iq} + Re^{-iq} \ ,$$
$$Y_{-N-1} = F \ , \ Y_{-N} = \kappa F \ . \tag{22}$$

Here T and R are the transmission and reflection amplitudes. F and D describe the exponentially decaying amplitudes in the closed Y-channel, where the degree of localization is connected with the coefficient $\kappa \equiv e^{\lambda}$:

$$\kappa = \frac{1}{2C}\left[-(\Omega - \omega_q) + \sqrt{(\Omega - \omega_q)^2 - 4C^2}\right] . \tag{23}$$

The transfer matrix is a 4×4 matrix, which is defined by (18,19) at $n = 0$. After the corresponding solving of four linear equations we obtain

$$|T|^2 = \frac{4\sin^2 q}{\left(2\cos q - a - \frac{d^2\kappa}{2-b\kappa}\right)^2 + 4\sin^2 q} , \tag{24}$$

$$a = \frac{-\omega_q + V_x}{C} \; , \; b = \frac{-(\Omega - \omega_q) + V_y}{C} \; , \; d = \frac{V_a}{C} . \tag{25}$$

This central result allows one to conclude that total reflection is obtained when the condition

$$2 - b\kappa = 0 \tag{26}$$

is realized. It is equivalent to the condition

$$\omega_q = \omega_L^{(y)} , \tag{27}$$

which has a very physical meaning: perfect reflection is obtained when a local mode, originating from the closed Y-channel, is resonating with the spectrum ω_q of plane waves from the open X-channel. The only condition is that the interaction V_a is nonzero. Remarkably, the resonance position does not depend on the actual value of V_a, so 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 not of any importance. This resonant total reflection is very similar to the Fano resonance effect, as it is unambiguously related to a local state resonating and interacting with a continuum of extended states. The fact that the resonance is independent of V_a is due to the assumed local character of the coupling between the local mode (originating from the Y-channel) and the open channel. If this interaction is assumed to have some finite localization length by itself, then the resonance condition (27) may be renormalized[13].

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 (24,25) and obtain the following expression for the transmission T_b:

$$|T_b|^2 = \frac{4\sin^2 q}{\left(-\frac{2\Omega_b}{C} - \frac{\Omega_b^2}{2C^2}\frac{\kappa_b}{2C - \cos q\kappa_b}\right)^2 + 4\sin^2 q} \tag{28}$$

with

$$\kappa_b = \frac{1}{2C}\left(-(2\Omega_b - \omega_q) + \sqrt{(2\Omega_b - \omega_q)^2 - 4C^2}\right) . \tag{29}$$

The result is that any breather solution of the DNLS close to the anticontinuous limit yields perfect reflection close to $q = \pi/2$. In the very anticontinuous limit perfect reflection is obtained precisely at $q = \pi/2$. Indeed, if we expand (28) in $\frac{C}{\Omega_b}$ we obtain in the lowest order

$$|T_b|^2 \approx \frac{4C^4}{\Omega_b^4} \sin^2 2q , \tag{30}$$

provided $\frac{C}{2|\Omega_b|} \ll |\cos q|$. At the same time the DNLS breather is linearly stable, so another conclusion is that total reflection is not related to stability or instability of the scattering periodic orbit. The reason for the appearance of total reflection at the anticontinuous limit is that the closed channel has distance $2\Omega_b$ from the open channel, but the local state of the closed channel is located at the same distance $2\Omega_b$ from the closed channel, leading to a resonance with the open channel.

References

1. A. J. Sievers and J. B. Page, in *Dynamical properties of solids VII phonon physics the cutting edge*, Elsevier, Amsterdam, 1995; S. Aubry, Physica D, **103**, 201 (1997); S. Flach and C. R. Willis, Phys. Rep. **295**, 181 (1998).
2. E. Trias, J. J. Mazo and T. P.Ornaldo, Phys. Rev. Lett. **84**, 741 (2000); B. Binder, D. Abraimov, A. V. Ustinov, S. Flach and Y. Zolotaryuk, Phys. Rev. Lett. **84**, 745 (2000).
3. B. I. Swanson, J. A. Brozik, S. P. Love, G. F. Strouse, A. P. Shreve, A. R. Bishop and W.-Z. Wang, Phys. Rev. Lett. **82**, 3288 (1999).
4. U. T. Schwarz, L. Q. English and A. J. Sievers, Phys. Rev. Lett. **83**, 223 (1999).
5. R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
6. B. Dey, M. Eleftheriou, S. Flach and G.P. Tsironis, Phys. Rev. E **65**, 017601 (2001).
7. S. Flach, Phys. Rev. E **51**, 1503 (1995).
8. S. Flach, Physica D **91**, 223 (1996).
9. J. Dorignac and S. Flach, in preparation.
10. S. Flach, and C. R. Willis, in: *Nonlinear Excitations in Biomolecules*, ed. by M. Peyrard, Editions de Physique, Springer-Verlag, 1995; S. Kim, C. Baesens, and R. S. MacKay, Phys. Rev. E **56**, R4955 (1997); T. Cretegny, S. Aubry and S. Flach, Physica D **199**, 73 (1998); S. W. Kim, and S. Kim, Phys. Rev. B **63**, 212301 (2001).
11. S. W. Kim and S. Kim, Physica D **141**, 91 (2000); S. Flach, A. E. Miroshnichenko and M. V. Fistul, submitted to CHAOS, cond-mat/0209427.

12. P. Tong, B. Li and B. Hu, Phys. Rev. B **59**, 8639 (1999).
13. S. Flach, V. Fleurov, A. E. Miroshnichenko and M. V. Fistul, in preparation.