q Breathers in Finite Lattices: Nonlinearity and Weak Disorder

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Nonlinearity and disorder are the recognized ingredients of the lattice vibrational dynamics, the factors that could be diminished, but never excluded. We generalize the concept of q breathers—periodic orbits in nonlinear lattices, exponentially localized in the linear mode space—to the case of weak disorder, taking the Fermi-Pasta-Ulan chain as an example. We show that these nonlinear vibrational modes remain exponentially localized near the central mode and stable, provided the disorder is sufficiently small. The instability threshold depends sensitively on a particular realization of disorder and can be modified by specifically designed impurities. Based on this sensitivity, an approach to controlling the energy flow between the modes is proposed. The relevance to other model lattices and experimental miniature arrays is discussed.

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Nonlinearity and disorder are ubiquitous and unavoidable features of discrete extended systems, the key players in a wealth of fundamental dynamical and statistical physical phenomena such as thermalization, thermal conductivity, wave propagation, electron and phonon scattering. Lattice vibrational modes are central to these processes. Nonlinearity induces interaction between normal modes, but may or may not lead to the energy equipartition [the Fermi-Pasta-Ulam (FPU) problem] [1], and makes possible time-periodic solutions exponentially localized in direct space (discrete breathers) [2]. Linear systems with disorder yield exponentially localized Anderson modes (AMs) [3]. But while the individual effects of nonlinearity and disorder are well-established, a satisfactory full understanding of their concurrent effect is missing. This gap is being progressively filled for strongly disordered and weakly nonlinear lattices by intensive research on continuation of AMs into nonlinear regime [4], wave packet spreading [5], light propagation in photonic lattices [6], and Bose-Einstein condensate (BEC) localization in random optical potentials [7].

Little, however, is known on how the systems with pronounced nonlinearity and weak disorder behave. Remarkably, it is a demand in a number of experimental and applicational contexts, beside a challenge from theory. Micro- and nano-electro-mechanical systems are rapidly developing components in microinstruments design [8]. Their array structures offer broadband excitations, elastic waves, and effects of dispersion to be utilized [9,10]. They are often suggested to operate in the nonlinear regime, while maturing technology reduces fabrication errors, hence diminishing spatial disorder. On the atomic scale, surface vibrational modes of three-dimensional gold nanoclusters may stay behind active and selective catalytic properties [11].

One of the fundamental types of nonlinear oscillatory modes are q breathers (QBs)—exact time-periodic solutions continued from linear modes and exponentially localized in the linear mode space. Originally proposed to explain the FPU paradox (the energy locking in low-frequency modes, recurrencies, and size-dependent stochasticity thresholds) [12], they have been discovered in two and three-dimensional finite and infinite lattices, discrete nonlinear Schrödinger (DNLS) arrays, and quantum Bose-Hubbard chains [13]. QBs have been suggested as major actors in a BEC pulsating instability and a four-wave mixing process in a nonlinear crystal [14].

In this Letter we extend the concept of QBs to weakly random nonlinear lattices, exemplifying in the FPU chain. The cornerstones of our approach are continuation of QBs into nonzero "frozen" disorder and statistical analysis of constructed solutions. QBs demonstrate the crossover from the exponential localization near the central mode to plateaus at a distance, and complete delocalization if a determined threshold is overcome. The average stability threshold in nonlinearity remains the same in the first order of approximation. In contrast, the standard deviation increases linearly with disorder, manifesting a high sensitivity on realizations. We analyze and explain the effect of the particular inhomogeneities and discuss the energy flow control by impurities design. The developed theory applies to physical arrays that are insufficiently large or disordered to display AMs, but manifest pronounced interplay between nonlinearity and disorder. It suggests a way to approach strongly disordered systems in terms of QBs on top of the AMs space.

The FPU-β chain of N equal masses, coupled by springs with disorder in linear coefficients and quartic nonlinearity in potential, is described by the Hamiltonian

$$H=\frac{1}{2}\sum_{n=1}^{N}p_n^2+\sum_{n=1}^{N+1}\left[\frac{1}{2}(1+D\kappa_n)(x_n-x_{n-1})^2+\frac{\beta}{4}(x_n-x_{n-1})^4\right], \quad (1)$$

where $x_n(t)$ is the displacement of the nth particle from its original position, $p_n(t)$ its momentum, $x_0 = x_{N+1} = 0$, $\kappa_n \in [-1/2, 1/2]$ are random, uniformly distributed, and uncorrelated with $\langle \kappa_n \kappa_m \rangle = \sigma_\kappa^2 \delta_{n,m}$, $\sigma_\kappa^2 = 1/12$ in our case. A canonical transformation $x_n(t) = \sqrt{\frac{2}{N+1}} \times \sum_{q=1}^{N} Q_q(t) \sin(\frac{\pi q n}{N+1})$ defines the reciprocal wave number space with N normal mode coordinates $Q_q(t)$, being solutions to the linear disorder-free case. The normal mode space is spanned by q and represents a chain similar to the situation in real space. It yields

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\beta}{2(N+1)} \times \sum_{p,r,s}^{N} C_{q,p,r,s} \omega_q \omega_p \omega_r \omega_s Q_p Q_r Q_s - \frac{D}{\sqrt{N+1}} \sum_{p}^{N} \omega_q \omega_p K_{q,p} Q_p. \quad (2)$$

Here $\omega_q = 2 \sin\frac{\pi q}{2(N+1)}$ are the normal mode frequencies. The coupling coefficients $C_{q,p,r,s}$ [12] induce the selective nonlinear interaction between distant modes and $K_{q,p} = \frac{2}{\sqrt{N+1}} \sum_{n=1}^{N+1} \kappa_n \cos\frac{\pi q(n-1/2)}{N+1} \cos\frac{\pi p(n-1/2)}{N+1}$ reflect the all-to-all linear interaction due to disorder. Nonlinearity and disorder parameters $\nu = \beta/(N+1)$, $d = D/\sqrt{N+1}$ are assumed to be small: $\nu, d \ll 1$.

Our methodology is two step. First, we take a known QB solution for $\nu \neq 0$ [12]. A particular realization of $\{\kappa_n\}$ is fixed and an asymptotic expansion in powers of $\{\nu, d\}$ is developed. Linear stability analysis of the constructed solution is carried out. Second, we study the statistical properties of the QB solution and instability threshold calculating respective averages and variances.

Note, that an alternative reciprocal space can be given by the modes of the disordered linear array. Still, the current choice allows for a detailed analytical study. In general, the theory of QBs can be formulated in the disordered modes space, their continuation into nonzero nonlinearity being proved by Albanese and Froehlich [4]. It offers a promising approach to the wave packet spreading problem in nonlinear strongly disordered lattices [4].

Continuation of QBs to $\beta, D \neq 0$ from $\beta \neq 0, D = 0$ employs the same technique as to $\beta \neq 0, D = 0$ from $\beta = D = 0$ [12]. For $\nu, d \ll 1$ and small amplitude excitations the q oscillators get effectively decoupled, their harmonic energy $E_q = \frac{1}{2}(\dot{Q}_q^2 + \omega_q^2 Q_q^2)$ being almost conserved in time. Single q-oscillator excitations are trivial time-periodic and q-localized solutions for $\beta = D = 0$.

For $d = 0$ such periodic orbits can be continued into $\beta \neq 0$ at fixed total energy [12] because the nonresonance condition $n\omega_{q_0} \neq \omega_{q \neq q_0}$ (integer n) holds for any finite size [15] and the Lyapunov theorem [16] applies. Same ideas are expected to work for $d \ll 1$, as the spectrum remains nonresonant with the probability 1 [4]. Such continuation succeeded for all parameters we took.

Numerically, we continue QBs from $\beta \neq 0$, $D = 0$ solutions increasing D and keeping $\{\kappa_n\}$ fixed. The total energy of the chain is $E = 1$ in all examples, and 100 realizations of disorder are generated. Dependence of the average QB energy distribution on the level of disorder is reported in Fig. 1. We observe an exponentially localized profile on the almost flat disorder-induced background. The plateau grows with D gradually absorbing localized modes. For $\beta = 0.01$, $q_0 = 5$, $N = 32$ the plateau overcomes E_{3q_0} near $D = 0.01$, but E_{q_0} holds beyond $D > 2$, as interpolation predicts. Interestingly, representation in the disordered modes space (filled diamonds) exhibits a typical QB profile with reduced background. It indicates that the theory of QBs in case of strong disorder should be developed in this reciprocal space.

Recall, that in case $D = 0$ the QB solution $\hat{Q}_q^{\mathrm{NL}}(t)$ with a low-frequency seed mode number q_0 can be written as an asymptotic expansion in powers of ν [12]. The energies of the modes $q_0, 3q_0, \ldots, (2n+1)q_0, \ldots \ll N$ read

$$E_{(2n+1)q_0}^{\mathrm{NL}} = \lambda^{2n} E_{q_0}, \qquad \lambda = \frac{3\beta E_{q_0}(N+1)}{8\pi^2 q_0^2}, \quad (3)$$

and the frequency $\omega^{\mathrm{NL}} = \omega_{q_0}(1 + 9/4\nu E_{q_0})$. Now we develop a perturbation theory to (2) in terms of the small disorder parameter d: $\hat{Q}_q(t) = Q_q^{(0)}(t) + dQ_q^{(1)}(t) + \ldots$, its frequency being $\hat{\omega} = \omega^{(0)} + d\omega^{(1)} + \ldots$, substituting $Q_q^{(0)}(t) = \hat{Q}_q^{\mathrm{NL}}(t)$ and $\omega^{(0)} = \omega^{\mathrm{NL}}$. In the first order approximation (2) becomes the equation of a forced oscillator: $\ddot{Q}_q^{(1)} + \omega_q^2 Q_q^{(1)} = -\omega_q \omega_{q_0} K_{q,q_0} Q_{q_0}^{(0)}$. It follows that all modes get excited by disorder, their amplitude the bigger the closer its frequency to ω_{q_0}:

$$A_q^{(1)} = -\frac{\omega_q \omega_{q_0}}{\omega_q^2 - \omega_{q_0}^2} K_{q,q_0} A_{q_0}, \qquad q \neq q_0, \quad (4)$$

the frequency being $\hat{\omega} = \omega_{q_0}(1 + 9/4\nu E_{q_0} + d/2K_{q,q_0})$. As $\langle K_{q,q_0} \rangle = 0$, the first order corrections in d vanish for the averages $\langle A_q^{(1)} \rangle = \langle \omega^{(1)} \rangle = 0$. Naturally, the variances are nonzero as the amplitude and frequency corrections vary depending on $\{\kappa_n\}$. The mode energy (averaged on $2\pi/\hat{\omega}$) approximately separates into nonlinearity and disorder-induced parts $E_q \approx E_q^{\mathrm{NL}} + E_q^{\mathrm{DO}}$, where

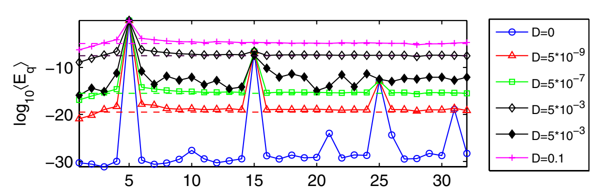

FIG. 1 (color online). The average mode energy distribution in QBs with $q_0 = 5$, $\beta = 0.01$, $N = 32$ under increasing disorder. Dashed lines are theoretical estimates (5). Filled diamonds: energy distribution in the disordered modes space for a particular realization, modes are sorted so that their frequencies increase with q.

$$\langle E_q^{\rm DO}\rangle = \frac{d^2 E_{q_0}\omega_q^4}{2(\omega_q^2-\omega_{q_0}^2)^2}\langle K_{q,q_0}^2\rangle = \frac{d^2 E_{q_0}\sigma_\kappa^2\omega_q^4}{2(\omega_q^2-\omega_{q_0}^2)^2}. \quad (5)$$

Two limit cases are of particular interest: (i) $q \gg q_0$, then $\langle E_q^{\rm DO}\rangle \approx d^2 E_{q_0}\sigma_\kappa^2/2$ that gives a q-independent plateau energy (dashed lines in Fig. 1), and (ii) $q = q_0 + 1$, then $\langle E_q^{\rm DO}\rangle \approx d^2\sigma_\kappa^2\omega_{q_0}^2(N+1)^2 E_{q_0}/2$, that yields the QB localization criterion $E_{q_0} \gg E_{q_0+1}$ if $\omega_{q_0} D\sigma_\kappa \ll 2E_{q_0}/(N+1)$. The condition $\langle E^{\rm DO}_{(2n+1)q_0}\rangle = E^{\rm NL}_{(2n+1)q_0}$ gives the crossover between the exponential localization and the plateau at $q_c \approx (\ln\frac{D\sigma_\kappa^2}{2(N+1)}/\ln\lambda + 1)q_0$. Expression (ii) suggests the 'small' $D\sigma_\kappa \ll \sqrt{2\pi^3/(N+1)^3}$ and 'large' $D\sigma_\kappa \gg \sqrt{8(N+1)}$ disorder criteria, corresponding to localization and delocalization of all QBs. Then $q_0^* \propto \sqrt{N+1}$ separates the localized (QBs) and delocalized in the q space (but localized in the direct space) solutions (AMs), that agrees with [17]. Note, that parameters in simulations correspond to the "small" disorder.

The linear stability of the continued periodic orbits is determined by linearizing the phase space flow around them and computing the eigenvalues θ_i, $i = \overline{1, 2N}$ of the corresponding symplectic Floquet matrix [12]. A QB is stable if $|\theta_i| = 1$, $\forall i$. The maximal and minimal absolute values of θ_i of QBs with $q_0 = 6$, $N = 64$ for several increasing values of D and two different $\{\kappa_n\}$ are plotted vs β in Fig. 2(a). Remarkably, while the instability threshold varies monotonically with D, it may not only decrease, but increase as well, depending on a particular $\{\kappa_n\}$. Moreover, stabilizing realizations are common, neatly balancing destabilizing ones. The observed deviation of the average instability threshold $\langle\beta^*\rangle$ from the disorder-free value β_0^* was much smaller that the variance [Fig. 2(b)]. The latter grows almost linearly in D, up to $\sigma_{\beta^*} \approx 0.25\beta_0^*$, as seen for $q_0 = 6$, $N = 64$ [Fig. 2(b); note that for larger D the linear fit may become violated, due to the lower bound $\beta^* > 0$].

The monotonic dependence of the instability threshold on D suggests that it is caused by the same resonance with the modes $q_0 \pm 1$ as in the disorder-free case. Let us explore the impact of disorder on this bifurcation. Linearizing equations of motion (2) around a QB solution $Q_q = \hat{Q}_q(t) + \xi_q(t)$, one gets

$$\ddot{\xi}_q + \omega_q^2\xi_q = -3\nu\omega_q E_{q_0}\cos^2(\hat\omega t)\sum_p C_{q,q_0,q_0,p}\,\omega_p\xi_p - d\omega_q\sum_p \omega_p K_{p,q}\xi_p + O(\nu^2, \nu d, d^2). \quad (6)$$

The strongest instability is due to primary parametric resonance in (6) and involves a pair of the resonant modes $\tilde q$, $\tilde p = q_0 \pm 1$. Omitting nonresonant and $O(\nu^2, \nu d, d^2)$ terms it is reduced to

$$\ddot{\xi}_{\tilde q} + \omega_{\tilde q}^2(1 + dK_{\tilde q,\tilde q})\xi_{\tilde q} = -3\nu\omega_{\tilde q}\omega_{\tilde p}E_{q_0}\cos^2(\hat\omega t)\xi_{\tilde p},$$
$$\ddot{\xi}_{\tilde q} + \omega_{\tilde p}^2(1 + dK_{\tilde p,\tilde p})\xi_{\tilde p} = -3\nu\omega_{\tilde p}\omega_{\tilde q}E_{q_0}\cos^2(\hat\omega t)\xi_{\tilde q}. \quad (7)$$

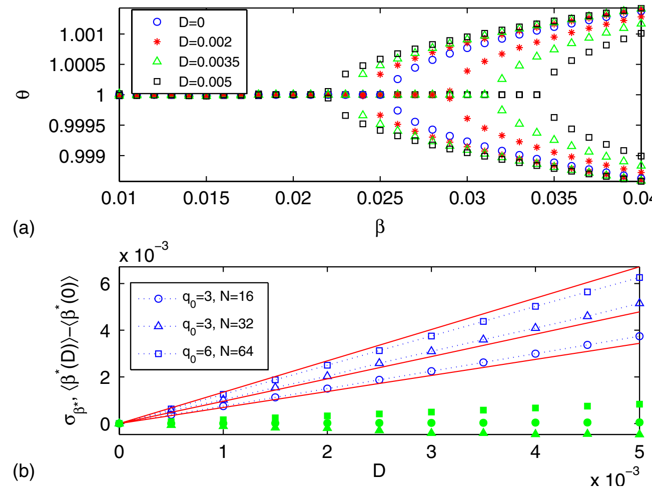

FIG. 2 (color online). (a) The maximal and minimal absolute values of the eigenvalues of the Floquet matrix if $q_0 = 6$, $N = 64$ for two realizations of $\{\kappa_n\}$ vs the nonlinearity coefficient β. For one realization the instability threshold in nonlinearity is increasing with D, for another—decreasing. (b) Empty markers, dotted line: dependence of the variance of the instability threshold σ_{β^*} on the disorder strength. Solid lines are theoretical estimates (8). Filled markers: $\langle\beta^*(D) - \langle\beta^*(0)\rangle$.

Thus, the disorder does not create new resonant terms, its impact being confined to the QB and resonant modes frequency shifts. The analysis analogous to [12] yields the instability threshold β^*, its mean and variance:

$$\beta^* = \beta_0^*\Big(1 - \frac{2d(N+1)^2}{\pi^2}\Delta K\Big), \qquad \langle\beta^*\rangle = \beta_0^*, \quad (8)$$
$$\sigma_{\beta^*} = 2\sigma_\kappa D\sqrt{N+1}/E_{q_0},$$

where the disorder-free value is $\beta_0^* = \frac{\pi^2}{6E_{q_0}(N+1)}$ and $\Delta K = K_{\tilde q,\tilde q} - 2K_{q_0,q_0} + K_{\tilde p,\tilde p}$. It agrees well with the numerical results [Fig. 2(b)].

One may ask now, which particular realizations favor or disfavor stability? Furthermore, can the results be used in controlling the energy flow in the mode space? The disorder-determined part of (8) can be rewritten as $\Delta K = -\frac{4}{\sqrt{N+1}}\sum_{n=1}^{N+1}\kappa_n\cos\frac{\pi 2q_0(n-0.5)}{N+1}\sin^2\frac{\pi(2n-1)}{2(N+1)}$. It is linear with respect to κ_n; thus, we can represent the latter as a sum of spatial Fourier components, their contributions being additive. Thus, consider $\kappa_n = 0.5\cos(\frac{\pi p(n-0.5)}{N+1} + \varphi)$, where φ is the phase shift. It is natural to expect the minimum of ΔK (and the maximal gain in stability), when $p = 2q_0$, and it indeed yields $\Delta K = 0.5\sqrt{N+1}\cos\varphi$, and the maximum $\beta^* = \beta_0^*(1 + D(N+1)^2/\pi^2)$ for $\varphi = 0$. Immediately, a high sensitivity on φ is seen: the zero shift $\beta^* = \beta_0^*$ for $\varphi = \pm\pi/2$; the minimum $\beta^* = \beta_0^*(1 - D(N+1)^2/\pi^2)$ for $\varphi = -\pi$. The effect of $p = 2q_0$ on adjacent QBs $q_0' = q_0 \pm 1$ is twice as small and reverse: for example, if $\varphi = 0$ then $\beta^* = \beta_0^*(1 - D(N+1)^2/(2\pi^2))$. Remarkably, while for $p = 2q_0$ extremal shifts correspond to $\varphi = 0$, π and

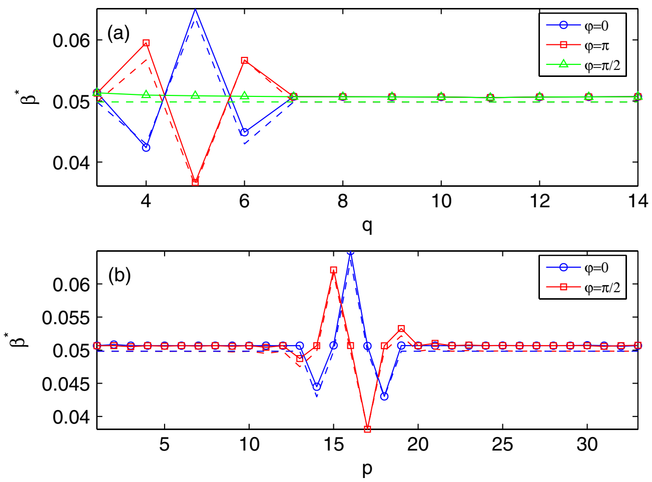

FIG. 3 (color online). QB stability in case of spatially harmonic modulations: $N = 32$, $D = 0.0025$ and (a) $p = 10$, the central mode q is changed, (b) the central mode $q = 8$, the modulation wave number p is varied. Dashed lines are theoretical estimates.

zero ones to $\varphi = \pm\pi/2$, for $p = 2q_0 \pm 1$ the zero shift appears for $\varphi = 0$, π, and the extrema for $\varphi = \pm\pi/2$: $\beta^* = \beta_0^*(1 \mp 8D(N+1)^2/(3\pi^3))$.

These results are illustrated in Fig. 3, and show a good correspondence to the numerically determined QB stability. That is, depending on the phase φ, the spatially harmonic modulation of springs elasticities with the wave number $p = 2q_0$, may significantly augment, weaken, or leave the stability intact [Fig. 3(a)]. Modulations with $p = 2q_0 \pm 2$ change the stability reversely and with twice a smaller amplitude for the same φ, and those with $p = 2q_0 \pm 1$—just a bit weaker than $2q_0$, but with a $\pi/2$ shift in φ [Fig. 3(b)]. Notably, modulations with other wave numbers have only a minor effect. Therefore, the spatial Fourier components of $\{\kappa_n\}$ with $p \in [2q_0 - 2, 2q_0 + 2]$ are decisive for the q_0-QB stability.

These findings suggest a possibility of controlling the energy flow between modes. For example, imposing a proper periodic modulation of the linear elasticity one can destabilize certain QB excitations and (i) promote equipartition or (ii) stabilize others, where the energy will be radiated; new QBs may also be subject to the same procedure to arrange the further energy flow. Experimentally, elasticity modulations could be achieved, for example, by laser heating, either as harmonic or spot impurities, like it was designed to control discrete breathers location in cantilever arrays [9].

In conclusion, we have demonstrated, that the concept of QBs can be successfully applied to analyzing nonlinear vibrational modes in weakly disordered lattices. They essentially retain exponential localization and stability in the mode space, if the disorder is sufficiently small. We show, that the stability trend depends sensitively on a particular realization of disorder, and deliberately created inhomogeneities offer a promising technique of controlling the energy flow between nonlinear modes. We expect that these ideas and methods to be applicable to a variety of nonlinear weakly disordered lattices—and we have already applied them to the DNLS chain (to be reported elsewhere)—including the contexts of a different source of disorder (masses, nonlinearities), higher dimensions, and quantum lattices. The results on the nonlinear modes sustainability, stability, and controlling are strongly expected to be in demand from experiments and applications. Another possibility is to develop the theory of QBs in the AMs space to target the localized wave packet spreading problem.

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