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q-BREATHERS IN FPU-LATTICES — SCALING AND PROPERTIES FOR LARGE SYSTEMS

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Recently q-breathers - time-periodic solutions which localize in the space of normal modes and maximize the energy density for some mode vector q_0 - were obtained for finite nonlinear lattices. We scale these solutions to arbitrarily large lattices in various lattice dimensions. We study the scaling consequence for previously obtained analytical estimates of the localization length of q-breathers for β-FPU and α-FPU lattices. The first finding is that the degree of localization depends only on intensive quantities and is size independent. Secondly a critical wave vector k_m is identified, which depends on one effective nonlinearity parameter. q-breathers minimize the localization length at $k_0 = k_m$ and completely delocalize in the limit $k_0 \rightarrow 0, \pi$.

Keywords: Nonlinearity; normal modes; localization.

1. Introduction

Recently it was shown[1], that a one-dimensional anharmonic atomic chain allows for exact time-periodic solutions which localize exponentially in the space of normal modes and have their maximum energy on a mode with mode number q_0. The existence and properties of these q-breathers allowed to explain the major ingredients of the famous Fermi-Pasta-Ulam problem (FPU)[2,3,4] in a clear and constructive way. The FPU problem concerns the nonequipartition of normal mode energies on time scales which can be many orders of magnitude larger than the characteristic vibration periods. The key ingredient for the construction of q-breathers is a finite nonlinear system[1]. This is a very general condition and may apply to many other systems as well. It has been recently successfully tested[5] by considering FPU models with lattice dimension $d = 2, 3$ and also discrete nonlinear Schrödinger models (DNLS) in various lattice dimensions[6]. A q-breather, being periodic in time, can be viewed as one normal mode which is dressed by several other normal modes in a neighbourhood of q_0 and has an infinite lifetime. Further studies also revealed the persistence of q-breathers in thermal equilibrium[1], which shows their relevance for statistical properties of extended systems.

Here we show that q-breathers persist and have invariant properties for large system sizes by using real space renormalization procedures. We then reveal intriguing new localization properties of q-breathers for large lattices. These results are particularly important because they apply to macroscopic systems.

Consider a generic model of a D-dimensional nonlinear lattice of size $N_1 \times \ldots \times N_D$, defined by a Hamiltonian

$$H = \sum_{\boldsymbol{n}} \left[\frac{p_{\boldsymbol{n}}^2}{2} + U(x_{\boldsymbol{n}}) + \sum_{l=1}^{D} V(x_{\boldsymbol{n}+\boldsymbol{e}_l} - x_{\boldsymbol{n}}) \right] \tag{1}$$

where $x_{\boldsymbol{n}}$, $p_{\boldsymbol{n}}$ are canonical variables. $U(x)$ and $V(x)$ are anharmonic on-site and interaction potentials, respectively. Their Taylor expansion around $x = 0$ starts with quadratic terms. $\boldsymbol{n} = \{n_1, \ldots, n_D\}$ is a D-dimensional lattice vector with $n_l = \overline{1, N_l}$. $\boldsymbol{e}_l$ denotes a unitary lattice vector along the dimension l. We will consider the cases of fixed, free and periodic boundary conditions (BC). Note that $x_{\boldsymbol{n}} = 0$ is an equilibrium state of the system.

This Hamiltonian can be expressed in terms of normal modes $P_{\boldsymbol{q}}$, $Q_{\boldsymbol{q}}$ of the linearized problem, obtained by skipping all anharmonic terms in the potentials:

$$H = \sum_{\boldsymbol{q}} E_{\boldsymbol{q}} + H^{int}(Q_{\boldsymbol{q}}) \ , \ E_{\boldsymbol{q}} = \frac{1}{2} \left(P_{\boldsymbol{q}}^2 + \omega_{\boldsymbol{q}}^2 Q_{\boldsymbol{q}}^2 \right) \tag{2}$$

where $E_{\boldsymbol{q}}$ is the energy of a given normal mode and H^{int} is the mode interaction part of the Hamiltonian which appears due to anharmonicity. The integer components of the mode vector $\boldsymbol{q}$ enumerate the modes. That is a class of models for which exact q-breather solutions may exist[1,5]. Such solutions are time-periodic and the normal mode energies are exponentially localized around a mode vector $\boldsymbol{q}_0$.

2. Scaling and real space renormalization

We search for a way of scaling a given solution $Q_{\boldsymbol{q}}(t)$ of a system (2) of size N to a solution $\tilde{Q}_{\tilde{\boldsymbol{q}}}(t)$ of a system of scaled size. It consists of scaling the values of mode variables $\sqrt{r}$ times and scaling their indices r times, filling the gaps with zeros:

$$\tilde{Q}_{\tilde{q}_l}(t) = \begin{cases} \sqrt{r} Q_{q_l}(t), & \tilde{q}_l = r q_l \\ 0, & \tilde{q}_l \neq r q_l \end{cases} , \tag{3}$$

where we omitted all mode indices except the l-th component. In case of fixed BC $q_l = \overline{1, N_l}$, and the scaled system size is assumed $\tilde{N}_l + 1 = r(N_l + 1)$. In cases of free and periodic BC $q_l = \overline{0, N_l - 1}$, and the system size is scaled as $\tilde{N} = rN$. The phase space of the scaled system then possesses an invariant subspace (also coined a bush of modes[7]). This procedure can be applied to construct a solution to a system

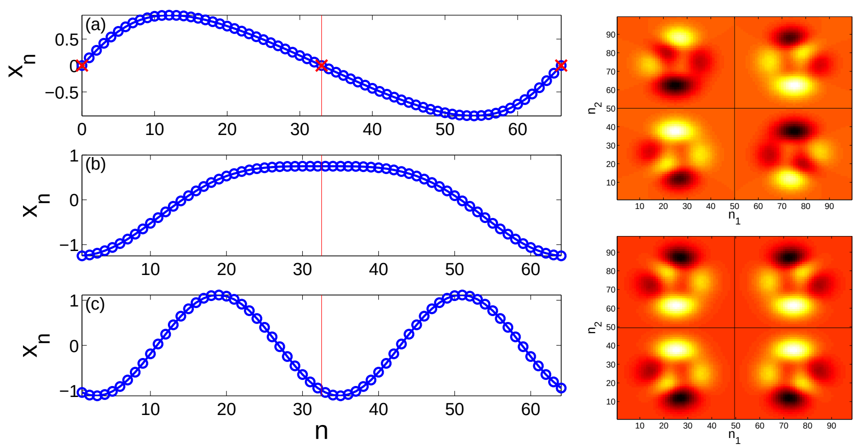

Fig. 1. Left panel: Constructing a solution in a chain of double size in real space, cases of fixed (a), free (b) and periodic (c) boundary conditions. In (a) boundaries and the additional lattice site in the center are marked with crosses. Initial size is $N = 32$. The momentary displacements versus lattice site are shown. Right panel: Scheme of constructing a solution in real space of a 2d lattice with fixed (upper plot) and open (bottom plot) BC, scaled twice along both dimensions. Thin lines denote borders between blocks. Initial size is 49×49. Color coding schematically represents the oscillator displacements in real space.

of arbitrarily large size, increasing r. In order to identify the applicability of (3) in systems with each of the three mentioned types of boundary conditions, we will use a renormalization in real space which is equivalent to (3).

Consider $D = 1$ in (1). The equations of motion read

$$\ddot{x}_n = f(x_n) + \varphi(x_{n+1} - x_n) - \varphi(x_n - x_{n-1}) \,. \tag{4}$$

Here $f(x) = -U'(x)$, $\varphi(x) = V'(x)$ and $n = \overline{1, N}$. We start with fixed BC $x_0 = x_{N+1} = 0$ and odd restoring force $f(x) = -f(-x)$. Then (4) is invariant under the following combined parity and sign reversal symmetry: $x_n \to -x_{N+1-n}(t)$. The real-space representation of transformation (3) for fixed BC is given by an alternation of spatial blocks constructed by parity and sign reversal transform. The blocks are separated by additional nonexcited lattice sites (see Fig. 1(a)):

$$\tilde{x}_n(t) = \{x_1(t), \ldots, x_N(t), 0, -x_N(t), \ldots, -x_1(t), 0, \ldots\}.$$

It is straightforward to observe that if $x_n(t)$ is a solution to the initial system, then $\tilde{x}_n(t)$ is a solution to the scaled-size system. For the case of free BC of the model (4) $x_0 = x_1, x_{N+1} = x_N$, we need odd $\varphi(x)$. Then the equations of motion are invariant under parity transform $x_n \to x_{N+1-n}(t)$. Consequently we can take a solution to a system of size N, and construct a solution to a system of a scaled size rN by the replacement of mode variables (3). The real-space representation of this transformation (see Fig. 1(b)) is given by

$$\tilde{x}_n(t) = \{x_1(t), \ldots, x_N(t), x_N(t), \ldots, x_1(t), \ldots\}.$$

In the case of periodic BC $x_{N+1} = x_1$, $x_0 = x_N$ the scaling consists of simply gluing together blocks of a given size, and we do not need to request any symmetry of the force functions. The scaling rule (3) is thus confirmed for 1D chains (4) with fixed, open and periodic BC.

We generalize the above results to higher lattice dimensions. The transformation to mode variables is a superposition of the corresponding 1D transforms applied along each lattice dimension. Then, the transformation (3) along a dimension l corresponds to one of the transforms already discussed for the $D = 1$ case. The force symmetry requirements for open and periodic BC are identical to the 1D case. For fixed BC we have to request odd $\varphi(x)$ in addition.

Given a q-breather solution for the original finite system, we can thus scale the q-breather solution to larger system sizes. Its total energy is scaled in all cases like $\tilde{E} = rE$, which is ensured by the block structure of the scaling and the local structure of the coupling in the Hamiltonian (1). The time-dependent mode energies E_q are transformed as $\tilde{E}_{\tilde{q}}(t) = rE_q(t)$ for $\tilde{q} = rq$, and $\tilde{E}_q = 0$ for other q. Introducing the energy density as $\varepsilon = E/(N+1)$ and wavenumber $k = \pi q/(N+1)$ for fixed BC ($\varepsilon = E/N$ for free and periodic BC, $k = \pi q/N$ for free BC, $k = 2\pi q/N$ for periodic BC), it is straightforward to observe that the scaling procedure leaves the energy density and the wave number (vector) of a q-breather invariant. Together with the rigorous proof of existence of q-breathers for finite systems[1] we arrive at a rigorous proof of existence of these excitations for infinite system sizes, with proper scaling and under certain restrictions for the potential functions. Since the scaled solutions are embedded on mode bushes[7], the question arises whether q-breathers with other (or any) values of k_0 exist in large systems as well. The fact that the scaling preserves the localization properties of the scaled excitations suggests a positive answer and was recently confirmed[8]. We also note that we needed certain symmetry properties of the potentials for the scaling to work. It however does not imply that for cases with less symmetries q-breathers do not exist.

3. Localization properties of q-breathers for large systems

The localization properties of q-breathers in the normal mode space have been obtained analytically using asymptotic expansions for FPU-models in various lattice dimensions. We will now analyze the consequences with respect to the above scaling results for fixed BC and $D = 1$.

3.1. β-FPU model

For $f = 0$ and $\varphi = x + \beta x^3$, the result[1] expressed in total energies and mode numbers reads $E_{(2n+1)q_0} = \lambda^n E_{q_0}$ with $\sqrt{\lambda} = 3\beta E_{q_0}(N+1)/(8\pi^2 q_0^2)$ for $D = 1$ and $q_0 \ll N$. In fact this relation holds also for q-breathers with frequencies close to the upper Debye cutoff, when q_0 in above expressions is formally replaced by $\tilde{q}_0 = N + 1 - q_0$. We conclude that it must be possible to substitute densities and wave numbers instead, and obtain an expression which is independent of the actual system size. Indeed the outcome of our substitution is written in the following way:

$$\ln \varepsilon_k = \left(\frac{k}{k_0} - 1\right) \ln \sqrt{\lambda} + \ln \varepsilon_{k_0}, \quad \sqrt{\lambda} = \frac{3\beta}{8} \frac{\varepsilon_{k_0}}{k_0^2}. \tag{5}$$

Similar expressions (differing only in a constant prefactor in $\sqrt{\lambda}$) are obtained for higher lattice dimensions. Let us analyze the k-dependence of (5). We compute q-breathers at fixed average energy density ε. In the approximation of exponential localization it follows $\varepsilon_{k_0} = (1-\lambda)\varepsilon$. Together with the definition of λ in (5) we find, that the inverse localization length in k-space is given by the absolute value of the slope S:

$$S = \frac{1}{k_0} \ln \sqrt{\lambda}\ , \ \sqrt{\lambda} = \frac{z^2}{2}(\sqrt{1+4z^{-4}} - 1)\ , \ z = \frac{k_0}{\nu}\ , \ \nu^2 = \frac{3\beta}{8}\varepsilon\ , \tag{6}$$

where z is a scaled wavenumber and ν the effective nonlinearity parameter. It follows, that $S = S_m/\nu$ where the master function $S_m = z^{-1} \ln \sqrt{\lambda}$ depends only on the scaled wavenumber z. S_m vanishes for $z \to 0$ and has its largest absolute value $max(|S_m|) \approx 0.7432$ at $z_{min} \approx 2.577$. For a fixed effective nonlinearity parameter ν the q-breather with $k_{min} = \nu z_{min}$ shows the strongest localization, while larger and smaller k_0 tend to weaken the localization. Especially for $k_0 \to 0$ the q-breather delocalizes completely. With increasing ν, the localization length of the q-breather for $k_0 = k_{min}$ increases. For $k_0 \gg \nu$ it follows $S_m \approx -2z^{-1}\ln(z)$ and for $k_0 \ll \nu$ we find $S_m \approx -z/2$ (see left panel in Fig.2). We test our prediction by computing

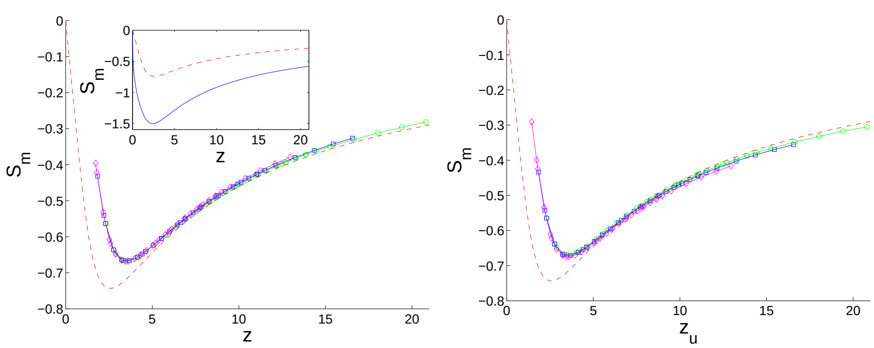

Fig. 2. Left panel: Dashed curve shows analytical estimation of S_m as a function of $z = k_0/\nu$ for the β-FPU chain. Symbols correspond to computed and scaled slopes of q-breathers for three different energy densities $\varepsilon = 6.08 \cdot 10^{-4}$ (circles), $9.6 \cdot 10^{-4}$ (squares), $1.57 \cdot 10^{-3}$ (diamonds) and two different sizes $N = 149, 359$ and $\beta = 1$. Inset: analytical S_m versus z for the α-FPU chain (bottom curve), curve for β-FPU also shown (top). Right panel: S_m as a function of $z_u = (\pi - k_0)/\nu$ for q-breathers with $|N - q_0| \ll N$ for the β-FPU chain, other parameters and notation same as in the left panel.

the scaled slope for various q-breathers of the β-FPU chain (symbols in left panel in Fig.2). We nicely observe an optimum wavenumber for localization. Deviations from the theoretical curves for small z are due to strong nonlinear corrections to our estimates, while deviations at larger z are finite size corrections to the analytical estimates. The numerically obtained values of slope as a function of wavenumber with different N at any given ε fit on a single smooth curve[8]. We note further, that the numerical data for different ε condense at small k_0 into a single universal dependence $S_m(z)$. Although it differs from the analytically obtained function, the scaling result from above is thus confirmed. In the right panel in Fig.2 we show the corresponding result for q-breathers with $|N - q_0| \ll N$. As predicted and expected, again an optimum wavenumber for strongest localization is found, and q-breathers delocalize completely at the Debye cutoff.

The reason for the weaker localization of q-breathers when $k_0 \gg \nu$ is the increasing distance $3k_0$ between modes excited in consecutive orders of perturbation theory. The delocalization for $k_0 \to 0$ and $k_0 \to \pi$ however is due to an approaching of resonances[1] $n\omega_{k_0} \to \omega_k$ for some integer n.

3.2. *α-FPU model*

For $f = 0$ and $\varphi = x + \alpha x^2$, the result[1,5] expressed in total energies and mode numbers reads $E_{nq_0} = n^2 \gamma^{n-1} E_{q_0}$ with $\gamma = \alpha^2 E_{q_0} (N+1)^3/(\pi^4 q_0^4)$ for $D = 1$. Substituting densities and wave numbers we find:

$$\ln \varepsilon_k = \left(\frac{k}{k_0} - 1 \right) \ln \gamma + 2 \ln \left(\frac{k}{k_0} \right) + \ln \varepsilon_{k_0} , \quad \gamma = \frac{\alpha^2 \varepsilon_{k_0}}{k_0^4} . \tag{7}$$

In the approximation of exponential localization it follows $\varepsilon_{k_0} = \frac{(1-\gamma)^3}{1+\gamma} \varepsilon$ and together with (7)

$$\gamma = z^{-4} \frac{(1-\gamma)^3}{1+\gamma} \ , \ z = \frac{k_0}{\xi} \ , \ \xi = \sqrt{\alpha} \varepsilon^{1/4} \ . \tag{8}$$

Here we again introduced a scaled wave number z and the effective nonlinearity parameter ξ. The inverse localization length S of a q-breather is then defined by a master slope S_m via

$$S = \frac{S_m}{\xi} \ , \ S_m = \frac{1}{z} \ln \gamma \ . \tag{9}$$

The dependence of $S_m(z)$ is shown in the inset in Fig.2. It has a minimum at $z_{min} \approx 2.39$ and a value $S_m(z_{min}) \approx -1.5$. At variance to the β-FPU case the dependence for small $z \ll 1$ is $S_m \approx -(2z)^{1/3}$. That may be related to the observation that the convergence of exponents describing the anomalous heat conductivity in these finite systems is much faster for the β-FPU case than for the α-FPU case (Ref. 9 and Fig.4 therein). There one needs to overcome a certain system size to replace the ballistic-type propagation of long wavelength modes by scattering, which may be related to the delocalization of q-breathers for small k_0.

4. Discussion

Let us estimate the minimum system size at which scattering processes for long wavelength modes become essential. The localization length of a q-breather is given by $|S|^{-1}$. The localization becomes meaningless when $|S|^{-1} \approx \pi$ which is the size of the Brillouin zone. With the above results we estimate the critical k_0 at which that happens, and finally assume that the system size is large enough to resolve this value, so $k_0 = \pi/N_c$. Then we obtain for the β-FPU chain $N_c(\beta) \approx \frac{8\pi^2}{6\beta\varepsilon}$, and for the α-FPU chain $N_c(\alpha) \approx \frac{2\pi^4}{\alpha^2\varepsilon}$. Taking the numbers from Ref. 9 ($\varepsilon = 0.1$, $\beta = 1$, $\alpha = 0.25$) we obtain $N_c(\beta) \approx 130$ and $N_c(\alpha) \approx 30000$. The numerical data for the β-FPU case in Fig.2 imply that these estimates are upper bounds. According to Lepri[9] $N_c(\beta) \approx 150$ and $N_c(\alpha) \approx 10000$ which shows good qualitative and semiquantitative agreement with our estimates.

We expect the above results to qualitatively hold independent of the dimension D. It remains a challenging task to perform computations for e.g. $D = 2$, since one needs about 10^5 lattice sites, which is presently not reachable with our numerical tools.

We fixed the average energy density in order to ensure finite temperatures. If the energy density ε_{k_0} is fixed, then q-breathers will delocalize for some nonzero value of k_0. For a finite lattice $\varepsilon \approx N\varepsilon_{k_0}$ at that point.

We also studied a DNLS model[6] in various lattice dimensions with similar results. We conclude that the power of nonlinearity and the type of the underlying lattice equations do not crucially change the above outcome.

For a spatially discrete system the normal mode spectrum has a finite width. It defines a critical nonlinearity value, for which k_m reaches the center of the band. It can be roughly estimated as $\nu \sim 1$. For larger values of ν the system will enter a regime of strong nonlinearity, where q-breathers may become meaningless.

We considered standing waves. We expect the results to be also of importance for travelling waves which are reflected at boundaries or inhomogeneities.

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