q-Breathers in Finite Two- and Three-Dimensional Nonlinear Acoustic Lattices

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In their celebrated experiment, Fermi, Pasta, and Ulam (FPU) [Los Alamos Report No. LA-1940, 1955] observed that in simple one-dimensional nonlinear atomic chains the energy must not always be equally shared among the modes. Recently, it was shown that exact and stable time-periodic orbits, coined q-breathers (QBs), localize the mode energy in normal mode space in an exponential way, and account for many aspects of the FPU problem. Here we take the problem into more physically important cases of two- and three-dimensional acoustic lattices to find existence and principally different features of QBs. By use of perturbation theory and numerical calculations we obtain that the localization and stability of QBs are enhanced with increasing system size in higher lattice dimensions opposite to their one-dimensional analogues.

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Nonlinearity induced interaction between normal modes of extended systems is crucial for many fundamental dynamical and statistical phenomena like thermalization, thermal expansion of solids, or turbulence in liquids. It is also important in many artificial systems where one aims at controlling the energy flow among the normal modes, preventing or efficiently channeling energy pumping due to resonances with external perturbations, etc. Among the many accumulated results in this area, a seminal one is due to Fermi, Pasta, and Ulam (FPU), who reported on the absence of thermalization of chains of atoms connected by weakly nonlinear springs [1]. They observed that the energy of an initially excited normal mode with frequency ω_q and mode number q did not spread over all other normal modes, staying almost completely locked within a few neighboring modes in the normal mode space [2,3]. Longer waiting times yielded another puzzle of energy recurrence to the originally excited mode. Many efforts to explain the FPU paradox resulted in extraordinary progress in this field: the observation of solitons [4], size-dependent stochasticity thresholds [5], nonlinear resonances [6], Kolmogorov-Arnold-Moser tori, Arnold diffusion, and many other issues [7–11]. The efforts to carry all these concepts into two-dimensional lattices have been also reported [12]. However, according to Ford [2], despite the richness of new topics, the original FPU problem was still waiting to be understood.

Recently it was shown that the major ingredients of the FPU problem can be addressed within the promising concept of q-breathers (QBs), which are exact time-periodic solutions in the nonlinear FPU chain [13]. These solutions are exponentially localized in the q space of normal modes and preserve stability for small enough nonlinearity. They continue from their trivial counterparts for zero nonlinearity at finite energy. In that limit they correspond to one mode with the seed mode number q_0 being excited, and all the other modes being at rest. The stability threshold of QB solutions coincides with the weak chaos threshold in [7]. Persistence of exact stable QB modes surrounded by almost quasiperiodic trajectories explains the origin of FPU recurrences and the absence of energy equipartition. The scaling of the localization exponents with the relevant control parameters relates to results on higher order nonlinear resonance overlaps [8]. But perhaps the most important result was that it needs only one ingredient to obtain QBs in FPU chains: a discrete nonequidistant frequency spectrum of normal modes, as induced by a finite system. Thus the door is opened to apply the concept of QBs to a variety of nonlinear finite systems—truly common objects in nature and applications. One of such challenges is an extension of the notion of QBs into more physically realistic two- and three-dimensional FPU-type systems.

In this Letter we report on the existence and remarkable properties of q-breathers in finite two- and three-dimensional nonlinear acoustic lattices. For fixed energy, the nonlinearity coefficient and seed mode vector the QB localization length stays finite in the 2D case and tends to zero in the 3D case with increasing size of the system. For both 2D and 3D cases the nonlinearity coefficient at the QB stability threshold increases in the same limit. These findings differ crucially from the 1D case [13] where QBs delocalize and the nonlinearity threshold of the instability tends to zero in the limit of large chains.

We consider quadratic and cubic lattices of N^d ($d = 2$ and 3, respectively) equal masses coupled by nonlinear springs with the Hamiltonian

$$H = \frac{1}{2}\sum_{\boldsymbol{n}}\left(p_{\boldsymbol{n}}^2 + \sum_{\boldsymbol{m}\in D(\boldsymbol{n})}\left[\frac{1}{2}(x_{\boldsymbol{m}} - x_{\boldsymbol{n}})^2 + \frac{\beta}{4}(x_{\boldsymbol{m}} - x_{\boldsymbol{n}})^4\right]\right), \tag{1}$$

where $x_{\boldsymbol{n}}(t)$ is the displacement of the $\boldsymbol{n} = (n_1, \ldots, n_d)$th particle from its original position, $p_{\boldsymbol{n}}(t)$ its momentum,

$D(\boldsymbol{n})$ is the set of its nearest neighbors, and fixed (zero) boundary conditions are taken: $x_{\boldsymbol{n}} = 0$ if $n_l = 0$ or $n_l = N + 1$ for any of the components of $\boldsymbol{n}$.

A canonical transformation

$$x_{\boldsymbol{n}}(t) = \left(\frac{2}{N+1}\right)^{d/2} \sum_{q_1,\text{ldots},q_d=1}^{N} Q_{\boldsymbol{q}}(t) \prod_{i=1}^{d} \sin\left(\frac{\pi q_i n_i}{N+1}\right) \quad (2)$$

takes into the reciprocal mode vector space with N^d normal mode coordinates $Q_{\boldsymbol{q}}(t) \equiv Q_{q_1,\ldots,q_d}(t)$. The normal mode space is spanned by $\boldsymbol{q}$ and represents a d-dimensional lattice similar to the situation in real space. The equations of motion then read

$$\ddot{Q}_{\boldsymbol{q}} + \Omega_{\boldsymbol{q}}^2 Q_{\boldsymbol{q}} = -\frac{16\beta}{(2N+2)^d} \sum_{\boldsymbol{p},\boldsymbol{r},\boldsymbol{s}} C_{\boldsymbol{q},\boldsymbol{p},\boldsymbol{r},\boldsymbol{s}} Q_{\boldsymbol{p}} Q_{\boldsymbol{r}} Q_{\boldsymbol{s}}. \quad (3)$$

Here $\Omega_{\boldsymbol{q}}^2 = 4\sum_{i=1}^{d} \omega_{q_i}^2$ are the squared normal mode frequencies with $\omega_{q_i} = \sin[\pi q_i/2(N+1)]$. Note that all linear modes but the diagonal ones $Q_{q_1=\cdots=q_d}$ are at least d-fold degenerate with respect to their frequencies. The coupling coefficients $C_{\boldsymbol{q},\boldsymbol{p},\boldsymbol{r},\boldsymbol{s}}$ induce a selective interaction between distant modes in the normal mode space similar to the 1D case.

For small amplitude excitations the nonlinear terms in the equations of motion can be neglected, and according to (3) the q oscillators get decoupled, each conserving its harmonic energy $E_{\boldsymbol{q}} = \frac{1}{2}(\dot{Q}_{\boldsymbol{q}}^2 + \Omega_{\boldsymbol{q}}^2 Q_{\boldsymbol{q}}^2)$ in time. Especially, we may consider the excitation of only one of the q oscillators, i.e., $E_{\boldsymbol{q}} \neq 0$ for $\boldsymbol{q} \equiv \boldsymbol{q}_0$ only. Such excitations are trivial time-periodic and q-localized solutions (QBs) for $\beta = 0$.

For the 1D chain, such periodic orbits can be continued into the nonlinear case at fixed total energy [13] because the nonresonance condition $n\Omega_{\boldsymbol{q}_0} \neq \Omega_{\boldsymbol{q}\neq\boldsymbol{q}_0}$ (here n is an integer) holds for any finite size [14]. This argument can be used straightforwardly for $d = 2, 3$ and large seed mode components $\boldsymbol{q}$ on the main diagonal such that $2\Omega_{\boldsymbol{q}} > 4$. For all other seed mode vectors on the main diagonal we checked that the nonresonance condition holds as well. For seed mode vectors off the main diagonal the above mentioned d-fold degeneracies could be lifted by considering anisotropic lattices. In fact, these degeneracies are lifted by the nonintegrability of the nonlinear lattice (3), and a discrete set of periodic orbits will remain. QBs are successfully observed in numerical experiments in the presence of the degeneracy, and we did not find substantial difficulties in computing them.

In the following we compute QBs as well as their Floquet spectrum numerically using the same algorithms as for the 1D atomic chain [13], and compare the results with analytical predictions, derived by means of asymptotic expansions.

First, we turn to the case $d = 2$. We obtain various symmetric [with $(q_0)_1 = (q_0)_2$, Figs. 1 and 2] and asymmetric [with $(q_0)_1 \neq (q_0)_2$] QBs in the lower frequency range, which are exponentially localized in q space. Note that due to the parity symmetry of the model [Eq. (1) is invariant under $x_{\boldsymbol{n}} \to -x_{\boldsymbol{n}}$ for all $\boldsymbol{n}$] only modes with odd components (q_1, q_2) are excited by the $\boldsymbol{q} = (3,3)0$ mode. In contrast to $d = 1$, the decay of the energy distribution [especially along the diagonal $\boldsymbol{q}(n) = (2n-1)\boldsymbol{q}_0$] remains almost constant with increase of the lattice size (Fig. 2).

The above-mentioned degeneracy of the frequency spectrum supports the existence of multimode QBs, namely, those that have two (or more) excited seed mode vectors. Indeed, we continued multimode periodic solutions of the linear lattice $E_{\boldsymbol{q}} \neq 0$ for $\boldsymbol{q} \in S(\boldsymbol{q}_0) = \{\boldsymbol{q}:\Omega_{\boldsymbol{q}} = \Omega_{\boldsymbol{q}_0}\}$ into the nonlinear regime. For example, the set $\boldsymbol{q}_0 = (2,3)$, $\boldsymbol{q}_0^* = (3,2)$ allows for two asymmetric QB solutions with the energy mainly concentrated in one of the two seed modes and two symmetric multimode QB solutions with the same energy in each of the seed modes, and oscillations being in or out of phase.

By an asymptotic expansion of the solution to (3) in powers of the small parameter $\sigma = \beta/(N+1)^2$ (in anal-

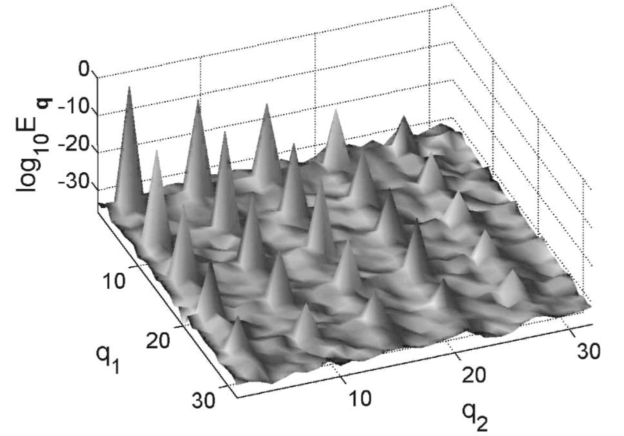

FIG. 1. A QB for $d = 2$ with $\boldsymbol{q}_0 = (3,3)$ for $\beta = 0.5$, $E_{\text{tot}} = 1.5$, frequency $\hat{\Omega} \approx 0.403$, $N = 32$.

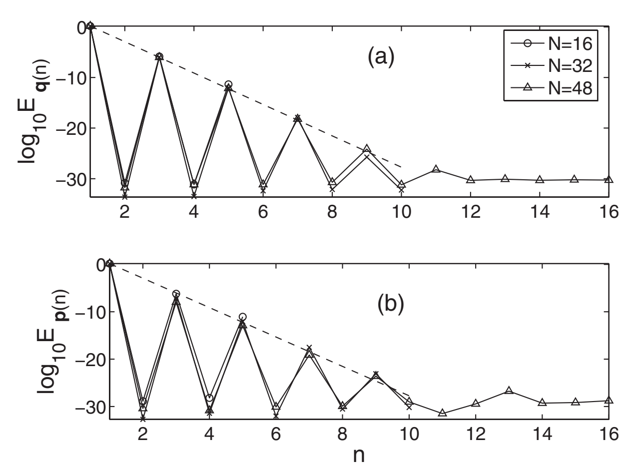

FIG. 2. The normal mode energies along (a) the diagonal $\boldsymbol{q}(n) = n\boldsymbol{q}_0$ and (b) the side direction $\boldsymbol{p}(n) = (q_{0,1}, nq_{0,2})$ for a QB with $\boldsymbol{q}_0 = (3,3)$, $\beta = 0.5$, $E_{\text{tot}} = 1.5$, $N = 16, 32, 48$, and the analytical estimate (4) (dashed lines).

ogy to [13]) we estimate the shape of a QB solution $\hat{Q}_{\boldsymbol{q}}(t)$ with a low-frequency seed mode vector $\boldsymbol{q}_0$ belonging to the diagonal. The energies of the modes on the diagonal $\boldsymbol{q}_0$, $3\boldsymbol{q}_0, \ldots, (2n+1)\boldsymbol{q}_0, \ldots, \ll (N, N)$, read

$$E_{(2n+1)\boldsymbol{q}_0} = \lambda_d^{2n} E_{\boldsymbol{q}_0}, \qquad \lambda_d = \frac{3\beta E_{\boldsymbol{q}_0} N^{2-d}}{2^{2+d}\pi^2|\boldsymbol{q}_0|^2}. \tag{4}$$

The dashed lines in Fig. 2(a) are obtained using (4) and show very good agreement with the numerical results. The energy distribution between other modes involved in the QB is more complicated, but the decay along the diagonal (4) gives a good estimate for it [Fig. 2(b)]. Note that the QB localization along the diagonal is the weakest, at least for large N. The shape of the QB in the q space then possesses the following properties: (i) the localization remains constant when the lattice size tends to infinity with all other parameters fixed, in contrast to the 1D case where QBs delocalize as $\lambda \propto (N+1)$; (ii) for constant *energy density* $\varepsilon = E_{\boldsymbol{q}_0}/(N+1)^2$ and the *wave vector* of the QB $\boldsymbol{\kappa}_0 = \boldsymbol{q}_0/(N+1)$ the degree of localization remains constant for $N \to \infty$ (similar to the 1D case); (iii) for smaller β, $E_{\boldsymbol{q}_0}$, and larger $|\boldsymbol{q}_0|$, QBs compactify. These results are a consequence of fundamental scaling properties of finite to infinite systems.

We analyze the stability of the obtained periodic orbits with standard methods of linearizing the phase space flow around the solutions and computing the eigenvalues and eigenvectors of a corresponding symplectic Floquet matrix [13]. The orbits are stable if all complex eigenvalues lie on the unit circle. The absolute values of the Floquet eigenvalues of QBs for symmetric $\boldsymbol{q}_0 = (3, 3)$ and asymmetric $\boldsymbol{q}_0 = (2, 3)$ are plotted versus β for different system sizes N in Fig. 3. Similar to the 1D case, QBs are stable for sufficiently weak nonlinearities. When β exceeds a certain threshold β^*, some eigenvalues get absolute values larger than unity (and some of them less than unity) and the QB becomes unstable. In remarkable contrast to the 1D case, β^* rapidly increases with the size of the system [Fig. 3(a)]. For a series of computationally accessible large lattices $N = 20, 30, 40$ [not plotted in Fig. 3(a)] we found the QB with $\boldsymbol{q}_0 = (3, 3)$ to be stable at least up to $\beta = 10.0$. For insufficiently large N the dependence $\beta^*(N)$ may become nonmonotonous [Fig. 3(b)]. It may be quite sensitive to the chosen seed wave number $\boldsymbol{q}_0$; compare Figs. 3(a) and 3(b).

The observed instabilities can be traced analytically, similar to the 1D case. Using standard secular perturbation techniques we approximate the frequency of the QB solution as $\hat{\Omega} = \Omega_{\boldsymbol{q}_0}(1 + 9h\rho) + O(h^2)$, where $h = 3\beta E_{\boldsymbol{q}_0}/(N+1)^2$ is a small parameter and $\rho = (w^2_{(q_0)_1} + w^2_{(q_0)_2})/\Omega^4_{\boldsymbol{q}_0}$. Linearizing the equations of motion (3) around a QB solution $Q_{\boldsymbol{q}} = \hat{Q}_{\boldsymbol{q}}(t) + \xi_{\boldsymbol{q}}$ we obtain

$$\ddot{\xi}_{\boldsymbol{q}} + \Omega^2_{\boldsymbol{q}}\xi_{\boldsymbol{q}} = -4h(1 + \cos 2\hat{\Omega}t)\sum_{\boldsymbol{p}} C_{\boldsymbol{q},\boldsymbol{q}_0,\boldsymbol{q}_0,\boldsymbol{p}}/\Omega^2_{\boldsymbol{q}_0}\xi_{\boldsymbol{p}} + O(h^2). \tag{5}$$

The strongest instability, caused by primary parametric resonance in (5), comes from pairs of resonant modes $\boldsymbol{q} + \boldsymbol{p} = 2\boldsymbol{q}_0$ with a nonzero vector $\boldsymbol{k} = \boldsymbol{q} - \boldsymbol{q}_0 = \boldsymbol{q}_0 - \boldsymbol{p}$. The bifurcation point and the absolute values of the Floquet multipliers involved in the resonance in its vicinity are represented by a complex expression, which demonstrates good agreement with the numerical results (Fig. 3). We assume $|k_{1,2}| \ll (q_0)_{1,2} \ll N$ and approximate

$$3\beta^* E_{\boldsymbol{q}_0}/(N+1)^2 = 8(\Omega_{\boldsymbol{q}} + \Omega_{\boldsymbol{p}} - 2\Omega_{\boldsymbol{q}_0})/\Omega_{\boldsymbol{q}_0} \approx 8\left(\frac{(q_0)_2 k_1 - (q_0)_1 k_2}{\boldsymbol{q}_0^2}\right)^2. \tag{6}$$

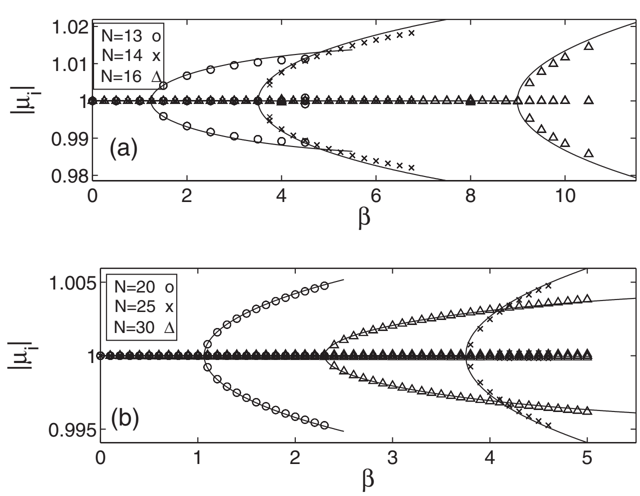

FIG. 3. Absolute values of Floquet eigenvalues (symbols) and analytical curves (solid lines) for QBs with $E_{\mathrm{tot}} = 1.5$ and (a) $\boldsymbol{q}_0 = (3, 3)$, $N = 13, 14, 16$ [the instabilities correspond to $\boldsymbol{k} = (1, 2)$ and $\boldsymbol{k} = (2, 1)$] and (b) $\boldsymbol{q}_0 = (2, 3)$, $N = 20, 25, 30$ [the instabilities correspond to $\boldsymbol{k} = (1, 1)$ for $N = 20, 25$ and $\boldsymbol{k} = (1, 2)$ for $N = 30$].

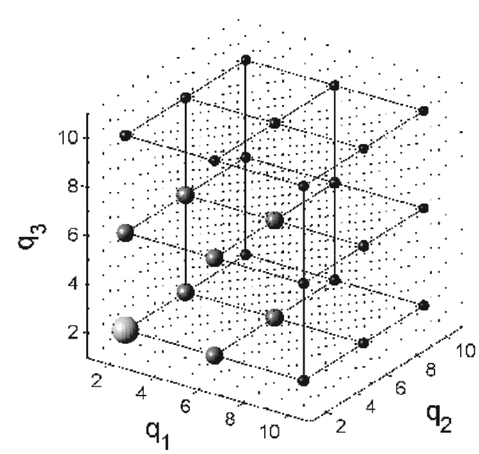

FIG. 4. The structure of the QB with $\boldsymbol{q}_0 = (2, 2, 2)$ on the three-dimensional lattice $N = 11$, $\beta = 0.5$, $E_{\mathrm{tot}} = 1.5$, $\hat{\Omega} \approx 0.897$. The size of spheres is a linear function of the decimal logarithm of the linear mode energy $E_{\boldsymbol{q}}$.

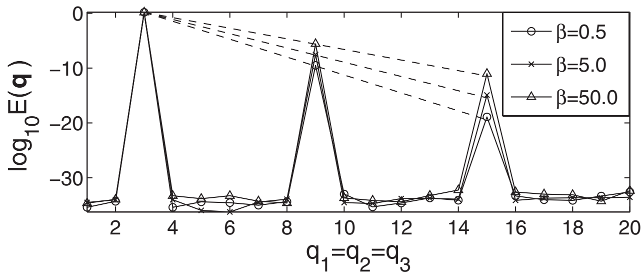

FIG. 5. The normal mode energies along the leading direction $\boldsymbol{q}(n) = (n, n, n)$ for $\boldsymbol{q}_0 = (3, 3, 3)$, $E_{\rm tot} = 1.5$, $N = 20$, and the analytical estimate (4) (dashed lines).

This estimate explains the following basic features of the observed instability. The instability of the type $\boldsymbol{k}$ that minimizes $|(q_0)_2 k_1 - (q_0)_1 k_2|$ is the first to occur. It results in a nonmonotonous and discontinuous dependence of $\beta^*(\boldsymbol{q}_0, N)$ for small lattices. It monotonously increases with N while $\boldsymbol{k}$ is constant [Fig. 3(a)]; when $\boldsymbol{k}$ changes, β^* changes as well [Fig. 3(b)]. Besides, the instability threshold scales as $\beta^* \propto \boldsymbol{q}_0^{-2}$ and $\beta^* \propto N^2$.

The 2D lattice supports also the existence of QBs with $\boldsymbol{q}_0$ located in the intermediate and high-frequency parts of the normal mode spectrum.

Let us turn to the case $d = 3$. We again compute QB solutions as in the 2D case (Fig. 4). A similar analysis shows that for the low-frequency seed mode vector $\boldsymbol{q}_0$ the decay of the normal mode energies along the leading direction $3\boldsymbol{q}_0, \ldots, (2n+1)\boldsymbol{q}_0, \ldots, \ll (N, N, N)$ is given by (4) with $d = 3$, and fits well the shape of the numerically computed QBs with $\boldsymbol{q}_0 = (3, 3, 3)$ (Fig. 5). In contrast to the 2D case, the localization length even decreases with increasing lattice size $\lambda_{3D} \propto (N+1)^{-1}$. For constant energy density $\varepsilon = E/(N+1)^3$ and wave vector of the QB $\boldsymbol{\kappa}_0$, the degree of localization is independent of the lattice size, as it is for the 1D and 2D cases. Despite having difficulties when calculating the stability of QBs in sufficiently large 3D lattices due to limited machine performance, the analytical treatment has been done similar to lower lattice dimensions. We find that $\beta^* \propto (N+1)^3$ for constant energy of the lattice and does not increase for fixed ε and $\boldsymbol{q}_0$. We also predict its sensitive dependence upon the choice of the seed mode vector of the QB and the size of the lattice when being small.

The main reason for the improvement of localization and stability of QBs in higher dimensions is due to (i) the decrease of the effective strength and (ii) the almost one-dimensional character of successive mode excitation by Q_{q_0} due to the selection rules of the nonlinear mode coupling.

In conclusion, we report on the existence and remarkable properties of q-breathers as exact time-periodic solutions in nonlinear two- and three-dimensional acoustic systems, thus extending the concept of one-dimensional QBs to more physically relevant objects. They are exponentially localized in the q space of the normal modes and preserve stability for small enough nonlinearity. In the limit of infinite lattice size, the localization length stays constant for $d = 2$ and tends to zero for $d = 3$ when fixing $\boldsymbol{q}_0$ and the total energy. At the same time the localization length does not depend on the lattice size N when fixing the energy density and the wave vector $\boldsymbol{\kappa}_0 = \boldsymbol{q}_0/(N+1)$. In contrast to the one-dimensional case, the observed instability threshold in the nonlinear coupling strength increases with increasing lattice size, and stays constant if the energy density is fixed.

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