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Double scaling in the relaxation time in the β -FPUT model

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We consider the original β -Fermi-Pasta-Ulam-Tsingou (β -FPUT) 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 interactions 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 Chirikov overlap criterium identifies a transition region between two different relaxation time scaling.

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In 1923 at the age of 22 E. Fermi published one of his first papers [1] in which the goal was to show that Hamiltonian systems are in general quasi-ergodic. 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 [4] for a discussion on 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 to the macroscopic Fourier law) heat conduction in solids could be obtained only in the presence of nonlinearity, see [5] for recent developments. They simulated a system of harmonic oscillators perturbed by a cubic (α -FPUT) or quartic potentials (β -FPUT). 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 the simulations of the FPUT system were performed, Kolmogorov enunciated the 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 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 criterium, 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 has been followed and different numerical studies confirmed the presence of a threshold above which the FPUT system reaches a fast thermalized state (see for example [11–13] for a study on β -FPUT). However, more recently, numerical simulations of the α -FPUT [14, 15] have shown that even for small nonlinearity the system does reach a thermalized state. The explanation of this result was given in [15] where it has been shown that for the finite dimensional system of certain size, six-wave resonant interactions are responsible for equipartition and only after very long time the system reaches a thermalized state.

In this Letter we perform a detailed study of the β -FPUT with a finite number of masses and, as a first result, we show that, as for the α -FPUT, the weak nonlinear regime is dominated by discrete six-wave resonant interactions which are responsible for thermalization. Such 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 angleaction variables and by using the Wick decomposition, we find an explicit formula for the broadening of the frequencies. When such broadening is larger than the spacing between frequencies, the Chirikov regime is observed. Therefore, the Chirikov criteria identifies 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

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

$$H_4 = \frac{\beta}{4} \sum_{j=1}^{N} (q_j - q_{j+1})^4.$$
(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 to 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, iii) the time scale of 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

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

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 procedure, is well documented in the general case in [16] and in the α -FPUT case in [15]). The following reduced Hamiltonian is obtained (the new variable has been renamed a_k and higher order terms have been neglected):

$$\tilde{H}_{2} = N \sum_{k=0}^{N-1} \omega_{k} |a_{k}|^{2}$$

$$\tilde{H}_{4} = \frac{N}{2} \beta \sum_{k_{1}k_{2}k_{3}k_{4}}^{N-1} T_{k_{1},k_{2},k_{3},k_{4}} a_{k_{1}}^{*} a_{k_{2}}^{*} a_{k_{3}} a_{4} \delta_{1+2,3+4},$$
(4)

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

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

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

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

that 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:

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

where $\Re[...]$ implies the real part. From this equation we obtain the frequency by applying the averaging operator $\langle ... \rangle$ over random frequencies and using the 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:

$$\tilde{\omega}_{k_1} = \langle \frac{d\theta_k}{dt} \rangle \simeq \omega_{k_1} + \epsilon 2 \sum_{k_2 \neq k_1} T_{k_1, k_2, k_1, k_2} I_{k_2}$$
 (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 [17, 18]. More interestingly, one can estimate half-width Γ_k of the frequency by calculating the second centred 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 equations (8), (10), the Wick's decomposition and under the assumption of thermal equilibrium (equipartition of linear energy), we obtain:

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

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

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

According to Chirikov, the stochastization takes place when $R_k = 1$. If we define $\epsilon_{\rm cr}$ as the value for which $R_k=1$, then it is straightforward to observe that $\epsilon_{\rm cr}$ is k dependent and $\epsilon_{\rm cr}$ 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 $H_{\rm 2cr}(t=0)=2N/(3\beta k)$. Full stochasticization of all wave numbers takes place for $\epsilon_{\rm cr}\simeq 0.6$ (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 follows 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 solution for integer values of k:

$$k_1 + k_2 + \dots + k_l = k_{l+1} + k_{l+2} + \dots + k_n$$

$$\omega_{k_1} + \omega_{k_2} + \dots + \omega_l = \omega_{l+1} + \omega_{l+2} + \dots + \omega_n.$$
(14)

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

An estimation of the time scale of such interactions can be obtained following the argument developed in [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 the 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 [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 infinite, keeping constant the linear density of masses, then it can be shown that the Fourier space becomes dense $(k \in \mathbb{R})$: four-wave exact resonances exists and the standard four-Wave Kinetic Equation can be recovered (see [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 [26]. We run the simulations for different values of β , keeping always the same initial conditions which is formulated in Fourier

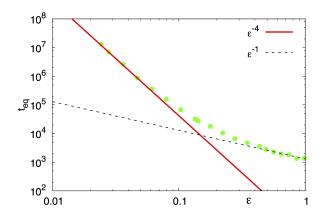


FIG. 1: Equilibrium time t_{eq} as a function of ϵ in Log-Log coordinates. Dots represent numerical experiments The straight line corresponds to power law of the type $1/\epsilon^4$, red line, and $1/\epsilon$, black dashed line.

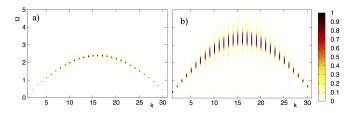


FIG. 2: $\langle |a(k,\Omega)|^2 \rangle$ for a) ϵ =0.12 and b) ϵ =1 obtained from numerical simulations.

space in normal variables as

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

related to the original variables by equation (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 by 2000 realizations. In order to establish the time of thermalization, we have considered the following entropy [11]:

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

and $\langle ... \rangle$ defines the average over the realizations. Note that the larger is the number of the members of the ensemble, the lower is the stationary values reached by s. In our numerics we have followed the procedure outlined in [15] to identify the time of equipartition. We present in Figure 1 such time, t_{eq} , as a function of ϵ for the simulations considered in a Log-Log plot. The figure also

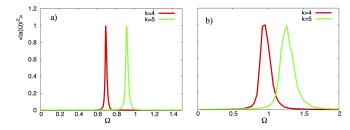


FIG. 3: $\langle |a(\Omega)|^2 \rangle$ for k=4 and 5 for a) ϵ =0.12 where there is no overlapping of the resonances of two nearby wave numbers and b) ϵ =1 where there is a **noticeable** overlapping of the resonances of the nearby wave numbers

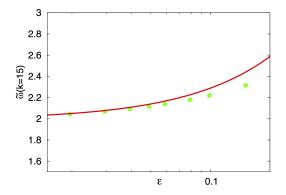


FIG. 4: Frequency shift as a function of the nonlinear parameter ϵ for k=15. The solid line corresponds to equation (10), dots correspond to the position of the peak of the distribution $\langle |a(\Omega)|^2 \rangle$ for k=15 computed numerically.

shows two straight lines (power laws) with slope -4 and -1. The steepest one (in red color) 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. Similar transition has also been observed in [27] where the α -FPUT has been integrated.

In order to understand such behaviour, 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 let the simulation run on a time window over which, for each mode, a Fourier transform (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 . Would the system be 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 Figure 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 stronger nonlinear

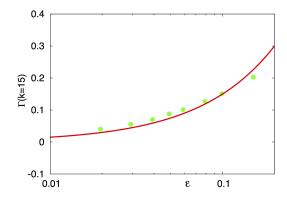


FIG. 5: Width of the distribution of the frequencies shift as a function of the nonlinear parameter ϵ for k=15. The solid line corresponds to equation (11), dots correspond to the standard deviation of the distribution $\langle |a(\Omega)|^2 \rangle$ for k=15 computed numerically.

regime, $\epsilon=1$. The plots appear to be very different: first we notice that for the stronger nonlinear case the dispersion curved 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 wavenumber, there is a distribution of frequencies characterized by some width. Due to such width, for two adjacent discrete wavenumbers, the frequencies overlaps (Chirikov criterium). In order to have a clearer picture of such overlap, we show a slice of Figure 2 taken at k = 4 and k = 5 for both cases, see Figure 3. The distribution of the frequencies are 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 exact six-wave resonant interaction starts failing and an other scaling is observed (see Figure 2).

We compare the shifts and the broadening of the frequencies of our theoretical predictions with the one obtained from numerical simulations, see Figures 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 correlation between wave numbers. Such departure of the theory is consistent also with the one observed in Figure 1.

Conclusions- In this Letter we have considered the original β -FPUT model and found that the system reaches a thermalized state, even for very small nonlinearity. In this regime and for 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 sys-

tem 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 be possibly captured directly as is done in [28], where a nonequilibrium spatiotemporal kinetic formulation that accounts for the existence of phase correlations among incoherent waves is developed.

For $\epsilon \gtrsim 0.1$ a different scaling, $t_{eq} \sim \epsilon^{-1}$, 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 val-

ues of nonlinearities. Chirikov criterion approximately separates regimes of slow equipartition due to six-wave resonant interactions to 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 behaves exactly in the same way and we expect that the same mechanism be responsible for explaining the equipartition in systems where metastable states has been observed as in the Nonlinear Klein-Gordon equation [29].

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