Instabilities and relaxation to equilibrium in long-range oscillator chains

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We study instabilities and relaxation to equilibrium in a long-range extension of the Fermi-Pasta-Ulam-Tsingou (FPU) oscillator chain by exciting initially the lowest Fourier mode. Localization in mode space is stronger for the long-range FPU model. This allows us to uncover the sporadic nature of instabilities, i.e., by varying initially the excitation amplitude of the lowest mode, which is the control parameter, instabilities occur in narrow amplitude intervals. Only for sufficiently large values of the amplitude, the system enters a permanently unstable regime. These findings also clarify the long-standing problem of the relaxation to equilibrium in the short-range FPU model. Because of the weaker localization in mode space of this latter model, the transfer of energy is retarded and relaxation occurs on a much longer timescale.

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The relaxation to equilibrium in nonlinearly coupled oscillators is still an open problem [1,2]. Starting with the pioneering work of Fermi-Pasta-Ulam-Tsingou (FPU) [3], these studies led to important discoveries in both statistical mechanics and nonlinear science. In most cases, the analysis was restricted to one-dimensional (d = 1) lattices where oscillators interact only with nearest neighbors, i.e., to short-range interactions. However, in recent years there has been a growing interest in systems with long-range interactions [4,5]. In such systems, either the two-body potential or the coupling at separation r decays with a power-law $r^{-\alpha}$. When the power $\alpha$ is less than the dimension of the embedding space d, these systems violate additivity, a basic feature of thermodynamics, leading to unusual properties like ensemble inequivalence, broken ergodicity, quasistationary states.

The extension of the FPU problem to include long-range couplings is rarely considered [6–8]. Moreover, attention has been focused mainly on finding conditions for the existence of localized solutions like solitons or breathers. No one, to the best of our knowledge, has tackled, in the context of long-range systems, the original question posed by FPU on the time-scales for relaxation to equilibrium when the energy is fed into the lowest Fourier mode. This is the subject of this paper. Moreover, we here show that the lessons learned from the long-range FPU model can be used to clarify key features of the original short-range model.

Long-range coupled oscillator models have been previously introduced to cope with dipolar interaction in mechanistic DNA models [9]. They describe also ferroelectric [10] and magnetic [11] systems, where the long-range coupling is provided again by dipolar forces. Other candidates for application are cold gases: dipolar bosons [12,13], Rydberg atoms [14], atomic ions [15,16]. Moreover, one can mention optical wave turbulence [17] and scale-free avalanche dynamics [18], where such long-range couplings appear.

In this paper, we consider a generalization of the FPU model by introducing a long-range coupling in the linear term, while keeping the nonlinear term short-range. Choosing the power $1 < \alpha \leq 3$, the results do not depend much on the specific value. Dipolar systems correspond, as mentioned, to the power $\alpha = 3$, while the power $\alpha = 2$ has been considered for crack front propagation along disordered weak planes between solid blocks [18] and contact lines of liquid spreading on solid surfaces [19].

Here, we repeat the FPU experiment by putting the energy initially in the lowest Fourier mode. As for the short-range FPU model, an exponential spectrum involving only odd modes forms on a short-time scale [20,21]. However, energy localization in Fourier space is much stronger, as we will comment in the following. By increasing the initial amplitude, a parametric instability sets in where the energy is transferred to even modes [22–25].

For the long-range FPU this instability has a sporadic nature, i.e., by increasing the amplitude one observes instability islands, narrow amplitude intervals where instability sets in. Similar sporadic instabilities (so-called induction phenomenon [26]) have been observed in the short-range FPU when exciting higher modes. As we will show below, these instabilities play a much more important role in the long-range FPU than in the short-range one. This is due to the strong localization in mode space, which is ultimately determined by the nonequidistant character of the unperturbed frequency spectrum; see Fig. 1(a). This instability drives the long-range system to energy equipartition on a short time-scale. For the short-range FPU, the simultaneous presence of sporadicity and weak localization in mode space, which is due to the equidistant character of the frequency spectrum shown in Fig. 1(a), delays the convergence to energy equipartition. Therefore, the study of these instabilities for long-range systems clarifies an important aspect of the relaxation to equilibrium in the traditional short-range FPU model.
where \( n \) is the normal mode number, and \( q_n = 2\pi n/N \), one can rewrite Eq. (3) in the following form:

\[
Q_n = -(\Omega_n^0)^2 Q_n - \sum_{(m,r,p)} G_{n,m,r}^n Q_m Q_r Q_p. (5)
\]

where normal mode numbers satisfy the condition \( m + r + p - n = 0, 2N \) and \( (m,r,p) \) further restricts the sum so that each triplet of modes \((m,r,p)\) is present only once. \( G_{n,m,r}^n \) are mode coupling constants where \( \omega_n = 2\sin(q_n/2) \) and \( D_{m,r,p} \) stand for the number of permutations of the set \((m,r,p)\), while \( \Omega_n^0 \) are unperturbed frequencies of the long-range normal modes:

\[
\Omega_n^0 = \sqrt{2 \sum_{m=1}^{N} \frac{1 - \cos(q_n m)}{m^\alpha}}. (6)
\]

These frequencies are plotted in Fig. 1 for both a long-range and a short-range case. As mentioned above the spectrum is not equidistant in the long-range case. Originally, the FPU paradox involved exciting the first Fourier mode \( n = 1 \) and looking for the equipartition of energy with respect to all other modes. Thus, we consider the following initial condition

\[
u_1 = A [e^{i(\Omega_1 t - j\Omega_1 t)} + \text{c.c.}], (7)
\]

which implies that energy is carried by normal modes \( Q_1 = A e^{i\Omega_1 t} \) and \( Q_{N-1} = (Q_{N-1})^\dagger \). In what follows we will study the evolution and instability of this initial excitation.

First of all, let us note that this mode could be treated, in the first approximation, as a source field and causes a nonlinear frequency shift to all normal modes. Indeed, examining nonlinear terms in Eq. (5) for \( Q_n \) normal mode evolution containing \( G_{n,1,N-1}^n Q_n Q_1 Q_{N-1} \), we conclude that the expression for renormalized frequencies is

\[
\Omega_n = \sqrt{\left(\Omega_n^0\right)^2 + G_{n,1,N-1}^n |Q_1|^2}. (8)
\]

In addition, this source mode excites the branch of odd modes (often referred to as normal mode bush or q-breather [21,24,25]). For instance, the initially absent \( Q_3 \) mode is generated according to the perturbation analysis of Eq. (5),

\[
Q_3 = -\left(\Omega_3^0\right)^2 Q_3 - \frac{G_{3,11}^3}{\Omega_3} Q_1 Q_3^\dagger, (9)
\]

Thus, in addition to the triple source harmonic \( Q_3 = 3\Omega_3 \), \( Q_3 \) acquires the harmonic pair \( \pm\Omega_3 \) as well. In the long-range case, the perturbation analysis is well justified since low frequencies \( \Omega_3 \) are not equidistant, i.e., the ratio \( (3\Omega_3 - \Omega_2)/\Omega_3 \) remains finite even in the \( N \to \infty \) limit, in contrast to the short-range FPU system. This itself guarantees the perturbative scaling \( |Q_1| \gg |Q_3| \) and, as we will see below, leads to an excellent agreement between analytical predictions and numerical results. Proceeding further, we can derive perturbatively the expression for \( Q_n \) with harmonics \( \pm\Omega_3, \pm\Omega_1 + 2\Omega_2, \) and \( 5\Omega_2 \), and then for all odd normal modes, which have exponentially decaying amplitudes with increasing mode number. We define such a steady distribution set of multicomponent and multifrequency odd modes as \( Q_r^{(a)} \), where \( (a) \) indicates different harmonics of the \( r \)th odd mode. Further,
we should discuss how to derive the instability properties of this group of lowest energy modes.

First of all, we note that the initially excited lowest mode \( Q_1 \) alone (when all other modes are not excited) is parametrically stable in both long- and short-range cases: thus, in order to analyze the instability process, it is necessary to consider the combination of odd modes created by the initial excitation of the first mode. Following a parametric instability approach, we consider pair of equations from the set Eq. (5)

\[
\dot{Q}_n = - (\Omega_m)^2 Q_n - G_m^* Q_n Q_m (Q_n^{(a)} - Q_m^{(b)}), \\
\dot{Q}_m = - (\Omega_m)^2 Q_m - G_m^* Q_m (Q_m^{(a)} - Q_n^{(b)}),
\]

where we have restricted the sum to mode harmonics such that the relative frequency,

\[
\Delta = \Omega_n^{(a)} + \Omega_m^{(b)} - \Omega_m - \Omega_n,
\]

is close to zero. Then, introducing the transformations \( Q_n = Q_n \exp(i\Omega_m t) \) and \( Q_m = Q_m \exp(-i\Omega_n t) \), we get

\[
\dot{Q}_n + 2i\Omega_n Q_n = - G_m^* Q_m Q_n (Q_n^{(a)} - Q_m^{(b)}), \\
\dot{Q}_m + 2i\Omega_m Q_m = - G_m^* Q_m Q_n (Q_m^{(a)} - Q_n^{(b)}).
\]

The instability takes place when the approximate resonance condition \( \Delta \approx 0 \) holds. We can compute more precisely this threshold assuming a slow time evolution in Eq. (12) and neglecting second-order time derivatives there. Thus, seeking a solution of the form

\[
Q_n = F_1 \exp(i\nu t - i\Delta t/2) \quad \text{and} \quad Q_m = F_2 \exp(i\nu t + i\Delta t/2),
\]

with \( F_1, F_2 \) constants and real growth increment \( \nu \), we get two coupled algebraic equations,

\[
\Omega_n (\Delta + 2i\nu) F_1 - G_m^* Q_m Q_n^{(a)} F_2 = 0, \\
\Omega_m (\Delta - 2i\nu) F_2 - G_m^* Q_m Q_n^{(a)} F_1 = 0.
\]

The solvability condition of this system leads to the growth rate

\[
\nu = \frac{1}{\pi} \sqrt{G_m^* Q_m Q_n^{(a)} Q_n^{(a)}}, \quad \nu = \frac{1}{\pi} \left( \Omega_n Q_m - \Omega_m Q_n \right) - \Delta^2.
\]

Usually the first term under the square root is very small but the growth rate could still be real (inducing the instability) if the resonance condition \( \Delta = 0 \) is realized. Thus, changing \( A \), we monitor the variation of \( \Delta \) given by Eq. (11). We check for which set of the renormalized frequencies of the modes the resonance condition is fulfilled. As long as \( Z = m = 5, r = 1, p = 3 \) with frequencies \( \Omega_z, \Omega_r, 2\Omega_1, 3\Omega_1 \), respectively, one gets \( \Delta = 0 \) for \( A = 1.425 \). For slightly smaller or larger values of \( A \), the resonance condition is violated and the system becomes stable again. It is possible to check these theoretical predictions via direct numerical simulations of Eqs. (3) and initial condition Eq. (7) with \( A = 1.4225 \). The results are displayed in Fig. 2(a), where the inset shows the dependence of growth rate calculated from Eq. (15) on \( A \), while numerical simulations are presented in the main plot. It is seen that even modes grow first with growth rate \( \nu = 0.0006 \), which is in good agreement with the theoretical value. It is remarkable that the first modes to participate in the growth almost in unison are indeed \( \Omega_z \) and \( \Omega_r \).

Furthermore, it is possible to find a scenario where odd modes grow first. This is realized for the set of modes \( n = 9, m = 5, r = 1, p = 3 \) with frequencies \( -\Omega_5, \Omega_6, \Omega_1, -\Omega_1 \), respectively. One gets the \( \Delta = 0 \) resonance condition for the value \( A = 1.97 \): the corresponding numerics and analytical results are presented in Fig. 2(b).

Now it is straightforward to extend the study of this unusual instability behavior to the conventional short-range FPU model. Indeed, mode evolution, Eq. (5), is applicable for the short-range case as well; the only difference is contained in the unperturbed frequencies \( \Omega_0 \). Note that in the short-range FPU unperturbed frequencies of low modes are almost equidistant, see Fig. 1(a), in contrast to the long-range case. Therefore, the denominator in Eq. (9) is close to zero, which is the reason for the well-known phenomenon of FPU recurrences (large energy transfer between the low modes) [1–3]. Thus, although the instability mechanism is present in short-range as well, the energy exchange among modes does not allow steady exponential growth of the unexcited modes. The short-range

\[
\dot{Q}_{n+2} = - (\Omega_{n+2})^2 Q_{n+2} - G_{n+2}^* Q_n Q_1, \quad (16)
\]

derived from Eq. (5).

From the above analytic consideriations, it is evident that in order to find the instability islands, one should analyze the effective frequency difference, Eq. (11). It is clear that when it vanishes, the growth rate, Eq. (15), becomes real and the instability takes place. In other words, one has to find the set of modes \( m, n, r, p \) and the amplitude \( A \) such that \( \Delta \to 0 \). For our initial condition, it is natural to seek resonances with the primary harmonic \( \Omega_1 \) and perhaps the harmonics of the third mode \( \Omega_3 \), which can be more easily excited.

We have found multiple sets of these parameters for which either odd or even mode instabilities occur. For instance, if one chooses the set \( n = 6, m = 2, r = 1, p = 3 \) with frequencies \( \Omega_6, \Omega_2, \Omega_1, 3\Omega_1 \), respectively, one gets \( \Delta = 0 \) for \( A = 1.425 \). For slightly smaller or larger values of \( A \), the resonance condition is violated and the system becomes stable again. It is possible to check these theoretical predictions via direct numerical simulations of Eqs. (3) and initial condition Eq. (7) with \( A = 1.4225 \). The results are displayed in Fig. 2(a), where the inset shows the dependence of growth rate calculated from Eq. (15) on \( A \), while numerical simulations are presented in the main plot. It is seen that even modes grow first with growth rate \( \nu = 0.0006 \), which is in good agreement with the theoretical value. It is remarkable that the first modes to participate in the growth almost in unison are indeed \( \Omega_3 \) and \( \Omega_2 \).

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\]
normal modes from numerical simulations on Eq. (3) with initial model, one finds the set the amplitude
FPU instability develops completely only for larger values of

\[
\Delta_1 \text{ and } A = 1.2425 \text{ [graph (a)] and } A = 1.97 \text{ [graph (b)].}
\]

Curves are color-coded according to the same principle as described in the legend of Fig. 1. Insets show the dependence of growth rates on the initial lowest mode amplitude according to the theoretical Eq. (15). Dashed lines show the estimated grow rates for even (a) and odd (b) modes.

FPU instability develops completely only for larger values of the amplitude \(A\), when instabilities are not sporadic.

Seeking for the resonant modes in the short-range FPU model, one finds the set \(n = 2, m = N - 2, r = 1, p = 3\) with frequencies \(\Omega_2, \Omega_1, 1, 3\Omega_1\), respectively. Then the condition \(\Delta = 0\) is reached for \(A = 0.29\). Plotting again the growth rate \(\nu\) versus \(A\) according to Eq. (15), we get the dependence presented in Fig. 3(a). The instability is no more sporadic: instead, after it is triggered at a given value of \(A = 0.249\), it persists for all larger values. In Figs. 3(b)–3(d), we plot the modes amplitude evolution for different values of \(A\). Instability develops in the range \(A = 0.24–0.26\), in excellent agreement with theoretical predictions.

Finally, as concluding remarks, we address the question of estimating the threshold amplitude \(A_{th}\) below which no sporadic instability takes place in the large \(N\) limit. The total number of harmonics in the \(N\) modes [see, e.g., Eq. (9) for the third mode] scales as \(N! \sim N^N\); consequently, the distance between neighboring harmonics decreases as \(N^{-N}\). Therefore, the average detuning \(\Delta\) in Eq. (15) should be of the same order and thus \(\Delta^2 \sim N^{-2N}\). On the other hand, the first term under the square root scales as \((A_{th}^2/N^4)^N\) in the perturbative limit. From the condition that the growth rate in Eq. (15) is real it follows that \(A_{th} \sim N\) (this estimate is compatible with recent unpublished numerical experiments [28]). Therefore, the energy density threshold remains finite at large \(N\), \(\epsilon_{th} = E_{th}/N \sim A_{th}^2/N^2 \sim \text{const.}\)

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