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Scaling properties of q-breathers in nonlinear acoustic lattices

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Abstract

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 together with the size of the system to arbitrarily large 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 $k_0 \to 0$.

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Spatially extended nonlinear Hamiltonian systems serve as starting models for the study of excitations in many branches in physics, e.g. anharmonic vibrations of crystal lattices, mesoscopic and nanoscopic systems, molecules, but also of electromagnetic, acoustic and other waves in nonlinear media, to name a few. They have been studied over many decades in order to understand such intriguing material properties as heat conductivity, thermal expansion, turbulence, confinement of light, but also general mathematical aspects such as thermalization, mode–mode interactions, etc. While in any realistic situation damping and energy input have to be considered as well, these dissipative effects are often weak enough to allow the observation of the underlying Hamiltonian excitations.

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. 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. The existence and properties of these q-breathers allowed to explain the major ingredients of the famous Fermi–Pasta–Ulam problem (FPU) [2–4] 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 with dispersion [1]. This is a very general condition and may apply to many other systems as well. It has been recently successfully tested by considering FPU models with lattice dimension $d = 2, 3$ [5] and also discrete nonlinear Schrödinger models (DNLS) in various lattice dimensions [6]. Further studies also revealed the persistence of q-breathers in thermal equilibrium [1], which shows their relevance for statistical properties of extended systems. Previous studies of the FPU problem suggested that the effect of nonequipartition will disappear for large system sizes [3,4]. That seems to imply a disappearance of q-breathers in that limit. Here we show that q-breathers persist and have invariant properties for large system sizes. These results are particularly important because they apply to macroscopic systems.

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

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

where $x_{\mathbf{n}}$, $p_{\mathbf{n}}$ are canonical variables. $U(x)$ and $V(x)$ are anharmonic on-site and interaction potentials, respectively, such that $x_{\mathbf{n}} = 0$ is a stable equilibrium state of the system, and at least one of $U(x)$ and $V(x)$ has a non-zero quadratic Taylor expansion term. $\mathbf{n} = \{n_1, \ldots, n_D\}$ is a D-dimensional lattice vector with $n_l = \overline{1, N_l}$. $\mathbf{e}_l$ denotes a unitary lattice vector along the dimension l. We will consider the case of fixed boundary conditions (BC). We have also studied free and periodic BC with similar results.

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

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

where $E_{\mathbf{q}}$ 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 $\mathbf{q}$ 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 $\mathbf{q}_0$.

We search for a size scaling transformation which maps a given solution $Q_{\mathbf{q}}(t)$ of a system (2) of size N to a solution $\tilde{Q}_{\tilde{\mathbf{q}}}(t)$ of a system of scaled size. Consider a mapping which consists of scaling the values of mode variables $\sqrt{r}$ times and scaling their indices r times along a chosen lattice dimension l, filling the gaps with zeros:

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

and all the other components of $\mathbf{q}$ are equal on both sides. For fixed BC, $q_l = \overline{1, N_l}$, and the scaled system size is assumed $\tilde{N}_l + 1 = r(N_l + 1)$. In order to identify the applicability of (3), we will rewrite it in real space and insert into the equations of motion.

Consider $D = 1$ in (2). 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 $n = \overline{1, N}$. For fixed BC, $x_0 = x_{N+1} = 0$. The normal modes are defined by a discrete sine transform. The transformation (3) is then expressed in real space by an alternation of spatial blocks, obtained from the previous by parity and sign reversal transform $x_n \to -x_{N+1-n}$. The blocks are separated by additional nonexcited lattice sites (see Fig. 1):

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

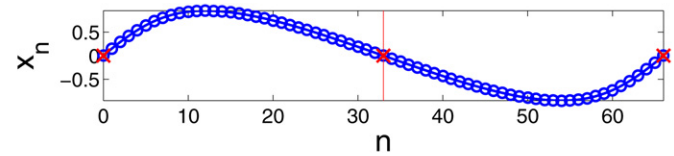

Fig. 1. (Colour online.) Constructing a solution in a chain of double size in real space. Boundaries and the additional lattice site in the center are marked with crosses. Initial size is $N = 32$. The momentary displacements versus lattice site are shown.

We further assume an odd restoring force $f(x) = -f(-x)$. Then it is straightforward to observe that for $x_n(t)$ being a solution to the initial system, $\tilde{x}_n(t)$ is a solution to the scaled-size system. The scaling rule (3) is thus confirmed for 1D chains (4).

We generalize the above results to higher lattice dimensions. The transformation to mode variables is a superposition of 1D transforms along each dimension. Then, the transformation (3) along a lattice direction l corresponds to the real-space transform already discussed for the $D = 1$ case. It yields a solution to a scaled-size system if both $f(x)$ and $\varphi(x)$ are odd functions.

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 of arbitrarily large size, increasing r.

Given a q-breather solution for the original finite system, we can thus scale the solution to larger system sizes. Its total energy is scaled like $\tilde{E} = rE$, which is ensured by the block structure of the scaling and the local structure of the coupling in the Hamiltonian (2). 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 wave number $k_q = \pi q/(N+1)$ and average energy densities $\varepsilon = E/(N+1)$, $\varepsilon_{k_q} = E_q/(N+1)$, it is straightforward to observe that the scaling transform leaves these intensive quantities invariant in the sense that $\tilde{\varepsilon} = \varepsilon$ and $\tilde{\varepsilon}_{\tilde{k}} = \varepsilon_k$ for $\tilde{k} = k$. 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. It also implies, that any observable (in particular, the k-space localization length of a q-breather) which is defined in terms of intensive quantities must be invariant to scaling transform.

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. Below we will address this question. 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.

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. For $f = 0$ and $\varphi = x + \beta x^3$, the result from [1,5] is expressed in total energies and mode numbers $E_{(2n+1)q_0} = \lambda^n E_{q_0}$ with

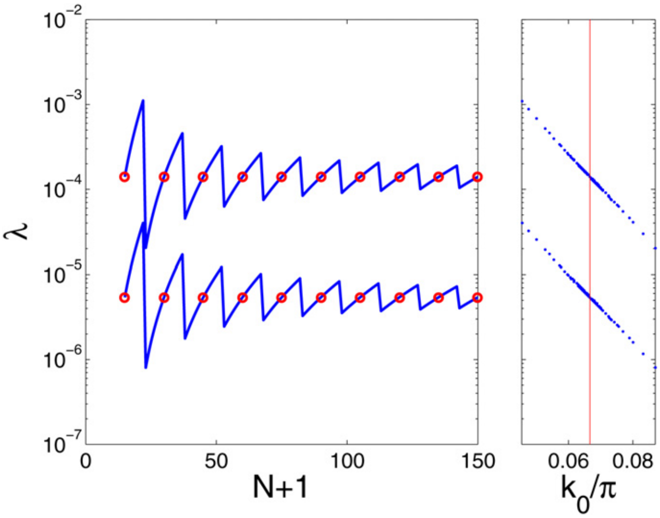

Fig. 2. (Colour online.) Dependence of the localization parameter λ on the system size N of a q-breather (left panel) for the β-FPU chain at constant energy density, $\varepsilon = 4 \times 10^{-4}$ and 2×10^{-3} (for lower and upper curves, respectively) and $\beta = 1$. q_0 is chosen to be the nearest integer to $k_0(N+1)/\pi$, $k_0 = \pi/15$. Open circles mark system sizes $N+1 = r(N_0+1)$, $N_0 = 15$, for which the prediction is that λ should be invariant on the integer r. The right panel shows the smooth dependence of the measured λ values on the actual wave numbers k_0 used in the left panel.

$\sqrt{\lambda} = 3\beta E_{q_0}(N+1)/(8\pi^2 q_0^2)$ for $D = 1$ and $q_0 \ll N$. 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:

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

Note that these results hold actually for $D = 1, 2, 3$ [5]. This expression does not depend explicitly upon N as suggested by the scaling invariance from above. Note however, that N determines the grid of allowed wave number values k_q.

We test the size-dependence of λ, when the size of the system takes different values, and the new wave number $\tilde{k}_0$ is chosen to be the nearest one to the original k_0 value. We compute q-breathers for that model with $D = 1$ for various system sizes starting with $N_0 = 15$ and plot the numerically found λ as a function of N in the left panel in Fig. 2. The mode number q_0 is chosen to be the nearest integer to $k_0(N+1)/\pi$, $k_0 = \pi/15$. We obtain λ from the ratio of the energy densities $\varepsilon_{5q_0}/\varepsilon_{3q_0}$. First we observe that λ is independent on N when $N+1 = r(N_0+1)$. Secondly we observe fluctuations of λ around a mean value for other values of N due to the fact that for these system sizes the closest wave number to k_0 will nevertheless be slightly different. Thus we probe λ with wave numbers slightly varying around k_0. These deviations decrease with increase of the system size. The fluctuation amplitude in Fig. 2 decreases as well due to a smooth dependence of λ on k_0, which is confirmed in the right panel in Fig. 2.

Let us analyze the k-dependence of (5) for $D = 1$. For q-breathers at fixed average energy density ε it follows within the approximation of exponential localization that $\varepsilon_{k_0} = (1-\lambda)\varepsilon$.

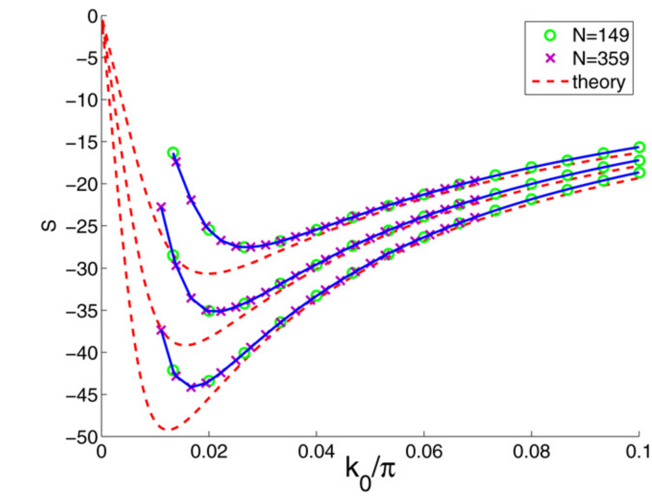

Fig. 3. (Colour online.) The slope S as a function of k_0 for the β-FPU chain and three different energy densities $\varepsilon = 6.08 \times 10^{-4}$, 9.6×10^{-4}, 1.57×10^{-3} and $\beta = 1$ (dashed curves, from bottom to top). Symbols and eye-guiding solid lines: estimate of the slope from numerical computations of q-breathers for $N = 149$ and $N = 359$.

Inserting this expression into (5) and resolving it in terms of $\sqrt{\lambda}$, we calculate the slope S whose absolute value is the inverse localization length in k-space:

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

S is negative, vanishes for $k_0 \to 0$ and has its largest absolute value $\max(|S|) \approx 0.7432/\nu$ at $k_{\min} \approx 2.577\nu$. For a fixed effective nonlinearity parameter ν the q-breather with $k_0 = k_{\min}$ shows the strongest localization. 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 $S \approx 2/k_0 \ln(\nu/k_0)$ and for $k_0 \ll \nu$ we find $S \approx -k_0/(2\nu^2)$.

We plot in Fig. 3 the dependence $S(k_0)$ for the β-FPU chain according to (6) (dashed curves) at three different energy densities. If ν or N are small enough, then the first non-zero k_0 value will appear for $k_0 > k_{\min}$. Increasing ν or N we shift some allowed low lying k values to the left of the minimum $k_0 < k_{\min}$. For very large systems (dense filling of the x-axis in Fig. 3 with allowed k_0 values) we thus expect that among them there is an optimum wavelength which provides strongest localization.

We test our prediction by computing the slope for various q-breathers of the β-FPU chain. The results are shown in Fig. 3 (symbols). We nicely observe an optimum value of k_0 for localization. Increasing the nonlinearity parameter (by either increasing the nonlinearity strength or the energy density) the critical wavenumber is shifted further away from the edge of the spectrum and gets shallower, as predicted. Deviations from the theoretical curves for small k_0 are due to strong nonlinear corrections to our estimates, while deviations at larger k_0 are finite size corrections to the analytical estimates. Note the smooth dependence of S on k_0 which does not depend on the system size, thus confirming the scaling results from above.

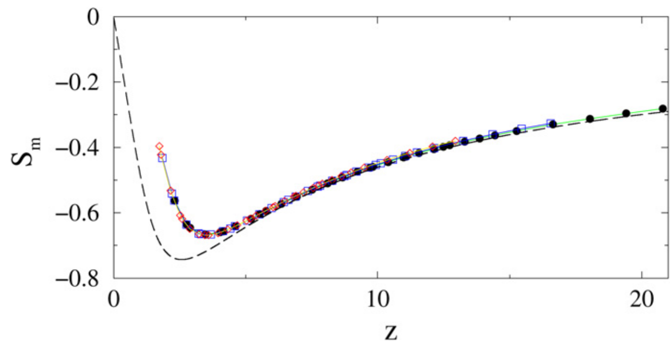

Fig. 4. (Colour online.) The master slope function $S_m(z)$ (dashed line). Different symbols correspond to the numerically obtained slopes from Fig. 3 which are scaled accordingly and fall on a single curve.

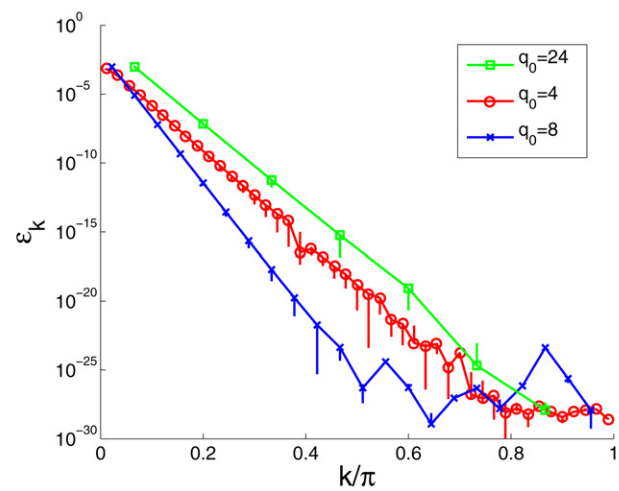

Fig. 5. (Colour online.) The profiles of q-breather solutions for $N = 359$, $\beta = 1$, $\varepsilon = 9.6 \times 10^{-4}$ and three different values of q_0 which yield $k_0/\pi = 0.011, 0.022, 0.067$ and correspond to the most left point on the middle curve in Fig. 3, its minimum and a point to the right of it. Symbols denote the mode energies at the moment of vanishing coordinates $x_l = 0$. The vertical bars denote the range of mode energy values taken during one period of the q-breather.

We plot in Fig. 4 the single master slope function $S_m(z) = \nu S$ with $z = k_0/\nu$ and scale all numerically obtained slopes as well. The numerical data all condense on one single curve at small k_0. Thus higher order corrections to the decay law do not alter the scaling properties of q-breathers in the limit of small k_0.

The profiles of three q-breather solutions for $\varepsilon = 9.6 \times 10^{-4}$ are shown in Fig. 5. The symbols correspond to normal mode energies at the moment when all coordinates vanish. Among them is the q-breather with the strongest localization. The precision of computation is 10^{-8} (see [1] for details). Since the normal mode energies are not conserved quantities, we show as well the fluctuation range for each of them. These fluctuations become stronger at particular k-values and are possibly due to a closely nearby lying resonance, which nevertheless does not destroy the localization profile.

Let us discuss the obtained results. 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 $k_0 \to 0$ however is due to an approaching of resonances $n\omega_{k_0} \to \omega_k$ for some integer n [1]. Note that the same approaching of resonances holds at the upper frequency cutoff where the frequency detuning is quadratic in k and the relevant integer $n = 1$. We computed the dependence of the slope S there and obtained a behaviour similar to the one in Fig. 3. Similar results were also obtained for free BC at the lower and the upper spectrum edges. 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 non-zero value of k_0. For a finite lattice $\varepsilon \approx N\varepsilon_{k_0}$ at that point.

We derived similar results for the α-FPU model with $\varphi = x + \alpha x^2$ using the estimates from [1]. We obtain strongest localization for $k_m \approx 2.39\xi$ and $\max(|S|) \approx 1.5/\xi$ with the effective nonlinearity parameter $\xi = \sqrt{\alpha/\pi}\,\varepsilon^{1/4}$. For small k_0 the slope $S \sim -(2k_0/\xi)^{1/3}$.

In all cases the localization becomes meaningless when $|S|^{-1} \approx \pi$ which is the size of the first Brillouin zone. That happens at $\tilde{k}_0 \approx 3\beta\varepsilon/(4\pi)$ (β-FPU) and at $\tilde{k}_0 \approx \alpha^2\varepsilon/(2\pi^5)$ (α-FPU). Well defined and localized q-breathers exist for $k_0 \gg \tilde{k}_0$. Strong resonances destroy them for $k_0 \ll \tilde{k}_0$ and lead to an effective redistribution of mode energy in that regime. The same reasoning defines a critical nonlinearity value, for which k_m reaches the center of the band. It can be roughly estimated as $\nu, \xi \sim 1$. For larger values of ν, ξ the system will enter a regime of strong nonlinearity, where q-breathers may become meaningless for any k_0.

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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