Route to thermalization in the α-Fermi–Pasta–Ulam system

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We study the original α-Fermi–Pasta–Ulam (FPU) system with $N = 16$, 32, and 64 masses connected by a nonlinear quadratic spring. Our approach is based on resonant wave–wave interaction theory; i.e., we assume that, in the weakly nonlinear regime (the one in which Fermi was originally interested), the large time dynamics is ruled by exact resonances. After a detailed analysis of the α-FPU equation of motion, we find that the first nontrivial resonances correspond to six-wave interactions. Those are precisely the interactions responsible for the thermalization of the energy in the spectrum. We predict that, for small-amplitude random waves, the timescale of such interactions is extremely large and it is of the order of $1/\epsilon^8$, where ϵ is the small parameter in the system. The wave–wave interaction theory is not based on any threshold: Equipartition is predicted for arbitrary small nonlinearity. Our results are supported by extensive numerical simulations. A key role in our finding is played by the Umklapp (flip-over) resonant interactions, typical of discrete systems. The thermodynamic limit is also briefly discussed.

α-Fermi–Pasta–Ulam chain | thermalization | wave–wave interactions | FPU recurrence | resonant interactions

The Fermi–Pasta–Ulam (FPU) chains is a simple mathematical model introduced in the 1950s to study the thermal equipartition in crystals (1). The model consists of N identical masses, each one connected by a nonlinear spring; the elastic force can be expressed as a power series in the spring deformation Δx:

$$F = -\gamma\Delta x + \alpha\Delta x^2 + \beta\Delta x^3 + \ldots, \qquad [1]$$

where γ, α, and β are elastic, spring-dependent, constants. The α-FPU chain, the system studied herein, corresponds to the case of $\alpha \neq 0$ and $\beta = 0$. Fermi, Pasta, and Ulam integrated numerically the equation of motion and conjectured that, after many iterations, the system would exhibit a thermalization, i.e., a state in which the influence of the initial modes disappears and the system becomes random, with all modes excited equally (equipartition of energy) on average. Contrary to their expectations, the system exhibited a very complicated quasiperiodic behavior. This phenomenon has been named "FPU recurrence," and this finding has spurred many great mathematical and physical discoveries such as integrability (2) and soliton physics (3).

More recently, very long numerical simulations have shown clear evidence of the phenomenon of equipartition (see, for instance, ref. 4 and references therein). However, despite substantial progress on the subject (5–10), to our knowledge no complete understanding of the original problem has been achieved so far, and the numerical results of the original α-FPU system remain largely unexplained from a theoretical point of view. More precisely, the physical mechanism responsible for a first "metastable state" (4) and the observation of equipartition for very large times have not been understood.

In this manuscript, we study the FPU problem using an approach based on the nonlinear interaction of weakly nonlinear dispersive waves. Our main assumption is that the irreversible transfer of energy in the spectrum in a weakly nonlinear system is achieved by exact resonant wave–wave interactions. Such resonant interactions are the base for the so-called "wave turbulence theory" (11, 12) and are responsible for the phenomenon of thermalization. Specifically, we will show that, in the α-FPU system, six-wave resonant interactions are responsible for an effective irreversible transfer of energy in the spectrum.

The Model

The equation of motion for a chain of N identical particles of mass m, subject to a force of the type in Eq. **1** with $\alpha \neq 0$ and $\beta = 0$, has the following form:

$$m\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j)\left(\gamma + \alpha(q_{j+1} - q_{j-1})\right), \qquad [2]$$

with $j = 0, 1, .., N-1$. Here, $q_j(t)$ is the displacement of the particle j from the equilibrium position. We consider periodic boundary conditions, i.e., $q_N = q_0$. Our approach is developed in Fourier space and the following definitions of the direct and inverse discrete Fourier transform are adopted:

$$Q_k = \frac{1}{N}\sum_{j=0}^{N-1} q_j e^{-i2\pi kj/N}, q_j = \sum_{k=-N/2+1}^{N/2} Q_k e^{i2\pi jk/N}, \qquad [3]$$

where k are discrete wave numbers and Q_k are the Fourier amplitudes.

Normal Modes. We then introduce the complex amplitude of a normal mode $a_k = a(k,t)$ as follows:

$$a_k = \frac{1}{\sqrt{2\omega_k}}(P_k - i\omega_k Q_k), \qquad [4]$$

where $\omega_k = \omega(k)$ is the angular frequency related to wave numbers as follows:

Significance

Despite the fact that more than 60 years have passed, the α-Fermi–Pasta–Ulam (FPU) system has not yet been fully understood. Their seminal work stimulated many interdisciplinary research topics in mathematics and physics like integrable systems, soliton theory, ergodic theory, and chaos. In this article, we theoretically investigate the original problem by applying the wave–wave interaction theory. By using this mathematical approach, we are able to explain why the emergence of equipartition requires very long times (inaccessible when the original numerical experiments were performed but nowadays recently observed using computer power). Our approach is general and can be used to attack other problems of weakly nonlinear dispersive waves.

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$$\omega_k = 2\sqrt{\frac{\gamma}{m}}|\sin(\pi k/N)|, \quad [5]$$

and P_k is the momentum, $P_k = \dot{Q}_k$. Substituting the above definitions into the equation of motion (Eq. **2**) and introducing the nondimensional variables,

$$a'_k = \frac{(\gamma/m)^{1/4}}{\sqrt{\sum_k \omega_k |a_k(t=0)|^2}} a_k, \quad t' = \sqrt{\frac{\gamma}{m}} t, \quad \omega'_k = \sqrt{\frac{m}{\gamma}} \omega_k, \quad [6]$$

we get the following evolution equation:

$$i\frac{\partial a_1}{\partial t} = \omega_1 a_1 + \epsilon \sum_{k_2,k_3} V_{1,2,3}\left(a_2 a_3 \delta_{1,2+3} + 2a_2^* a_3 \delta_{1,3-2} + a_2^* a_3^* \delta_{1,-2-3}\right), \quad [7]$$

where primes have been omitted for brevity and the summation on k_2 and k_3 is intended from $-N/2+1$ to $N/2$; $a_i = a(k_i, t)$, $\delta_{i,j} = \delta_{k_i,k_j}$ is the Kronecker delta that should be understood with "modulus N," i.e., it is also equal to 1 if the argument differs by N. The dispersion relation becomes now $\omega_k = 2|\sin(\pi k/N)|$. The matrix $V_{1,2,3}$ weights the transfer of energy between wave numbers k_1, k_2, and k_3 and is given by the following:

$$V_{1,2,3} = -\frac{1}{2\sqrt{2}} \frac{\sqrt{\omega_1\omega_2\omega_3}}{\mathrm{sign}[\sin(\pi k_1/N)\sin(\pi k_2/N)\sin(\pi k_3/N)]}. \quad [8]$$

The parameter ϵ, given by the following:

$$\epsilon = \frac{\alpha}{m}\left(\frac{\gamma}{m}\right)^{1/4}\sqrt{\sum_k \omega_k |a_k(t=0)|^2}, \quad [9]$$

is the only free parameter of the model. If $\epsilon = 0$, the system is linear; in the present manuscript, we are interested in the weakly nonlinear regime, i.e., $\epsilon \ll 1$.

Absence of Three-Wave Resonant Interactions and the Role of the Canonical Transformation. Eq. **7**, which has a Hamiltonian structure with canonical variables $\{ia_k, a_k^*\}$, describes the time evolution of the amplitudes of the normal modes of the α-FPU system. It is characterized by a quadratic nonlinearity, i.e., a three-wave interaction system. Wave numbers k_1, k_2, and k_3 are called "resonant" if they satisfy the following equations:

$$k_1 \pm k_2 \pm k_3 \overset{N}{=} 0, \quad \omega_1 \pm \omega_2 \pm \omega_3 = 0, \quad [10]$$

where the $\overset{N}{=}$ sign means "equal modulus N," i.e., wave numbers may scatter over the edge of the Brillouin zone because of the Umklapp (flip-over) scattering (13). Using prosthaphaeresis formulas, one can show that it is impossible to find nonzero k_1, k_2, and k_3 satisfying Eq. **10** with $\omega(k)$ given in Eq. **5**. This observation leads to a first important consideration: the Fourier modes a_k in the α-FPU system can be divided into "free" and "bound" modes. To illustrate the concept of the bound modes, we refer to the classical hydrodynamic example of the Stokes wave in surface gravity waves (see, e.g., ref. 14). The Stokes wave is a solution of the Euler equations and is characterized by a primary sinusoidal wave plus higher harmonics whose amplitudes depend on the primary wave. Those higher harmonics are bound to the primary free sinusoidal mode and they do not obey the linear dispersion relation. Cnoidal waves and solitons are similar objects: they are characterized by a large number of harmonics that are not free to interact with each other. In the light of the above comments, we then make the following statement: the equipartition phenomenon is not to be expected for the Fourier modes of the original variables $a(k,t)$ or $Q(k,t)$, but only for those that are free to interact. The rest of the modes in the spectrum do not have an independent dynamics and are phase-locked to the free ones. The question is then how to build a spectrum characterized only by free modes. From a theoretical point of view, the problem can be attacked by removing via an ad hoc canonical transformation all interactions that are not resonant. The transformation inevitably generates higher-order interactions that may or may not be resonant. If those are not resonant, then a new transformation can be applied to remove them; in principle, such operation can be iterated up to an infinite order in nonlinearity, as long as no resonant interactions are encountered. In the presence of resonant interactions, the transformation diverges because of the classical small divisor problem (15).

For the case of α-FPU, the following transformation from canonical variables $\{ia_k, a_k^*\}$ to $\{ib_k, b_k^*\}$:

$$a_1 = b_1 + \epsilon \sum_{k_2,k_3}\left(A^{(1)}_{1,2,3} b_2 b_3 \delta_{1,2+3} + A^{(2)}_{1,2,3} b_2^* b_3 \delta_{1,3-2} + A^{(3)}_{1,2,3} b_2^* b_3^* \delta_{1,-2-3}\right) + O(\epsilon^2), \quad [11]$$

removes the triad interactions in Eq. **7** and introduces higher-order nonlinearity. Here,

$$A^{(1)}_{1,2,3} = V_{1,2,3}/(\omega_3 + \omega_2 - \omega_1),$$
$$A^{(2)}_{1,2,3} = 2V_{1,2,3}/(\omega_3 - \omega_2 - \omega_1),$$
$$A^{(3)}_{1,2,3} = V_{1,2,3}/(-\omega_3 - \omega_2 - \omega_1).$$

Note that the denominators are never zero because of the nonexistence of triad resonant interactions. Higher-order terms in Eq. **11** will be considered in *The Reduced Dynamical Equation and Exact Resonances* and will involve four-, five-, and six-wave interactions. These higher-order terms will play a crucial role in the foregoing analyses. The procedure for calculations of such canonical transformations is well established (16) and may be implemented, for example, by use of diagrammatic technique, as was done in ref. 17.

To present a physical interpretation of the canonical transformation, we can write it in terms of the original variable $q_j(t)$. Using Eqs. **3** and **4**, the displacement of the masses can be written in the following form:

$$q_j(t) = i\sum_k\left[\frac{a_k}{\sqrt{2\omega_k}} e^{i2\pi jk/N} - c.c.\right], \quad [12]$$

where $c.c.$ stands for complex conjugate. We now plug Eq. **11** in Eq. **12**, and for simplicity we assume that the free modes are characterized by a monochromatic wave centered in k_0 of the form $b(k,t) = |\overline{b}|\delta_{k,k_0} e^{-i(\omega_{k_0}t - \phi_{k_0})}$, with $\omega_{k_0} = 2|\sin(\pi k_0/N)|$; $|\overline{b}|$, a constant; and ϕ_{k_0}, an arbitrary phase; after some algebra, the following result is obtained for the displacement (see also ref. 18):

$$q_j(t) = A\sin(\theta) + \epsilon\, B\sin(2\theta) + O(\epsilon^2), \quad [13]$$

with $\theta = 2\pi k_0 j/N - \omega_0 t + \phi_{k_0}$, $A = -2|\overline{b}|/\sqrt{2\omega_{k_0}}$, and $B = 2V_{2k_0,k_0,k_0}\sqrt{2\omega_{k_0}}|\overline{b}|^2/(-4\omega_{k_0}^2 + \omega_{2k_0}^2)$. Note that B is proportional to A^2 and the second harmonic $2k_0$ does not oscillate with frequency $\omega(2k_0)$ but with $2\omega(k_0)$, i.e., it does not obey the linear dispersion relation. Higher-order terms in the canonical transformation would bring higher harmonics. It is clear that the spectrum associated to the variable b_k (in the present case, a single mode) is different from the one associated to the variable a_k or Q_k (where multiple bound harmonics appear). Eq. **13** is nothing but the second-order Stokes series solution of the α-FPU system. The initial stage of the α-FPU system initialized by a single mode k_0 would then be characterized by the generation of the higher harmonics of the type in Eq. **13**.

The Reduced Dynamical Equation and Exact Resonances. We now turn our attention to the dynamical equation that results after the canonical transformation has been performed; the equation reads as follows:

$$i\frac{\partial b_1}{\partial t}=\omega_1 b_1+\epsilon^2\sum_{k_2,k_3,k_4}T_{1,2,3,4}b_2^*b_3b_4\delta_{1+2,3+4}+O(\epsilon^3). \quad [14]$$

Note that similar terms including the Kroneker deltas $\delta_{1,3+4+2}$, $\delta_{1,-3-4-2}$, $\delta_{1,4-3-2}$, should also appear in Eq. **14** as a result of the transformation (Eq. **11**); however, those terms are not resonant and can be removed by higher-order terms in the transformation. The matrix $T_{1,2,3,4}$ has an articulated analytical form that depends on $V_{1,2,3}$ and is given, for example, in ref. 17 or 19. Due to the Hamiltonian structure of the original system, $T_{1,2,3,4}$ has the following symmetries: $T_{1,2,3,4}=T_{2,1,3,4}=T_{3,4,1,2}$. We underline that the same equation but with a different matrix $T_{1,2,3,4}$ can be obtained directly for the so-called β-FPU or for the $\alpha+\beta$-FPU chains. If higher-order terms are neglected, the equation admits a Birkhoff normal form (20) (see also ref. 21). Eq. **14**, with different linear dispersion relation, different matrix $T_{1,2,3,4}$, and with integrals instead of sums, is the equivalent of the Zakharov equation for one-directional water waves (22).

Eq. **14** describes the reduced α-FPU model where three-wave interactions have been removed by the canonical transformation (Eq. **11**). The resonant interactions associated with Eq. **14** are described by the following four-wave resonant conditions:

$$k_1+k_2-k_3-k_4\overset{N}{=}0, \quad \omega_1+\omega_2-\omega_3-\omega_4=0. \quad [15]$$

Solutions for $k_i\in\mathbb{Z}$ and $N=16$ or 32 or 64 particles, like in the original FPU problem, are reported below.

Trivial solutions. Trivial resonances are obtained when all wave numbers are the same or when the following:

$$k_1=k_3,\ k_2=k_4, \quad [16]$$

with permutations of 3 and 4. These trivial solutions are responsible for a nonlinear frequency shift and do not contribute to the energy transfer between modes, as discussed, for example, in ref. 12.

Nontrivial solutions. Nontrivial resonances exist and are the result of the following scattering process: when three waves interact to generate a fourth one, it can happen that the latter is characterized by a $k\notin[-N/2+1,\ldots,N/2]$, i.e., outside the Brillouin zone. The system flips back this energy into a mode contained in the domain; as mentioned, this is known as the Umklapp scattering process (13, 23). These resonant modes have the following structure:

$$(k_1,k_2,-k_1,-k_2), \quad [17]$$

with $k_1+k_2=mN/2$ and $m=0,\pm1,\pm2$. It is instructive to give an example: let us consider a chain of $n=32$ masses; the maximum wave number accessible is then $k_{max}=16$. One of the quadruplets satisfying the resonant condition (Eq. **15**) is $k_1=2$, $k_2=14$, $k_3=-14$, $k_4=30$. The first three wave numbers are contained in the domain, whereas k_4 is outside. The system will interpret $k_4=30$ as $k_4\rightarrow k_4-N=-2$.

To account for an effective energy mixing, the quadruplets (four modes satisfying the resonant conditions) should be interconnected, i.e., single wave numbers should belong to different quartets. However, a careful and straightforward analysis of Eq. **17** reveals that resonant quartets are not interconnected, that is, all of the quartets are isolated: if one puts energy into one of the quartets, and only weakly nonlinear resonant interactions are allowed, the energy will remain in the quartet. The above results has the important consequence that the four-wave interactions in the α-FPU model cannot possibly lead to equipartition of energy.

An efficient mixing mechanism should be searched by extending to higher order the canonical transformation. Five-wave interactions are nonresonant and can be removed by an appropriate choice of the higher-order terms in Eq. **11**. The resulting evolution equation for b_1 is a refinement of Eq. **14**, and it has the following form:

$$i\frac{\partial b_1}{\partial t}=\omega_1 b_1+\epsilon^2\sum T_{1,2,3,4}b_2^*b_3b_4 + \epsilon^4\sum W_{1,2,3}^{4,5,6}b_2^*b_3^*b_4b_5b_6\delta_{1+2+3,4+5+6}+O(\epsilon^5). \quad [18]$$

The explicit form of the matrix $W_{1,2,3}^{4,5,6}$ (for details, see refs. 12 and 24) is not necessary for the discussion of our results. Note that the four-wave interactions cannot be removed because, even though they do not contribute to the spreading of energy in the spectrum, they are resonant and a canonical transformation suitable for removing those modes would diverge.

For $N=16$ or 32 or 64, we have found that solutions of the following six-wave resonant conditions,

$$k_1+k_2+k_3-k_4-k_5-k_6\overset{N}{=}0, \qquad \omega_1+\omega_2+\omega_3-\omega_4-\omega_5-\omega_6=0, \quad [19]$$

exist for $k_i\in\mathbb{Z}$, and we report them below.

Trivial resonances. Trivial resonances are obtained when all six wave numbers are the same or when

$$k_1=k_4,\ k_2=k_5,\ k_3=k_6, \quad [20]$$

with all permutations of indices 4, 5, 6. These trivial solutions are responsible only for a nonlinear frequency shift.

Nontrivial symmetric resonances. These resonances are over the edge of the Brillouin zone and are given by the following:

$$(k_1,k_2,k_3,-k_1,-k_2,-k_3), \quad [21]$$

with $k_1+k_2+k_3=mN/2$ and $m=0,\pm1,\pm2,\ldots$.

Nontrivial quasisymmetric resonances. These resonances over the edge of the Brillouin zone are characterized by one repeated wave number:

$$(k_1,k_2,k_3,-k_1,-k_2,k_3), \quad [22]$$

with $k_1+k_2=mN/2$, $m=0,\pm1,\pm2,\ldots$, and all permutations of the indices. We have not found any other integer solutions to the resonant condition (Eq. **19**) for $N=16,32,64$, other than those in Eqs. **20**, **21**, and **22**.

Those resonant sextuplets are interconnected; therefore, they represent an efficient mechanism of spreading energy in the spectrum. Because of the existence of these exact resonant processes, we expect the equipartition to take place.

Estimation of the Equipartition Timescale

Thermal equilibrium is a statistical concept; therefore, an equation for the time evolution of the average spectral energy density is required. Within the wave turbulence theory, such equation is called a "kinetic equation." There are many techniques for deriving it that are object of intensive studies. We are mainly interested in the estimation of the timescale of equipartition; therefore, only the key steps are here considered (details can be found in ref. 11). We introduce the wave action, $n_k=n(k,t)$, defined as $\langle b_1b_2^*\rangle=n_1\delta_{1,2}$, where the brackets indicate ensemble averages and the $\delta_{1,2}$ is the Kronecker delta, the latter arising from the assumption of homogeneity of the wave field. To derive the evolution equation for n_1, Eq. **18** is multiplied by b_1^* and the ensemble averages are taken. The time evolution of the n_1 depends on the six-order correlator $\langle b_1^*b_2^*b_3^*b_4b_5b_6\rangle$ whose time evolution will be a function of higher-order correlators; this is the classical Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy problem. The time evolution of the six-order correlator turns out to be proportional to

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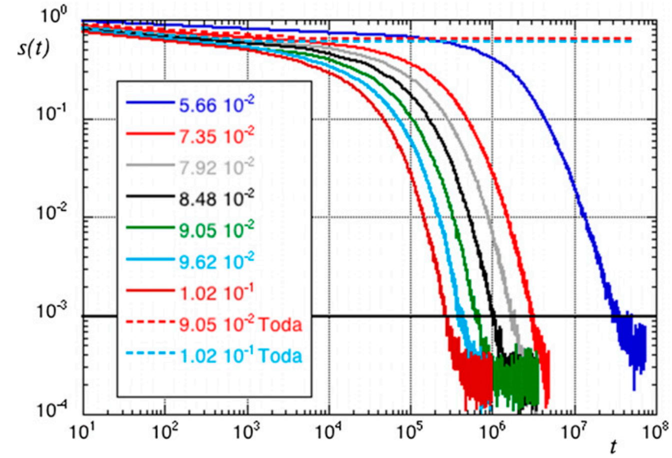

Fig. 1. Entropy $s(t)$ as a function of time for different simulations of the α-FPU system characterized by different values of ϵ. In the plot, two simulations of the Toda lattice are also presented. A horizontal line at $s = 0.001$ is also included as a threshold for estimating the equipartition time.

$\epsilon^4 W^{4,5,6}_{1,2,3}$. Indeed, assuming that the waves obey Gaussian statistics, we decompose the higher-order correlators into products of second-order correlators and, after taking the large time limit, the six-order correlator may be obtained explicitly. The result is then plugged into the equation for the time evolution of n_k, resulting in a collision integral proportional to $(\epsilon^4 W^{4,5,6}_{1,2,3})^2$ (see, for example, equation 6.89 in ref. 12). Consequently, the time evolution of the spectral energy density in the α-FPU problem is proportional to $1/\epsilon^8$. This is the main theoretical result of our work, which, as it will be shown, is supported by numerical simulations.

Relation to the Toda Lattice

Before showing our numerical simulation results, it is instructive to make a connection between the α-FPU and the integrable Toda system (25) (see also ref. 26 for a normal mode approach to the problem). In ref. 4, it has been shown that the α-FPU can be seen as a perturbation of the integrable Toda lattice (see also ref. 27). For the sake of clarity, we report this argument. We consider the general Hamiltonian for a discrete lattice:

$$H(p,q) = \frac{1}{2}\sum_{j=1}^{N} p_j^2 + \sum_{j=1}^{N} V(q_{j+1} - q_j); \qquad [23]$$

the potential V for the α-FPU case is given by the following:

$$V(r) = \frac{r^2}{2} + \varepsilon\frac{r^3}{3}. \qquad [24]$$

For the Toda lattice, instead, V results in the following:

$$V(r) = V_0\left(e^{\lambda r} - 1 - \lambda r\right), \qquad [25]$$

with V_0 and λ free parameters. For the particular choice of $V_0 = 1/(4\varepsilon^2)$ and $\lambda = 2\varepsilon$, upon Taylor expanding the exponential in the Toda lattice for small ε, we obtain the following:

$$V(r) = \frac{r^2}{2} + \varepsilon\frac{r^3}{3} + \varepsilon^2\frac{r^4}{6} + \ldots, \qquad [26]$$

which shows the α-FPU coincides with the Toda Lattice up to the order of ϵ (see Eqs. **24** and **26**).

Having made this introduction, using our approach based on resonant interactions and, following the fundamental work by Zakharov and Schulman (28), we are able to discern between integrable and nonintegrable dynamics. We underline that the Toda lattice has the same linear dispersion relation as the α-FPU, and, therefore, the possible resonant manifolds, being based on linear frequencies, are exactly the same. How then is it possible to explain that the Toda lattice never thermalizes, whereas the FPU does? For the Toda lattice, the same canonical transformation as in Eq. **11** can be performed and the three-wave interactions be removed (those correspond to the term proportional to ϵ in the potential in Eq. **26**). The equation of motion in Fourier space, neglecting higher-order terms, becomes the same as the one in Eq. **14**, with the only difference that the matrix $T_{1,2,3,4}$ is now modified due to the existence of the term proportional to ε^2 in the potential (Eq. **26**); such term is absent in the potential of the α-FPU. A straightforward but lengthy calculation shows that the matrix $T_{1,2,3,4}$ for the Toda lattice is identically zero on the resonant manifold. Indeed, this result has very profound origins and is based on the fundamental work by Zakharov and Schulman (28), where it is shown that, for an integrable system, either there are no resonances or all of the scattering matrices are zero at all orders on the resonant manifold. In principle, an infinite order canonical transformation would linearize an integrable system. Thus, integrable systems are characterized by trivial scattering processes, and a pure thermalization is never reached. The initial evolution of the spectrum observed in computations of the Toda lattice (see, for instance, ref. 4) is due to nonresonant interactions that are contained in the canonical transformation. On the other side, for nonintegrable systems such as the α-FPU nontrivial resonant interactions with nonzero scattering matrix exist and thermalization can be observed.

Numerical Simulations

A main result of this study is that the α-FPU model should reach thermal equilibrium on a timescale of $1/\epsilon^8$ for arbitrary small nonlinearity. Therefore, we use numerical simulations to support our theoretical finding. We integrate in time Eq. **2** with $N = 32$ particles and with $m = \gamma = 1$ by using the sixth-order symplectic integrator scheme described in ref. 29. Different values of ϵ have been considered between 0.0566 and 0.11; due to the slow time needed to reach thermalization, computations become soon prohibitive for smaller values of ϵ.

We emphasize that the thermal equilibrium is a statistical concept; therefore, averages should be taken to observe it. It may be possible to average over time, as in many previous simulations of the FPU model. We find such an approach to be problematic, because often the time window used is of the same order of the characteristic time to reach equipartition of energy. We have chosen to perform ensemble averaging, typically over 1,000 realizations (some convergence tests have also been made over 2,000 ensembles).

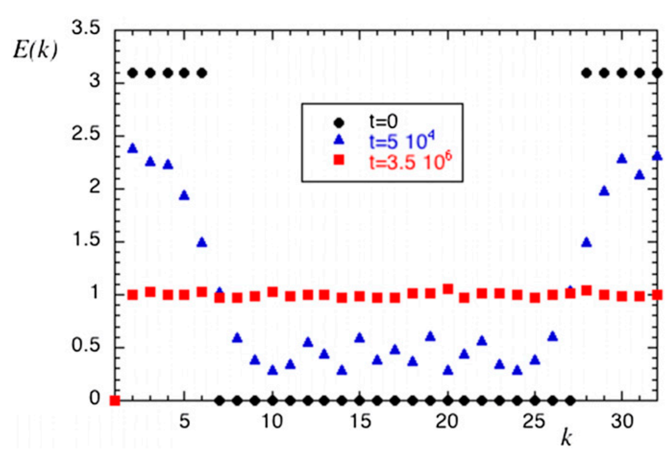

Fig. 2. Energy spectrum at different time steps from numerical simulations of the α-FPU system. Black dots correspond to the initial condition, blue triangles correspond to an intermediate stage, and red squares correspond to the final thermalized spectrum. Note that energy is presented in linear scale.

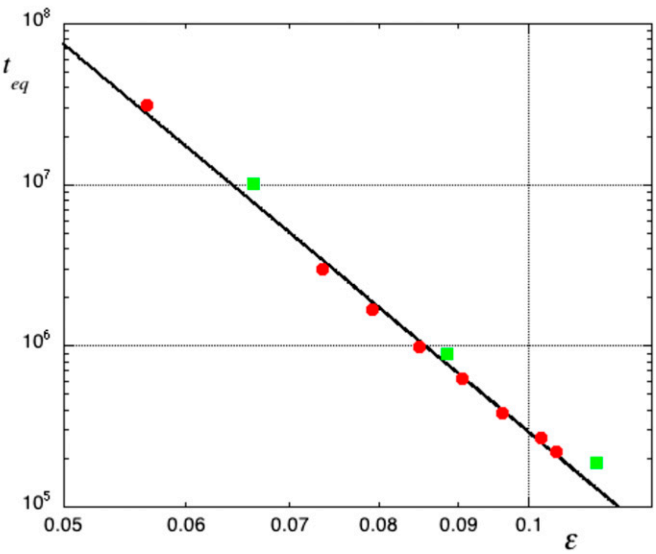

Fig. 3. Equilibrium time t_{eq} as a function of ϵ in log–log coordinates. Red dots represent numerical experiments of the α-FPU system with broad band initial conditions, i.e., modes $k=\pm1, \pm2 \pm3, \pm4, \pm5$ have been initially perturbed; green dots represent narrow-band initial conditions, i.e., modes $k=\pm1$ have been initially perturbed. The straight line corresponds to power law of the type $1/\epsilon^8$.

Two types of initial conditions have been considered: in the first one, we have initialized only the modes $k=\pm1$; in the second one, initial conditions are characterized by constant energy only over the modes $k=\pm1, \pm2, \pm3, \pm4, \pm5$. Different random phases are then applied to the Fourier amplitudes for each realization.

As in ref. 30, we have introduced, as an indicator of thermalization, the following entropy:

$$s(t) = \sum_k f_k \log f_k, \qquad [27]$$

with

$$f_k = \frac{N-1}{E_{tot}} \omega_k \left\langle |a_k|^2 \right\rangle, \quad E_{tot} = \sum_k \omega_k \left\langle |a_k|^2 \right\rangle, \qquad [28]$$

and $\langle \ldots \rangle$ defines the average over the realizations. We have used in the definition $N-1$ instead of N, because, with periodic boundary conditions, the modes that thermalize are $N-1$ and not N (the first mode $k=0$ is not involved in the dynamics). For a thermalized spectrum, the value of the entropy is theoretically 0. Through our numerical simulations, we have reached a minimum value of s very close to 10^{-4}. In Fig. 1, we show the evolution of the entropy for different values of ϵ. As one can observe, in the large time limit, the entropy reaches very small values. Two typical simulations of the Toda lattice are also included in the figure and show that, as expected, no thermalization is reached. Just as an example, we show in Fig. 2 the energy spectrum, defined as $E(k)=\omega_k\langle|a_k|^2\rangle$, at different time steps for the simulation with $\epsilon=0.0848$. The spectrum is normalized by $(N-1)/E_{tot}$ in such a way that, once thermalization has been reached, all values of the energy are around 1.

To verify the expected time scaling, we introduced an entropy threshold s_{thr} to estimate the time it takes for the system to reach thermodynamic equilibrium. Specifically, we have defined t_{eq} as the time in which the entropy s reaches the value of $s_{thr}=0.001$ (see a horizontal line at $s=0.001$ in Fig. 1). We present in Fig. 3 the log–log plot of this time t_{eq} as a function of ϵ for the two types of simulations considered. Fig. 3 also shows the straight line with slope −8. All of the points are pretty much aligned with this straight line. This numerical result is consistent with our analytic prediction that time t_{eq} is proportional to ϵ^{-8}. The last check on the validity of the theory, free of an arbitrary threshold, is made by rescaling the time evolution of the entropy: in Fig. 4, we show the evolution of the entropy as a function of $\epsilon^8 t$ for different values of ϵ. As predicted by our theory, the curves seem to collapse to a single one.

A Note on the Thermodynamic Limit

In statistical mechanics, one is usually interested in the thermodynamic limit. Assuming that the length of the chain is L and the spacing between masses is Δx, we let $N\to\infty$ and $L\to\infty$ in such a way that $\Delta x = L/N = const$. Wave numbers in Fourier space become dense, $\Delta k = 2\pi/L \to 0$. The dispersion relation now becomes $\omega(\kappa)=2|\sin(\kappa/2)|$, where we have set $\Delta x=1$ and $\kappa=k\Delta k$. Assuming that $\kappa\in\mathbb{R}$, the same approach based on resonant interactions can now be performed. It turns out that four-wave, nonisolated, resonant interactions exist. An example is provided by the following two connected quartets:

$$(-0.05710747907971836..., 1.604305030276316..., 1/2, \pi/3),$$
$$(-0.12747695473542747..., 2.198273281530324..., 1/2, \pi/2),$$

which can be found numerically using the resonant conditions (Eq. **19**). The existence of interconnected resonant quartets implies that, in the thermodynamic limit, the equipartition may be achieved by resonant four-wave interactions; in this case, the system is completely described by the traditional wave turbulence four-wave kinetic equation (11). The timescale of the resonant four-wave kinetic equation is given by the $1/\epsilon^4$, much shorter than $1/\epsilon^8$, i.e., the timescale of equipartition for a system of $n = 16,32,64$ masses.

A Short Discussion on Other Possible Scenarios

The FPU system has been the subject of many studies and a presentation of all of the different points of view developed in 60 years is merely impossible. However, here we briefly present some routes to equipartition that are accepted nowadays in the literature.

In the pioneering work of Izrailev and Chirikov (31), the idea that an initial energy larger than a critical value is needed to reach thermalization was put forward. Such concept is based on the fact that the nonlinearity changes the linear dispersion relation, and, consequently, the resonant condition in frequency is then modified. When the nonlinearity becomes large enough, a mechanism of "overlap of frequencies" may take place. Such phenomenon led to the introduction of the so-called "stochastic threshold." In the late 1960s, not everybody shared such an idea; indeed, for example, in 1970, Ford and Lunsford (32) insisted on the fact that mixing could be observed also in the limit as the nonlinearity goes to zero.

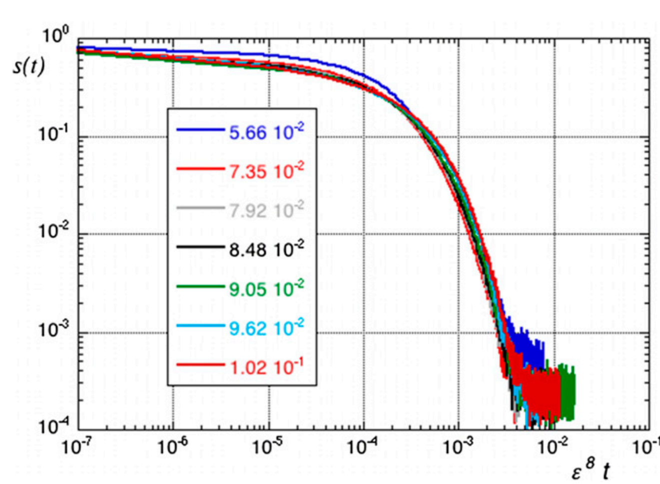

Fig. 4. Entropy $s(t)$ as a function of $\epsilon^8 t$ for different simulations of the α-FPU system characterized by different values of ϵ.

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In favor of the existence of a threshold, a large number of papers have been written and different scenarios have been presented (see, for example, ref. 30). A very interesting picture has been presented in ref. 33: the authors considered the β-FPU system with initial conditions characterized by the highest mode (also known as the π-mode). They showed that, above an energy threshold that can be computed analytically, the π-mode is modulationally unstable and gives rise to localized chaotic structures (breathers). They related the lifetime of the chaotic breathers to the time necessary for the system to reach equipartition. This interesting scenario cannot be directly applied to the α-FPU; the reason is that a straightforward calculation shows that a single mode in the α-FPU is modulationally stable. This does not imply that, in the α-FPU model, localized coherent structure does not exist. Indeed, being the system close to the Korteweg de Vries equation, solitary waves may be excited, if the initial energy is sufficiently large. However, our main finding is that such strong nonlinearity is not needed to reach equipartition. Our explanation is based only on resonant interactions, and, as a result, equipartition can take place for arbitrary small nonlinearity, as confirmed by numerical simulations.

We mention once more that our analyses are based on $n = 16$ or 32 or 64 masses, as the original simulations of Fermi, Pasta, and Ulam; by changing the number of masses, the solution to the resonant conditions may change; therefore, each case should be treated separately and possibly different scenarios may appear, as for example the thermodynamic limit described above.

Conclusion

i) Resonant triads are forbidden; this implies that, on a short timescale, three-wave interaction will generate a reversible dynamics. This is what has been observed originally by Fermi, Pasta, and Ulam and what is known as metastable state (see, for example, ref. 4).

ii) A suitable canonical transformation allows us to look at higher-order interactions in the system that are responsible for longer timescale dynamics.

iii) Four-wave resonant interactions exist; however, we have shown that, for $n = 16$, 32, 64, each resonant quartet is isolated, preventing the full spread of the energy across the spectrum and thermalization.

iv) Six-wave interactions lead to irreversible energy mixing.

v) The timescale of equipartition in a weakly nonlinear random system described by α-FPU system is $1/\epsilon^8$. The result is consistent with our numerical simulations.

vi) In the thermodynamic limit, nonisolated resonant quartets exits and the timescale of equipartition is $1/\epsilon^4$.

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