DISCRETE BREATHERS - RECENT RESULTS AND APPLICATIONS

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Nontopological spatially localized time periodic excitations - coined discrete breathers - are generic solutions for lattice Hamiltonians. I present recent results including the spatial decay of discrete breathers in systems with interactions decaying algebraically in space, the properties of the static deformation accompanying a breather excitation in low-symmetry lattice Hamiltonians with Goldstone modes, nonzero energy thresholds in lattice dimensions $d \geq 2$, models with analytic solutions and compact solutions. Finally I will discuss several experimental applications.

1 Introduction

The study of dynamical nontopological localization in nonlinear Hamiltonian lattices has experienced a considerable development during the past decade[1,2,3]. The discreteness of space - i.e. the usage of a spatial lattice - is crucial in order to provide structural stability for spatially localized excitations. Spatial discreteness is a very common situation for various applications from e.g. solid state physics.

To make things precise let us consider a d-dimensional hypercubic spatial lattice with discrete translational invariance. Each lattice site is labeled by a d-dimensional vector l with integer components. To each lattice site we associate one pair of canonically conjugated coordinates and momenta X_l, P_l which are real functions of time t. Let us then define some Hamiltonian H being a function of all coordinates and momenta and further require that H has the same symmetries as the lattice. The dynamical evolution of the considered system is given by the standard Hamiltonian equations of motion. Without loss of generality let us demand that H is a nonnegative function and that $H = 0$ for $X_l = P_l = 0$ (for all l). Call this state the classical ground state. Generalizations to other lattices and larger numbers of degrees of freedom per lattice site are straightforward.

When linearizing the equations of motion around $H = 0$ we obtain an eigenvalue problem. Due to translational invariance the eigenvectors will be spatially extended plane waves, and the eigenvalues Ω_q (frequencies) form a phonon spectrum, i.e. Ω_q is a function of the wave vector q. Due to the symmetry of the Hamiltonian Ω_q will be periodic in q. Moreover the phonon spectrum will be bounded, i.e. $|\Omega_q| \leq \Omega_{max}$. Depending on the presence or absence of Goldstone modes Ω_q might be gapless (zero belongs to the spectrum, spectrum is acoustic) or exhibit a gap ($|\Omega_q| \geq \Omega_{min}$, spectrum is optical). Increasing the number of degrees of freedom per lattice site induces several branches in Ω_q with possible gaps between them.

Let us search for spatially localized time periodic solutions of the full nonlinear equations of motion, i.e. $X_{|l|\rightarrow\infty} \rightarrow 0$ and $X_l(t) = X_l(t+T_b)$ (same for P). These solutions are coined discrete breathers. If a solution exists, we can expand it into a Fourier series in time, i.e. $X_l(t) = \sum_k A_{kl} \mathrm{e}^{\mathrm{i}k\omega_b t}$ ($\omega_b = 2\pi/T_b$). Spatial localization implies $A_{k,|l|\rightarrow\infty} \rightarrow 0$. Insert these series into the equations of motion. This results in a set of coupled algebraic equations for the Fourier amplitudes[3]. Consider the spatial tail of the solution where all Fourier amplitudes are small and should further decay to zero with growing distance from the excitation center. Since all amplitudes are small, we can linearize the equations. This procedure decouples interaction in k-space and we obtain for each k a linear equation for A_{kl} with interaction in l. This equation will contain $k\omega_b$. It will in fact be identical to the above discussed equation linearized around $H = 0$ and it will contain $k\omega_b$ instead of Ω_q[3]. If $k\omega_b = \Omega_q$ the corresponding amplitude A_{kl} will not decay in space, instead it will oscillate. To obtain localization we arrive at the nonresonance condition $k\omega_b \neq \Omega_q$[3]. This condition has to be fulfilled for all integer k. For an optical spectrum Ω_q frequency ranges for ω_b exist which satisfy this condition. For acoustic spectra $k = 0$ poses a problem. We will discuss this case below in more detail.

The nonresonance condition is only a necessary condition for generic occurence of discrete breathers. More detailed analysis shows that breathers being periodic orbits bifurcate from band edge plane waves[4]. The condition for this bifurcation is an inequality involving parameters of expansion of H around $H = 0$[4].

Discrete breathers (periodic orbits) appear generically as one-parameter families of periodic orbits. The parameter of the family can be e.g. the frequency (or the energy, action etc). Note that we do not need any topological requirement on H (no energy barriers). Indeed breather families have limits where the breather delocalizes and its amplitude becomes zero.

With the help of the nonresonance condition we can exclude the generic existence of spatially localized solutions which are quasiperiodic in time. Indeed in the simplest case we would have to satisfy a nonresonance condition $k_1\omega_1 + k_2\omega_2 \neq \Omega_q$ for ω_1/ω_2 being irrational and all possible pairs of integers k_1, k_2. This is impossible[5].

2 Spatial decay properties of discrete breathers

Consider

$$H = \sum_l \left[\frac{1}{2} P_l^2 + V(X_l) + \sum_{l' \neq l} W_{l-l'}(X_l - X_{l'}) \right] \tag{1}$$

with $V(z), W_l(z)$ being nonnegative functions and $V(0) = W_l(0) = 0$. If $\partial^2 V / \partial z^2$ is nonzero for $z = 0$ then Ω_q is optical. In the opposite case the phonon spectrum is acoustic. If Ω_q is optical and Ω_q^2 an analytical function in q (this is realized for any finite range interaction $W_{l>l_c} = 0$ but also e.g. for $W_l(z)$ exponentially decaying in l) the interaction part of H is called short-ranged. To compute the spatial decay of a breather solution we use the above mentioned linearized equations for its Fourier amplitudes A_{kl}. With the help of Green's function method we find[6]

$$A_{kl} \sim \int_{1.\mathrm{BZ}} \frac{\cos(ql)}{(k\omega_b)^2 - \Omega_q^2} \mathrm{d}^d q \quad . \tag{2}$$

Here the integration extends over the first Brillouin zone. Due to general properties of convergence of Fourier series[7] we conclude that for short-range interactions A_{kl} decay exponentially in l, where the exponents depend on k [5]. The exponent of A_{kl} tends to zero whenever $k\omega_b$ approaches an edge of Ω_q. Note that in such a limit the linearization of the algebraic equations in the tails of the breather ceases to be correct for a finite number of selected $k' \neq k$ and nonlinear corrections to (2) apply[8]. Still the spatial decay is exponential.

2.1 Algebraically decaying interactions

Consider a one-dimensional lattice with algebraically decaying interactions $W_l(z) \sim 1/l^s$ and $\partial^2 V / \partial z^2 |_{z=0} \neq 0$. Since Ω_q^2 is nonanalytic in q for this case, (2) implies that for large distances l the spatial decay of a breather will be algebraic[6]: $A_{kl} \sim 1/l^s$. However for $s \to \infty$ the spatial decay becomes short-ranged (nearest neighbour interactions). To understand the crossover to exponential decay in this limit, consider (2) for the case when $k\omega_b$ is very close to the edge of Ω_q which is characterized by some wave vector q_c. Since the integrand nearly diverges near q_c we may use a stationary phase approximation and expand Ω_q^2 around q_c taking into account only the leading order term. For $s > 3$ the leading order dependence of Ω_q^2 on q will be proportional to $(q - q_c)^2$. The nonanalytic behaviour is then hidden in higher order terms in $(q - q_c)$ and does not contribute within the approximation[6]. Since we approximate Ω_q^2 by an analytical function, we will obtain exponential decay in space. However we know that the asymptotic dependence of A_{kl} on l will be algebraic. We thus conclude that in the mentioned case of $k\omega_b$ being close to the edge of Ω_q the spatial decay will be exponential for intermediate distances, but becomes algebraic for distances larger than some crossover distance l_c. High-precision numerical computations confirm this prediction[6]. The crossover distance can be estimated to be given by

$$\frac{\ln l_c}{l_c} \approx \frac{\nu}{s} \tag{3}$$

where ν is the exponent of the spatial decay obtained within the stationary phase approximation[6]. From result (3) it follows that for $s \to \infty$ $l_c \to \infty$. This is an expected result, since in this short-range interaction limit we recover exponential decay in the whole space. More surprising is that also the limit $\nu \to 0$ (i.e. $k\omega_b \to \Omega_{q_c}$) yields $l_c \to \infty$. Exponential decay is thus also obtained in the whole space whenever the (multiple of a) frequency of the breather solution comes close to the edge of Ω_q.

2.2 Presence of Goldstone modes - acoustic breathers

When Ω_q contains zero, i.e. when the linearized equations around $H = 0$ yield Golstone modes, the dc component of a breather solution A_{kl} with $k = 0$ deserves special attention. All ac components ($k \neq 0$) can be analyzed similar to the case of an optical spectrum. If the Hamiltonian is invariant under the transformation $X_l \to -X_l$ then time-periodic solutions being invariant under this transformation will have $A_{kl} = 0$ for even k which includes $k = 0$. However if such a parity symmetry is broken, all Fourier components will become nonzero.

Assume that Ω_q^2 is analytical in q. Since the $k = 0$ component can not decay exponentially in space, at large distances from the breather the leading order part of the solution will be given by its slowly decaying dc part, the static lattice distortion. Its corresponding linearized equation will be similar to the equation for a strain in continuum mechanics, which is induced by some local deformation (the breather center) of the system[9]. The strain will decay algebraically in space. The constraint of finite energies leads to the requirement that the monopole contribution to the local deformation is zero for $d = 1, 2$. The resulting algebraic decay $A_{0l} \sim 1/|l|^{d-1}$ induced by a dipole has been numerically confirmed for $d = 2$ [9].

2.3 *Energy thresholds for discrete breathers*

A direct consequence of the spatial decay properties of discrete breathers is the possible appearance of nonzero energy thresholds. We remind that breathers show up as one-parameter families of time-periodic solutions in phase space. When sliding along such a family all parameters characterizing the breather will continuously change. Physically important is the presence or absence of an energy gap. First we observe that the only limit where the breather energy could vanish is the limit of zero amplitudes, i.e. the limit when ω_b approaches the edge of Ω_q. Let us estimate the far field energy part of a breather E_b

$$E_b \sim \int_1^\infty r^{d-1} F_d^2(\delta r) \mathrm{d}r \tag{4}$$

where the energy density is proportional to $A_{1r}^2 \sim F_d^2(\delta r)$. Since in the considered limit the spatial decay will be weakly exponential (no matter whether Ω_q^2 is analytical or not) the function $F_d(\delta r)$ is bounded by an exponential function with exponent δ. Assuming that the dispersion near the band edge in Ω_q is in leading order quadratic in $(q - q_c)$, we find $\delta \sim |\omega_b - \Omega_{q_c}|$. In the same limit, using perturbation theory for weakly nonlinear plane waves with amplitude A and frequency ω_b, we can estimate $|\omega_b - \Omega_{q_c}| \sim A^2$. Since the breather in the considered limit is a slightly distorted (localized) plane wave, we finally arrive at[10]

$$E_b \sim |\omega_b - \Omega_{q_c}|^{1-d/2} \quad . \tag{5}$$

This result implies that the breather energy can not assume arbitrary small values for $d \geq 2$. Consequently in such a case breathers have nonzero lower bounds on their energy (and similarly on their action). In some nongeneric cases nonzero energy gaps may occur even for one-dimensional systems[10]. Also nonanalytical dispersion Ω_q^2 may lower the critical lattice dimension[6].

3 Analytic discrete breather solutions

Although discrete breathers are generic solutions for lattice Hamiltonians, they are not easily obtained in a closed analytic form. In the following we will present classes of functions H for which closed expressions can be obtained, though no special integrability requirement for H has to be fulfilled. What is needed in first place is separability of time and space. This can be obtained for homogeneous potential functions. Consider the one-dimensional lattice

Hamiltonian

$$H = \sum_l \left[\frac{1}{2} P_l^2 + \frac{1}{2} (X_l - X_{l+1})^2 h(S_l) \right] \tag{6}$$

where $h(z)$ is some function and $S_l = \frac{X_l}{X_{l+1}} + \frac{X_{l+1}}{X_l}$. Making the ansatz $X_l(t) = u_l G(t)$ we find $\ddot{G} = -\kappa G$ and a set of nonlinear coupled algebraical equations for the amplitudes u_l which contains the separation parameter κ. These equations can be explicitely solved with e.g. $u_l = (-1)^l e^{-\beta|l|}$. A necessary and sufficient condition is that the function $h(z)$ satisfies

$$h(-z_0) = -z_0(z_0 + 1)h'(-z_0) \tag{7}$$

for a positive value of $z_0 > 2$ (note that (7) is not a differential equation)[11]. The exponent β is defined by $z_0 = 2\cosh\beta$. The locality of condition (7) allows to generate whole classes of $h(z)$.

It is also possible to define Hamiltonian functions in higher lattice dimensions with explicit breather solutions. Let us briefly introduce these models. Define $\hat{L}X_l = \sum_{l',|l-l'|=1} X_{l'}$ and $S_l = \frac{\hat{L}X_l}{X_l}$. Then the Hamiltonian

$$H = \sum_l \left[\frac{1}{2} P_l^2 + \frac{1}{2} (\hat{L}X_l)^2 h(S_l) \right] \tag{8}$$

allows for explicit breather solutions[11] if the function $g(z) = \frac{1}{2} z^2 h(z)$ satisfies two local equalities at z_0 and z_1:

$$g(z_0) = g(z_1) \ \ , \ \ g'(z_0) = g'(z_1) \ \ . \tag{9}$$

4 Compact discrete breather solutions

Compactons have been discussed for PDEs by Rosenau[12]. The basic idea is to consider field equations which lack linear dispersion terms. On a lattice it is easy to implement an analogous idea. All we have to require is that $\partial H / \partial X_l$ vanishes for $X_l = 0$ and arbitrary values of all other variables. This is satisfied for

$$H = \sum_l \left[\frac{1}{2} P_l^2 + V(X_l) + F(X_l) \sum_{l' \neq l} W_{l-l'} (X_l - X_{l'}) \right] \tag{10}$$

with $F(0) = F'(0) = 0$ (simplest choice is $F(z) = z^2$). Indeed in such a case it is possible to excite a cluster (or several clusters) of lattice sites with nonzero displacements and momenta, but the dynamics will be restricted to the initially excited sites, leaving all unperturbed sites with $X = P = 0$ unchanged.

5 Applications

The discrete breather concept has been recently used for different experimental situations. Light injected into a narrow waveguide which is weakly coupled to parallel waveguides (characteristic diameter and distances of order of micrometers, nonlinear optical medium based on GaAs materials) disperses to the neighbouring channels for small field intensities, but localizes in the initially injected wave guide for large field intensities[13].

Bound phonon states (up to seven participating phonons) have been observed by overtone resonance Raman spectroscopy in PtCl mixed valence metal compounds[14]. Bound states are quantum versions of classical discrete breather solutions.

Spatially localized voltage drops in Nb-based Josephson junction ladders have been recently observed and characterized[15] (typical size of junction is a few micrometers). These states correspond to generalizations of discrete breathers to dissipative systems.

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