# *q*-Breathers and the Fermi-Pasta-Ulam Problem

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The Fermi-Pasta-Ulam (FPU) paradox consists of the nonequipartition of energy among normal modes of a weakly anharmonic atomic chain model. In the harmonic limit each normal mode corresponds to a periodic orbit in phase space and is characterized by its wave number $q$. We continue normal modes from the harmonic limit into the FPU parameter regime and obtain persistence of these periodic orbits, termed here $q$-breathers (QB). They are characterized by time periodicity, exponential localization in the $q$-space of normal modes and linear stability up to a size-dependent threshold amplitude. Trajectories computed in the original FPU setting are perturbations around these exact QB solutions. The QB concept is applicable to other nonlinear lattices as well.

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Fifty years ago Fermi, Pasta, and Ulam (FPU) published their celebrated paper on thermalization of arrays of particles connected by weakly nonlinear strings [1], bringing forth a fundamental physical and mathematical problem of the energy equipartition and ergodicity in nonlinear systems. Series of numerical simulations showed that energy, initially placed in a low-frequency normal mode of the linear problem with a frequency $\omega_q$ and a corresponding wave number $q$, stayed almost completely locked within a few neighbor modes, instead of being distributed among all modes of the system. Moreover, recurrence of energy to the originally excited mode was observed.

Much effort has since been expended to understand and explain the FPU results (see [2–4] for reviews). Two major approaches were developed. The first one, taken by Zabusky and Kruskal, was to analyze dynamics of the nonlinear string in the continuum limit, which led to a pioneering observation of solitary waves [5]. The second approach, followed by Izrailev and Chirikov, pointed to the existence of a "stochasticity threshold" in the original FPU system [6]. For strong nonlinearity (or simply large energies) the overlap of nonlinear resonances [7] leads to strong dynamical chaos, destroying the FPU recurrence and ensuring fast convergence to thermal equilibrium. If nonlinearity is below a (size-dependent) "stochasticity threshold," the dynamics of the chain remains similar to that of the unperturbed (linear) system for large time scales. Later studies [8,9] showed that the "local" dynamics of four consecutive low-frequency modes may become substantially chaotic, while almost all initial energy stays localized in these modes during the time of computation. The redistributed mode energies fall exponentially with increasing mode numbers in this regime (coined "weak chaos") and the energy flow to higher frequency modes was argued to be exponentially slow (due to Arnold diffusion).

The results obtained through this second approach lead one to formulate some important questions. First, since the dynamics below the stochasticity threshold is localized in $q$-space for long times, do *time-periodic* trajectories with almost all energy locked in a single mode for *infinite times,* coined here *q-breathers* (QB), exist, and are they close to the ones studied by FPU? Second, are the stability thresholds of such QBs related to the various stochasticity thresholds mentioned above? And, finally, is the concept of QBs applicable also for other spatially extended nonlinear lattices, including generalizations to higher lattice dimensions? A strong motivation for this study is the fact that in the $q$-space representation we deal with oscillators that are uncoupled in the limit of small amplitudes, and, moreover, with frequencies being different for each mode. Nonlinearity induces coupling between oscillators. That is reminiscent of the case of *discrete breathers* (DB) that are time-periodic and spatially localized excitations on networks of interacting identical anharmonic oscillators, which survive continuation from the trivial limit of zero coupling [10]. Notably, DBs exist also in FPU lattices [11].

The FPU system is a chain of $N$ equal masses coupled by nonlinear strings with the equations of motion containing quadratic (the $\alpha$ model)

$$\ddot{x}_n = (x_{n+1} - 2x_n + x_{n-1}) + \alpha[(x_{n+1} - x_n)^2 - (x_n - x_{n-1})^2] \tag{1}$$

or cubic (the $\beta$ model)

$$\ddot{x}_n = (x_{n+1} - 2x_n + x_{n-1}) + \beta[(x_{n+1} - x_n)^3 - (x_n - x_{n-1})^3] \tag{2}$$

interaction terms, where $x_n$ is the displacement of the $n$th particle from its original position, and fixed boundary conditions are taken $x_0 = x_{N+1} = 0$. A canonical transformation $x_n(t) = \sqrt{\frac{2}{N+1}}\sum_{q=1}^{N} Q_q(t)\sin(\frac{\pi q n}{N+1})$ takes into the reciprocal wave number space with $N$ normal mode coordinates $Q_q(t)$. The equations of motion then read

 

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\alpha}{\sqrt{2(N+1)}} \sum_{i,j=1}^{N} A_{q,i,j} Q_i Q_j \quad (3)$$

for the FPU-$\alpha$ chain (1) and

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\beta}{2(N+1)} \sum_{i,j,m=1}^{N} C_{q,i,j,m} Q_i Q_j Q_m \quad (4)$$

for the FPU-$\beta$ chain (2), where $\omega_q = 2\sin[\pi q/2(N+1)]$ are the normal mode frequencies, and $A_{q,i,j}$ and $C_{q,i,j,m}$ are coupling coefficients [8]. For small amplitude excitations the nonlinear terms in the equations of motion can be neglected, and according to (3) and (4) the $q$ oscillators get decoupled, each conserving the energy $E_q = \frac{1}{2}(\dot{Q}_q^2 + \omega_q^2 Q_q^2)$ in time. Especially, we may consider the excitation of only one of the $q$ oscillators, i.e., $E_q = E \neq 0$ for $q \equiv q_0$ only. Such excitations are trivial and unique time-periodic and $q$-localized solutions (QBs) for $\alpha = \beta = 0$.

In order to guarantee continuation of this periodic orbit into the case $\beta \neq 0$ or $\alpha \neq 0$ and following [10], we conclude that it is enough to request the nonresonance condition $n\omega_{q_0} \neq \omega_{q \neq q_0}$, which is the generic case for a finite system size $N$ (here $n$ is an integer) (see also [12]). We show that the orbit will stay localized in $q$-space at least up to some critical nonzero value of $\beta$ or $\alpha$ [13]. The above mentioned value is correct also for free boundary conditions. For periodic boundary conditions twofold degeneracies of the normal modes at the harmonic limit have to be removed, allowing one again to construct QBs that are continued from standing waves.

We compute QBs as well as their Floquet spectrum numerically using well developed computational tools [11], and compare the results with analytical predictions, derived by means of asymptotic expansions. As a zero-order approximation for the numerical computation we take the $q_0$th linear mode: $x_n(t) = \sqrt{\frac{2}{N+1}} Q_{q_0}(t) \sin(\frac{\pi q_0 n}{N+1})$. For the $\beta$ model the initial conditions are $Q_q(t=0) = 0$ and $\dot{Q}_{q_0}(t=0) = \sqrt{2E - \Sigma_{q \neq q_0} \dot{Q}_q^2(t=0)}$. We map the space of $\vec{y} \equiv \{\dot{Q}_{q \neq q_0}\}$ onto itself by integrating the initial condition up to the time when $Q_{q_0}(t) = 0$, $\dot{Q}_{q_0}(t) > 0$ again: $\vec{y}^{n+1} = \vec{\mathcal{F}}(\vec{y}^n)$. A periodic orbit is a fixed point of that map. The vector function $\vec{\mathcal{G}} = \vec{\mathcal{F}}(\vec{y}) - \vec{y}$ is used to calculate the Newton matrix $\mathcal{N} = \partial \mathcal{G}(\vec{y})_i / \partial y_j$. The iteration procedure $\vec{y}' = \vec{y} - \mathcal{N}^{-1} \vec{\mathcal{G}}(\vec{y})$ continues until the required accuracy $\varepsilon$ is obtained: $\|\vec{\mathcal{F}}(\vec{y}) - \vec{y}\| / \|\vec{y}\| < \varepsilon$ (we have varied $\varepsilon$ from $10^{-5}$ to $10^{-8}$), where $\|\vec{y}\| = \max\{|y_i|\}$. For the $\alpha$ model we used a modified scheme choosing $x_s(t=0) = 0$ where $s = [(N+1)/2q_0]$ corresponds to the antinode of the mode $Q_{q_0}$. We map the phase space $\vec{r}$ (excluding $x_s$) onto itself integrating until $x_s(t) = 0$, $\dot{x}_s(t) > 0$ again. With the above notations we use a Gauss method to solve the equations $\vec{\mathcal{G}}(\vec{r}) = \mathcal{N}(\vec{r} - \vec{r}')$ for the new iteration $\vec{r}'$ and do final corrections to adjust the correct energy $E$. To compute the linear stability of the found QB, we linearize the phase space flow around it and map that flow onto itself by integrating over one period of the QB. The corresponding symplectic Floquet matrix can be computed numerically and subsequently diagonalized. If all eigenvalues $\mu$ have absolute value 1, the QB is stable; otherwise it is unstable [11].

First, we apply our method to the $\beta$ model with $q_0 = 3$ and $E = 1.58$, which is very close to the value 1.5 chosen in [8]. We obtain QBs that are exponentially localized in $q$-space (Fig. 1). The smaller $\beta$, the faster is the decay of the energy distribution with increasing wave number $q$. Note that because of the parity symmetry of the $\beta$ model [Eq. (2) is invariant under $x_n \to -x_n$ for all $n$] only odd $q$ modes are excited by the $q_0 = 3$ mode and get coupled [14]. In Fig. 2 we plot the absolute values of the Floquet eigenvalues of the computed QBs versus $\beta$ for different system sizes $N$. QBs are stable for sufficiently weak nonlinearities (all eigenvalues have absolute value 1). When $\beta$ exceeds a certain threshold, two eigenvalues get absolute values larger than unity (and, correspondingly, another two get absolute values less than unity) and a QB becomes unstable. Remarkably, unstable QBs can be traced far beyond the stability threshold, and, moreover, they retain their exponential localization in $q$-space (Fig. 1) [15]. As $\beta$ is increased further, new bifurcations of the same type are observed.

By an asymptotic expansion of the solution to (4) in powers of the small parameter $\sigma = \beta/(N+1)$, we estimate the shape of a QB solution $\hat{Q}_i(t)$ localized in the mode

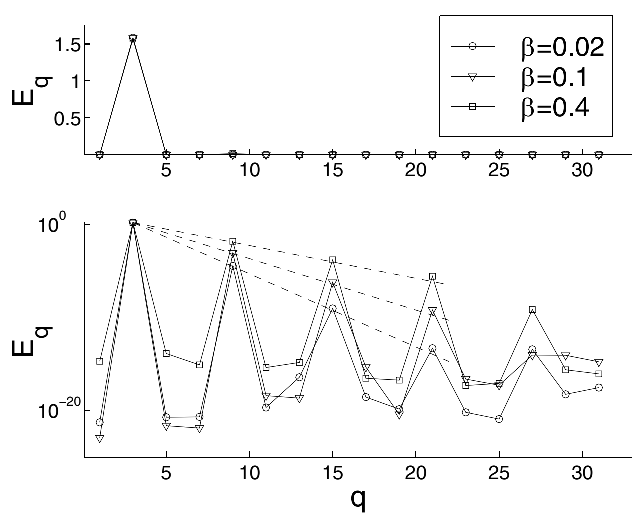


FIG. 1. Energy distributions between $q$ modes in QBs for different $\beta$ versus $q$ in linear and log scales with analytical estimations of the QBs exponential localization (dashed lines). Parameters are $E = 1.58$, $q_0 = 3$, $N = 32$. Only odd modes are shown (see text). The symbols for $q \neq 3, 9, 15, 21, 27$ represent upper bounds, and the real mode energies might be even less. Note that QBs persist even far beyond the stability threshold (see Fig. 2).

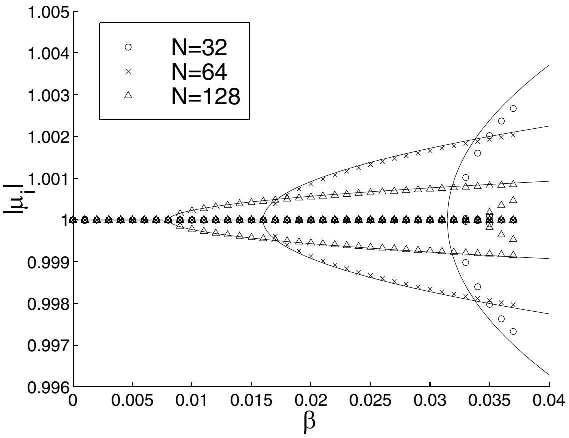


FIG. 2. Absolute values of Floquet multipliers $|\mu_i|$ of QBs with the energy $E = 1.58$ and $q_0 = 3$ and different $N$ versus $\beta$. Symbols: numerical results; lines: analytical results.

$q_0$. The energies of the modes $q_0, 3q_0, \ldots, (2n+1)q_0, \ldots$ are given by

$$E_{(2n+1)q_0} = \lambda^{2n} E_{q_0}, \qquad \lambda = \frac{3\beta E_{q_0}(N+1)}{8\pi^2 q_0^2}, \qquad (5)$$

up to an error of the order $(2n+1)^2 q_0^2/N^2$. Dashed lines in Fig. 1 are obtained using (5) and show very good agreement with the numerical results.

Using standard secular perturbation techniques, we approximate the frequency $\Omega$ of the QB solution as $\Omega = \omega_{q_0}[1 + \frac{9\beta E_{q_0}}{8(N+1)} + O(\frac{\beta^2}{(N+1)^2})]$. The instability threshold observed in Fig. 2 can be obtained analytically by making a replacement $Q_i = \hat{Q}_i(t) + \xi_i$ in the equations of motion (4) and linearizing the resulting equations with respect to $\xi$:

$$\ddot{\boldsymbol{\xi}} + \mathbf{A}\boldsymbol{\xi} + h(1 + \cos 2\Omega t)\mathbf{B}\boldsymbol{\xi} + O(h^2)\boldsymbol{\xi} = \mathbf{0}, \qquad (6)$$

where $\boldsymbol{\xi} = (\xi_i)$ is a vector, $\mathbf{A} = (\delta_{ij}\omega_i^2)$ is a diagonal matrix, $\mathbf{B} = (b_{ij})$ is a coupling matrix, and $h = 3\beta E/2(N+1)$ is a small parameter. We analyze parametric resonance in (6), treating $h$ and $\Omega$ as independent parameters. In the limit $h \to 0$ the equilibrium point $\boldsymbol{\xi} = \mathbf{0}$ is stable for all values of $\Omega$ except for those that satisfy $\omega_k + \omega_l = 2n\Omega \equiv 2n\Omega_{nkl}$ where $n \geq 1$, and the modes $k$ and $l$ belong to the same connected component of the coupling graph whose connectivity is defined by the matrix $\mathbf{B}$.

We seek for a solution to (6) at $\Omega = \Omega_{nkl}(1+\delta)$, $\delta = O(h)$, in the form $\boldsymbol{\xi} = \sum_{m=-\infty}^{+\infty} \boldsymbol{f}_m e^{(i\omega + z + 2im\Omega)t} + \text{c.c.}$, where $\tilde{\omega} = \omega_k(1+\delta) = -\omega_l(1+\delta) + 2n\Omega$, $\boldsymbol{f}_m$ are unknown complex vector amplitudes, and $z = O(h)$ is a small unknown complex number.

The nearest primary resonance corresponds to $k = q_0 - 1$, $l = q_0 + 1$, $n = 1$ [8]. In the vicinity of the bifurcation point the absolute values of the Floquet multipliers involved in the resonance are obtained as

$$|\mu_i| = 1 \pm \frac{\pi^3}{4(N+1)^2}\sqrt{R - 1 + O\left(\frac{1}{N^2}\right)}, \qquad (7)$$

where $R = 6\beta E(N+1)/\pi^2$. The bifurcation occurs at $R = 1 + O(1/N^2)$. The result (7) is plotted in Fig. 2 with solid lines for $N = 32$, 64, and 128, demonstrating good agreement with the numerical results. The agreement improves with increasing $N$ [16]. The instability threshold for QB orbits (Fig. 2), which is obtained analytically using the parameter $R$ (7), coincides with the criterion of transition to weak chaos reported by De Luca *et al.* [8].

We have used one of the original parameter sets of the FPU-$\alpha$ study $\alpha = 0.25$, $E = 0.077$, $N = 32$ [1] (and add to that the case $\alpha = 0.025$ as well for comparison) to find stable exponentially localized QB modes with most of the energy concentrated in $q_0 = 1$ (Fig. 3) [15]. We use again an asymptotic expansion of the solution to (3) in powers of the small parameter $\rho = \alpha/\sqrt{2(N+1)}$ and obtain that the energies of the modes $q_0, 2q_0, \ldots, nq_0$, are given by

$$E_{nq_0} = \epsilon^{2n-2} n^2 E_{q_0}, \qquad \epsilon = \frac{\alpha\sqrt{E_{q_0}^{(0)}}(N+1)^{3/2}}{\pi^2 q_0^2}. \qquad (8)$$

The dashed line in Fig. 3 is obtained using (8) in case $\alpha = 0.025$, $E = 0.077$, $N = 32$, $q_0 = 1$ and shows very good agreement with the numerical results [17].

How are QB solutions related to the original FPU studies? A QB requires specific initial conditions, which were not used in earlier numerical studies. However, nearby quasiperiodic solutions are expected to retain stability and exponential localization of their QB generator for times long compared to the QB period. In Fig. 4 we compare snapshots of displacements at different times obtained for the original FPU trajectory in [1] and for the

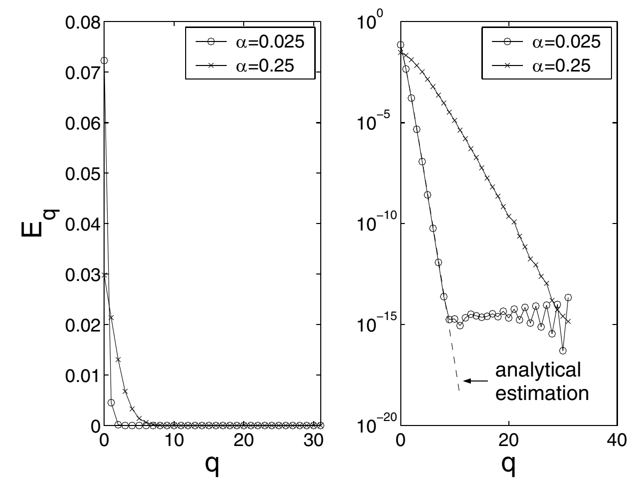


FIG. 3. Stable QB solutions for $\alpha = 0.025$ and $\alpha = 0.25$, $E = 0.077$, $N = 32$, and $q_0 = 1$; the latter corresponds to the original numerical FPU-$\alpha$ study [1]. An analytical estimation of the QB exponential localization in case $\alpha = 0.025$ is shown with a dashed line.

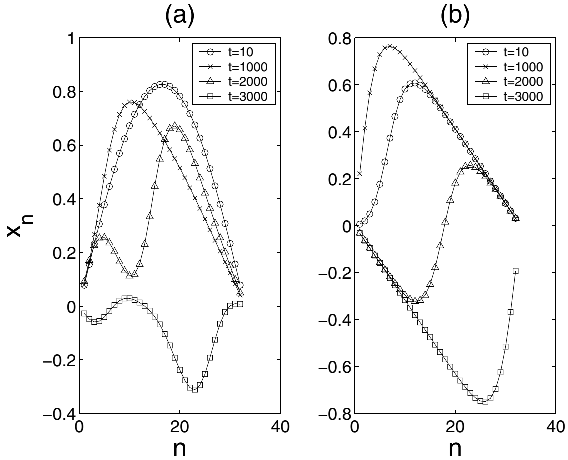


FIG. 4. Snapshots of displacements (a) of the original FPU trajectory for $\alpha = 0.25$, $E = 0.077$, $N = 32$ [1], and (b) of the corresponding exact QB solution from Fig. 3 taken at different times.

numerically exact QB solution from Fig. 3 for $\alpha = 0.25$ and observe similar evolution patterns. Moreover, we took a series of points on a line that connected initial conditions of the FPU trajectory ($E_{q\neq 1} = 0$) with the numerically exact QB solution from Fig. 3. For each of these points we integrated the corresponding trajectory and measured the average deviation $\Delta$ from the QB orbit. The dependence of $\Delta$ on the line parameter turns out to be an almost linear one, starting from zero when being very close to the QB orbit, and ending with a maximum value when being close to the FPU trajectory. That supports the expectation that the FPU trajectory is a perturbation of the QB orbit. The FPU recurrence is gradually appearing with increasing $\Delta$ and is thus directly related to the regular motion of a slightly perturbed QB periodic orbit, which we tested also numerically.

In conclusion, we report on the existence of $q$-breathers as exact time-periodic low-frequency solutions in the nonlinear FPU system. These solutions are exponentially localized in the $q$-space of the normal modes and preserve stability for small enough nonlinearity. They continue from their trivial counterparts for zero nonlinearity at finite energy. The stability threshold of QB solutions coincides with the weak chaos threshold in [8]. Persistence of exact stable QB modes is shown to be related to the FPU paradox. The FPU trajectories computed 50 years ago are perturbations of the exact QB orbits. Remarkably, localization in $q$-space persists even for parameters when the QBs turn unstable. The concept of stable QBs and their impact on the evolution of excitations in the FPU system is expected to apply far beyond the stability threshold of the QB solutions reported in the present work. Generalizations to higher dimensional lattices and other Hamiltonians are straightforward, due to the weak constraint imposed by the nonresonance condition needed for continuation. QBs can also be expected to contribute to peculiar dynamical features of nonlinear lattices in thermal equilibrium, e.g., the anomalous heat conductivity in FPU lattices [3].

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[13] Note that we do not demand specific symmetries leading to low-dimensional invariant manifolds in phase space, in contrast to the discussion in [14]. Consequently, our QB solutions must not be embedded in such subspaces.
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[15] Similar solutions are found for other values of $q_0$ (e.g., $q_0 = 1, 2, 3, 4$) provided $q_0 \ll N$.
[16] The subsequent bifurcations of the same type are associated with next primary resonances of the type $k = q_0 - m$, $l = q_0 + m$, $n = 1$, $m = 2, 3, \ldots$. The corresponding bifurcation points are located at $R = m^2 + O(1/N^2)$. Note that higher-order resonances at certain values of $q_0$ and $N$ may result in the appearance of narrow instability regions within the region $0 < R < 1$.
[17] To describe the energy distribution for $\alpha = 0.25$, a higher-order perturbation theory needs to be developed.