Double Scaling in the Relaxation Time in the β-Fermi-Pasta-Ulam-Tsingou Model

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We consider the original β-Fermi-Pasta-Ulam-Tsingou system; numerical simulations and theoretical arguments suggest that, for a finite number of masses, a statistical equilibrium state is reached independently of the initial energy of the system. Using ensemble averages over initial conditions characterized by different Fourier random phases, we numerically estimate the time scale of equipartition and we find that for very small nonlinearity it matches the prediction based on exact wave-wave resonant interaction theory. We derive a simple formula for the nonlinear frequency broadening and show that when the phenomenon of overlap of frequencies takes place, a different scaling for the thermalization time scale is observed. Our result supports the idea that the Chirikov overlap criterion identifies a transition region between two different relaxation time scalings.

In 1923 at the age of 22 Fermi published one of his first papers [1] in which the goal was to show that Hamiltonian systems are in general quasiergodic. At that time, the paper was considered interesting by the scientific community; however, it appeared later that the hypotheses needed for the proof are very restrictive ([2,3]). About thirty years later Fermi, in collaboration with Pasta, Ulam, and Tsingou (see Ref. [4] for a discussion of the role played by Tsingou), came back to the problem using a numerical approach. The goal was to study a simple mechanical system and verify that a small nonlinearity would be enough to let the system reach a thermalized state. Their research was also motivated by the work of Debye who in 1914 conjectured that normal (in accordance with the macroscopic Fourier law) heat conduction in solids could be obtained only in the presence of nonlinearity; see Ref. [5] for recent developments. They simulated a one dimensional lattice composed of coupled an harmonic oscillators with cubic and quartic potentials known as the $\alpha-$ and $\beta-$ Fermi-Pasta-Ulam-Tsingou (FPUT) models, respectively. The results they obtained numerically [6] were very different from expectations: instead of observing the equipartition of linear energy, they observed a recurrent phenomena known as the FPUT recurrence. This unexplained result triggered a surge of scientific activity and lead to the discovery of solitons [7] and integrability in infinite dimensional systems [8]. However, the FPUT system is only close to an integrable one [9] and soliton interactions are not elastic.

At the same time that the simulations of the FPUT system were performed, Kolmogorov enunciated the Kolmogorov-Arnold-Moser (KAM) theorem which loosely speaking describes how in a perturbed integrable Hamiltonian system the KAM tori survive if the perturbation is sufficiently small.

Chirikov and Izraielev [10] developed a method for estimating the threshold of the initial energy above which the KAM tori are destroyed. The basic idea is the following: in the presence of nonlinearity, linear frequencies are perturbed and, if the perturbation is larger than the frequency spacing (distance between two adjacent linear frequencies), then the trajectory may oscillate chaotically between the two frequencies. This idea, known also as the Chirikov overlap criterion, is very helpful but not rigorous. Indeed, for example, there exists a counter example: for the Toda lattice (or other integrable system) a threshold can be derived but the system is integrable, therefore never chaotic. The idea of Chirikov and Izrailev was followed and different numerical studies confirmed the presence of a threshold above which the FPUT system reaches a fast thermalized state (see, for example, Refs. [11–13] for a study of the β-FPUT model). However, more recently, numerical simulations of the α-FPUT model [14,15] have shown that even for small nonlinearity the system does reach a thermalized state. The explanation of this result was given in Ref. [15] where it has been shown that for the finite dimensional system of a certain size, six-wave resonant interactions are responsible for equipartition and only after a very long time does the system reach a thermalized state.

In this Letter we perform a detailed study of the β-FPUT model with a finite number of masses and, as a first result, we show that, as for the α-FPUT model, the weak nonlinear regime is dominated by discrete six-wave resonant interactions that are responsible for thermalization. Such a thermalization seems to occurs for any, even extremely small, levels of nonlinearity. We then estimate the time scale it takes to reach equipartition, and we confirm the result numerically. Moreover, we construct numerically the dispersion relation curve and show that equipartition is observed also in the

condition of no overlap of frequencies. By writing the equation of motion in angle-action variables and by using the Wick decomposition, we find an explicit formula for the broadening of the frequencies. When such a broadening is larger than the spacing between frequencies, the Chirikov regime is observed. Therefore, the Chirikov criteria identify a threshold for a more effective mechanism of thermalization. Consequently, there is a double time scaling to reach equipartition as a function of the nonlienarity parameter. Our results are fully supported by numerical simulations.

The model.—We consider the Hamiltonian for a chain of N identical particles of mass m of the type

$$H = H_2 + H_4 \tag{1}$$

with

$$H_2 = \sum_{j=1}^{N} \left(\frac{1}{2} p_j^2 + \frac{1}{2} (q_j - q_{j+1})^2 \right),$$

$$H_4 = \frac{\beta}{4} \sum_{j=1}^{N} (q_j - q_{j+1})^4. \tag{2}$$

$q_j(t)$ is the displacement of the particle j from its equilibrium position and $p_j(t)$ is the associated momentum; β is the nonlinear spring coefficient (without loss of generality, we have set the masses and the linear spring constant equal to 1).

Analytical results.—Before performing numerical simulations of the equations associated with the Hamiltonian (2), we first outline the derivation of some important theoretical predictions: (i) the nonlinear correction to the linear frequency, (ii) the broadening of the frequencies in the presence of nonlinearity, and (iii) the time scale of the equipartition. Those ingredients will help us in interpreting the numerical results.

Assuming periodic boundary conditions and the standard definition of the discrete Fourier transform, we introduce the following normal variable as

$$a_k = \frac{1}{\sqrt{2\omega_k}} (\omega_k Q_k + i P_k), \tag{3}$$

where $\omega_k = 2|\sin(\pi k/N)|$ and Q_k and P_k are the Fourier coefficients of q_j and p_j. Then, assuming small nonlinearity, we perform a near identity transformation to remove nonresonant four-wave interactions (such a procedure is well documented in the general case in Ref. [16] and in the α-FPUT case in Ref. [15]). The following reduced Hamiltonian is obtained (the new variable has been renamed a_k and higher order terms have been neglected):

$$\tilde{H}_2 = N \sum_{k=0}^{N-1} \omega_k |a_k|^2,$$

$$\tilde{H}_4 = \frac{N}{2} \beta \sum_{k_1 k_2 k_3 k_4} T_{k_1,k_2,k_3,k_4} a_{k_1}^* a_{k_2}^* a_{k_3} a_4 \delta_{1+2,3+4}, \tag{4}$$

where all wave numbers k_1, k_2, k_3, and k_4 are summed from 0 to $N-1$,

$$T_{k_1,k_2,k_3,k_4} = \frac{3}{4} e^{i\pi\Delta k/N} \prod_{j=1}^{4} \frac{2\sin(\pi k_j/N)}{\sqrt{\omega(k_j)}} \tag{5}$$

with $\Delta k = k_1 + k_2 - k_3 - k_4$, and $\delta_{i,j}$ is the generalized Kronecker delta that accounts for a periodic Fourier space. We then introduce scaled amplitudes $a_k' = a_k/\sqrt{H_2(t=0)/N}$ so that the equation of motion in the new variable reads

$$i \frac{da_{k_1}}{\partial t} = \omega_{k_1} a_{k_1} + \epsilon \sum_{k_i} T_{k_1,k_2,k_3,k_4} a_{k_2}^* a_{k_3} a_{k_4} \delta_{1+2,3+4}, \tag{6}$$

where primes have been omitted for brevity, the sum on k_i implies a sum on k_2, k_3, k_4 from 0 to $N-1$, and

$$\epsilon = \beta H_2(t=0)/N, \tag{7}$$

which implies that our nonlinear parameter is proportional to the linear energy density of the system at time $t = 0$ and to the nonlinear spring constant β. In terms of the angle-action variables $a_k = \sqrt{I_k} \phi_k$ with $\phi_k = \exp[-i\theta_k]$, the equation for θ reads

$$\frac{d\theta_{k_1}}{\partial t} = \omega_{k_1} + \epsilon \sum_{k_i} T_{k_1,k_2,k_3,k_4} \frac{\sqrt{I_{k_2} I_{k_3} I_{k_4}}}{\sqrt{I_{k_1}}}$$
$$\times \text{Re}[\phi_{k_1}^* \phi_{k_2}^* \phi_{k_3} \phi_{k_4}] \delta_{1+2,3+4}, \tag{8}$$

where $\text{Re}[\cdots]$ implies the real part. From this equation we obtain the frequency by applying the averaging operator $\langle \cdots \rangle$ over random phases and using Wick's contraction rule

$$\langle \phi_{k_1}^* \phi_{k_2}^* \phi_{k_3} \phi_{k_4} \rangle = \delta_{1,3}\delta_{2,4} + \delta_{1,4}\delta_{2,3}, \tag{9}$$

we get the instantaneous frequency:

$$\tilde{\omega}_{k_1} = \left\langle \frac{d\theta_k}{dt} \right\rangle \simeq \omega_{k_1} + 2\epsilon \sum_{k_2 \neq k_1} T_{k_1,k_2,k_1,k_2} I_{k_2}, \tag{10}$$

i.e., the nonlinear dispersion relation given by the linear dispersion relation plus amplitude corrections (recall that $I_k = |a_k|^2$), see also Refs. [17,18]. More interestingly, one can estimate the half-width Γ_k of the frequency by calculating the second centered moment of the equation (8) as

$$\Gamma_k = \sqrt{\left\langle \left(\frac{d\theta_{k_1}}{\partial t} - \tilde{\omega}_k \right)^2 \right\rangle}. \tag{11}$$

Using Eqs. (8) and (10), and Wick's decomposition, and under the assumption of thermal equilibrium (equipartition of linear energy), we obtain

$$\Gamma_k = \frac{3}{4}\epsilon\omega_k = \frac{3}{4}\frac{1}{N}\beta H_2(t=0)\omega_k. \qquad (12)$$

Once the broadening of the frequency is estimated, the Chirikov overlap parameter can be defined as

$$R_k = 2\frac{\Gamma_k}{\tilde{\omega}_{k+1} - \tilde{\omega}_k}\frac{3}{2}\frac{\omega_k}{\omega_{k+1} - \omega_k}\epsilon. \qquad (13)$$

According to Chirikov, the stochasticization takes place when $R_k = 1$. If we define ϵ_{cr} as the value for which $R_k = 1$, then it is straightforward to observe that ϵ_{cr} is k dependent and ϵ_{cr} becomes large for small values of k. This implies that a transition region between two regimes cannot be sharp. In the long wave limit the critical energy takes the following form $H_{2Cr}(t=0) = 2N/(3\beta k)$. Full stochasticization of all wave numbers takes place for $\epsilon_{cr} \simeq 0.6$ (as we will see below, for this value of ϵ we observe a new scaling of the equipartition time as a function of time).

We now turn our attention to the estimation of the time scale needed to reach equipartition. The theoretical predictions that follow are based on the assumption that an irreversible dynamics can be obtained only if waves interact in a resonant manner; i.e., for some n and l the following system has a solution for integer values of k:

$$k_1 + k_2 + \cdots + k_l = k_{l+1} + k_{l+2} + \cdots + k_n,$$
$$\omega_{k_1} + \omega_{k_2} + \cdots + \omega_l = \omega_{l+1} + \omega_{l+2} + \cdots + \omega_n. \qquad (14)$$

Just like for a forced harmonic oscillator, nonresonant interactions lead to periodic solutions, i.e., to recurrence. Based on the methodology developed in Ref. [15], we can state that for $N = 32$ (the number of masses in the original simulations of Fermi *et al.*) there are four-wave resonant interactions; however, those resonances are isolated and cannot lead to thermalization (see also Refs. [19,20]). Following the results in Ref. [15], efficient resonant interactions for the β-FPUT model take place for $l = 3$ and $n = 6$; i.e., six-wave resonant interactions are the lowest order resonant process for the discrete system. This implies that a new canonical transformation needs to be performed to remove nonresonant four-wave interactions and obtain a deterministic six-wave interaction equation whose time scale is $1/\epsilon^2$; see Ref. [21] for details on the canonical transformation.

An estimation of the time scale of such interactions can be obtained following the argument developed in Ref. [15] based on the construction of an evolution equation for the wave action spectral density $N_k = \langle|a_k|^2\rangle$, a_k being the new canonical variable [15]. Using Wick's rule to close the hierarchy of equations, it turns out $\partial N_k/\partial t \sim \epsilon^4$. The result is that the time of equipartition scales like $t_{eq} \sim 1/\epsilon^4$ (this coincides precisely with the time scale $1/\alpha^8$ given in Ref. [15] for the α-FPUT model). In the continuum limit (thermodynamic limit) in which the number of particles N and the length of the chain both tend to infinity, keeping the

linear density of masses constant,. it can be shown that the Fourier space becomes dense ($k \in \mathbb{R}$): four-wave exact resonances exist and the standard four-wave kinetic equation can be recovered (see Refs. [22–25]). In this latter case the time scale for equipartition should be $1/\epsilon^2$.

Numerical experiments.—We now consider numerical simulations of the β-FPUT system in the original q_j and p_j variables to verify our predictions. We integrate the equations with $N = 32$ particles using the sixth order symplectic integrator scheme described in Ref. [26]. We run the simulations for different values of β, keeping always the same initial conditions, which are formulated in Fourier space in normal variables as

$$a_k(t=0)$$
$$= \begin{cases} e^{i\phi_k}/(N\sqrt{\omega_k}), & \text{if } k = \pm 1, \pm 2, \pm 3, \pm 4, \pm 5, 0 \\ 0 & \text{otherwise} \end{cases}$$
$$(15)$$

related to the original variables by Eq. (3). ϕ_k are uniformly distributed phases. By changing β, different values of the nonlinear parameter ϵ are experienced.

We found out that a successful way of estimating the time of equipartition is to run, for each initial condition, different simulations characterized by a different set of random phases: our typical ensemble is composed of 2000 realizations. In order to establish the time of thermalization, we have considered the following entropy [11]:

$$s(t) = -\sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{H_2}\omega_k\langle|a_k(t)|^2\rangle,$$
$$(16)$$

and $\langle\cdots\rangle$ defines the average over the realizations. Note that the larger is the number of members of the ensemble, the lower are the stationary values reached by s. In our numerics we have followed the procedure outlined in Ref. [15] to identify the time of equipartition. We present in Fig. 1 such a time t_{eq} as a function of ϵ for the simulations considered in a log-log plot. The figure also shows two straight lines (power laws) with slopes -4 and -1. The steepest one (in red) is consistent with the six-wave interaction theory, while the blue one corresponds to the time scale associated with the nonlinearity in the dynamical equation. A clear transition between the two scalings is observed. A similar transition has also been observed in Ref. [27] where the α-FPUT model has been integrated.

In order to understand such behavior, we build the dispersion relation curve from numerical data and measure the shift and the width of the frequencies as a function of the parameter ϵ. After reaching the thermalized state, the procedure adopted consists in constructing the variable $a_k(t)$ from Eq. (3) and letting the simulation run on a time window over which, for each mode, a Fourier transform
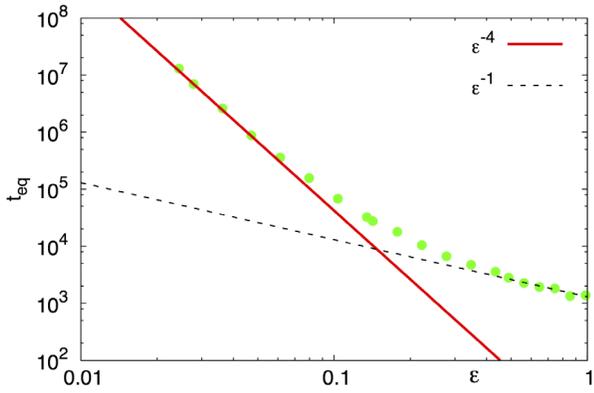
FIG. 1. Equilibrium time t_{eq} as a function of ϵ in log-log coordinates. The dots represent numerical experiments. The straight line corresponds to a power law of the type $1/\epsilon^4$ (red line) and $1/\epsilon$ (black dashed line).

(from variable t to Ω) is taken. This is done for all the members of the ensemble. Then, $\langle|a(k,\Omega)|^2\rangle$ is normalized by its maximum for each value of k and then plotted as a function of k and Ω. If the system were linear, only discrete Kronecker deltas would appear, placed exactly on the linear dispersion relation curve, i.e., $\langle|a(k,\Omega)|^2\rangle = \delta_{\Omega,\omega_k}$. In Fig. 2 we show two examples of the $(\Omega - k)$ plot: the first is calculated on the transition region, $\epsilon = 0.12$, and the other one in the stronger nonlinear regime, $\epsilon = 1$. The plots appear to be very different: first, we notice that for the stronger nonlinear case the dispersion curve is shifted towards higher frequencies. The shift is less pronounced for the smaller nonlinearity case $\epsilon = 0.12$ (in the linear case, the curve touches $\Omega = 2$).

The other important aspect is that a noticeable frequency broadening is observed for $\epsilon = 1$; that implies that for a single wave number, there is a distribution of frequencies characterized by some width. Because of such a width, for two adjacent discrete wave numbers, the frequencies overlaps (Chirikov criterion). In order to have a clearer picture of such an overlap, we show a slice of Fig. 2 taken at $k = 4$ and $k = 5$ for both cases, see Fig. 3. The distribution of the frequencies is separated for the weakly nonlinear case and visibly overlap for the stronger nonlinear case. Note that also for the weakly nonlinear case, for larger wave numbers an overlap starts to appear (not shown in the figure). This is the reason why the prediction made on the exact six-wave
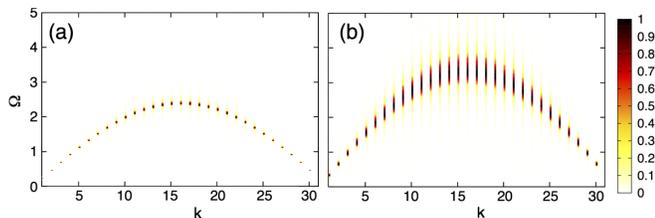

FIG. 2. $\langle|a(k,\Omega)|^2\rangle$ for (a) $\epsilon = 0.12$ and (b) $\epsilon = 1$ obtained from numerical simulations.
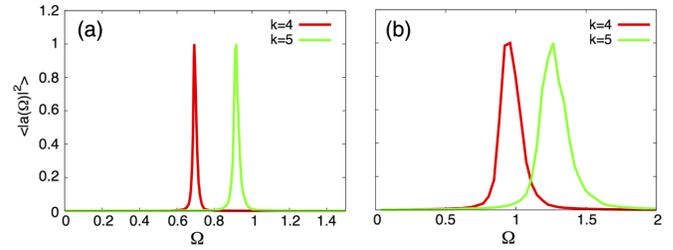

FIG. 3. $\langle|a(\Omega)|^2\rangle$ for $k = 4$ and 5 for (a) $\epsilon = 0.12$ where there is no overlapping of the resonances of two nearby wave numbers and (b) $\epsilon = 1$ where there is a noticeable overlapping of the resonances of the nearby wave numbers.

resonant interaction starts failing and another scaling is observed (see Fig. 2).

We compare the shifts and the broadening of the frequencies of our theoretical predictions with the one obtained from numerical simulations, see Figs. 4 and 5. Results are overall in agreement in the very weak nonlinear regime: the predictions are obtained by assuming the random phase approximation, which does not hold as soon as the nonlinearity starts creating a correlation between wave numbers. Such a departure from the theory is consistent also with the one observed in Fig. 1.

Conclusions.—In this Letter we have considered the original β-FPUT model and have found that the system reaches a thermalized state, even for very small nonlinearity. In this regime and for a small number of modes, three time scales may be identified: the linear time scale $1/\omega_k$, the nonlinear time scale of four wave interactions, and the time scale of irreversible six-wave interactions, $1/\epsilon^4$. In order to observe equipartition one needs to wait up to the $1/\epsilon^4$ time scale. If one is observing the system on a shorter time scale, using the original variables, then only reversible dynamics is seen, which might be an explanation for the celebrated FPUT recurrence. Such reversible dynamics can possibly be captured directly as is done in Ref. [28], where a nonequilibrium spatiotemporal kinetic
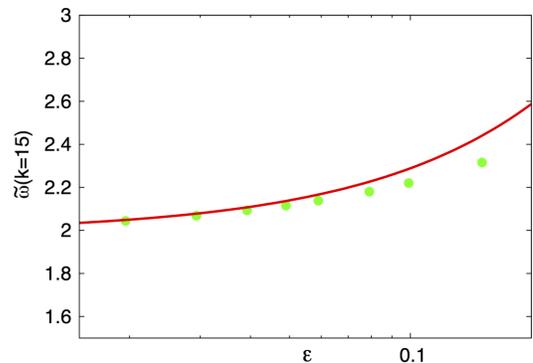

FIG. 4. Frequency shift as a function of the nonlinear parameter ϵ for $k = 15$. The solid line corresponds to Eq. (10); the dots correspond to the position of the peak of the distribution $\langle|a(\Omega)|^2\rangle$ for $k = 15$ computed numerically.
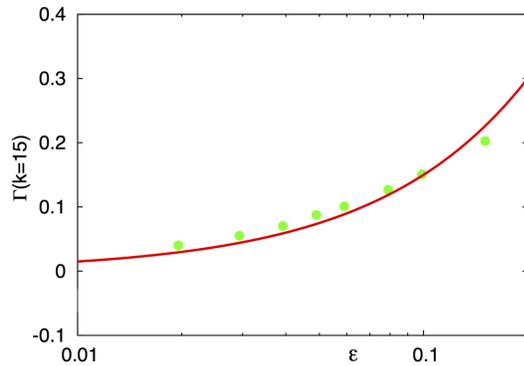
FIG. 5. Width of the distribution of the frequency shift as a function of the nonlinear parameter ϵ for $k = 15$. The solid line corresponds to Eq. (11); the dots correspond to the standard deviation of the distribution $\langle |a(\Omega)|^2 \rangle$ for $k = 15$ computed numerically.

formulation that accounts for the existence of phase correlations among incoherent waves is developed.

For $\epsilon \gtrsim 0.1$ a different scaling, $t_{\rm eq} \sim \epsilon^{-1}$, starts, which is consistent with the time scale of the nonlinearity of the dynamical equation. The transition region has been investigated by measuring the broadening of the frequencies: we observe that the phenomenon of frequency overlap suggested by Chirikov starts in the transition region; the breakdown of the prediction of the discrete weak wave turbulence theory is then observed for such values of nonlinearities. The Chirikov criterion approximately separates regimes of slow equipartition due to six-wave resonant interactions into the other, more effective mechanism for reaching thermal equilibrium. The mechanism that leads to equipartition for weakly nonlinear initial conditions seems to be universal; indeed, the α-FPUT model behaves exactly in the same way and we expect that the same mechanism will be responsible for explaining the equipartition in systems where metastable states have been observed as in the nonlinear Klein-Gordon equation [29].

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