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Abstract – We study the time of equipartition, T_{eq}, of energy in the one-dimensional Discrete Nonlinear Klein-Gordon (DNKG) equation in the framework of the Wave Turbulence (WT) theory. We discuss the applicability of the WT theory and show how this approach can explain qualitatively the route to thermalization and the scaling of the equipartition time as a function of the nonlinear parameter ϵ, defined as the ratio between the nonlinear and linear part of the Hamiltonian. Two scaling laws, $T_{eq} \propto \epsilon^{-2}$ and $T_{eq} \propto \epsilon^{-4}$, for different degrees of nonlinearity are explained in terms of four-wave or six-wave processes in the WT theory. The predictions are verified with extensive numerical simulations varying the system size and the degree of nonlinearity.

Introduction. – The behavior of the small perturbation of an integrable system is one of the fundamental problems of mechanics [1]. In particular, an important question is whether a system reaches thermalization (*e.g.*, equal distribution of energy among the degrees of freedom) given some initial distribution of energy. In this framework, Fermi, Pasta and Ulam (FPU) with the help of Tsingou [2] performed the very first numerical simulations of a nonlinear chain, obtaining puzzling results and then opening up the way to the modern nonlinear physics.

Almost at the same time, the same problem was tackled from a mathematical point of view by the Kolmogorov school, obtaining the fundamental result of the KAM (Kolmogorov-Arnold-Moser) theorem which is at the basis of modern perturbation theories [3–6]. A remarkable work was performed some years later by Zabusky and Kruskal [7] who showed that in the continuous limit the FPU system reduces to the celebrated Korteweg-de Vries equation which is known to be integrable via the inverse scattering transform. Interestingly, at the same time of the work of Zabusky and Kruskal, important advances in the statistical mechanics theory of weakly nonlinear interacting waves were developed [8,9]: this theory is called Wave Turbulence (WT) and has been applied to many physical situation since then [10,11], see also [12] for the concept of resonant interactions in discrete systems. Nevertheless, the understanding of the problem of ergodicity in nonlinear chains has been tackled mostly in terms of chaos tools, other than direct numerical simulations, as can be seen in the good reviews [13,14] and in more recent important results [15,16]. Only more recently, the wave turbulence approach has been used in relation with one-dimensional anharmonic chains [17–19].

In this letter, we deal with the problem of the dynamics of the Discrete Nonlinear Klein-Gordon (DNKG) or ϕ^4 model from generic initial data, using the tools of wave turbulence. The ϕ^4 chain has been already considered in an original way to shed light on the problem of thermalization in [20]. From extensive numerical simulations, it appears that thermalization takes place for very small nonlinearity in agreement with our predictions: in different regimes $T_{eq}(\epsilon)$ displays a power-law dependence on ϵ.

The model. – The equation of motion of a ϕ^4 chain reads

$$\ddot{\phi}_i = (\phi_{i+1} + \phi_{i-1} - 2\phi_i) - m\phi_i - g\phi_i^3, \qquad (1)$$

where $\phi_i \in \mathbb{R}$ and $i = 1, 2, \ldots, N$; m and g are two positive constants, the latter controls the strength of the nonlinearity. The Hamiltonian associated to eq. (1) is

$$H = \sum_i \frac{1}{2}\pi_i^2 + \frac{1}{2}(\phi_{i+1} - \phi_i)^2 + \frac{1}{2}m\phi_i^2 + \frac{1}{4}g\phi_i^4, \qquad (2)$$

with $\pi_i \equiv \dot{\phi}_i$. In order to characterize the degree of nonlinearity of the system, we introduce the following parameter:

$$\epsilon \equiv H_{nl}/H_l, \tag{3}$$

where H_l accounts for first three terms in eq. (2) and H_{nl} for the last one. For a given initial condition, a change of g leads to a change of the degree of nonlinearity ϵ of the simulation ($\epsilon \propto g$). We mention that ϵ is not constant throughout the evolution of the system. Nevertheless, for the weakly nonlinear regimes considered in our simulations, it will be shown that it is essentially equivalent for scaling considerations to use as a controlling parameter of the nonlinearity either g, or ϵ computed at the equipartition time, or ϵ computed at the initial conditions (that is, $\epsilon(t=0) \simeq \epsilon(t=T_{eq})$).

The linear version ($g = 0$) of eq. (2) can be diagonalized in the normal modes. Assuming periodic boundary conditions, we introduce the discrete Fourier transform of the ϕ_i and π_i,

$$\hat{\phi}_k \equiv \sum_{j=1}^{N} \phi_j e^{-i2\pi kj/N}, \quad \hat{\pi}_k \equiv \sum_{j=1}^{N} \pi_j e^{-i2\pi kj/N} \tag{4}$$

(note $\hat{\phi}_k^* = \hat{\phi}_{-k}$ and $\hat{\pi}_k^* = \hat{\pi}_{-k}$), and then normal modes are given by

$$a_k \equiv \left(\omega_k \hat{\phi}_k + i\hat{\pi}_k\right)/\sqrt{2\omega_k}, \tag{5}$$

where ω_k is the positive branch of the linear dispersion relation,

$$\omega_k \equiv \sqrt{m + 4\sin\left(k\pi/N\right)^2}. \tag{6}$$

In normal variables, the equation of motion reads

$$\begin{aligned} i\dot{a}_{k_1} = \omega_{k_1} a_{k_1} + g \sum_{k_2,k_3,k_4} V_{k_1k_2k_3k_4} (a_{k_2} a_{k_3} a_{k_4} \delta_1^{234} \\ + 3a_{k_2}^* a_{k_3} a_{k_4} \delta_{12}^{34} + 3a_{k_2}^* a_{k_3}^* a_{k_4} \delta_{123}^{4} + a_{k_2}^* a_{k_3}^* a_{k_4}^* \delta_{1234}), \end{aligned} \tag{7}$$

with the interaction coefficient $V_{1234} = 1/(4\sqrt{\omega_1\omega_2\omega_3\omega_4})$ and δ is the generalized Kronecker's delta,

$$\delta_{ab\ldots}^{\alpha\beta\ldots} \equiv \begin{cases} 1, & k_a + k_b + \ldots = k_\alpha + k_\beta + \ldots \mod (N), \\ 0, & \text{otherwise.} \end{cases} \tag{8}$$

Equation (7) describes a wave dynamics with a third-order nonlinearity [10,21].

The large-box limit and the weak WT theory. – In the framework of WT [8,10,21,22] one considers the evolution of a statistical ensemble of realisations, each characterized by random phases and amplitudes, in the limit of a large-box ($N \to \infty$) and small nonlinearity (small wave amplitude).

In the standard formulation of the WT, the physical space is considered continuous while our system will be considered always discrete (in physical space). Here, we consider the large-box limit of the system (1), assuming that, as $N \to \infty$, also the length of the chain, L, goes to infinity with their ratio constant, $\Delta x = L/N = 1$; this implies that the Fourier space becomes dense and the wave numbers are not discrete anymore, yet the dynamics in the physical space is intrinsically discrete, and therefore $k_{\max} = \pi$. In such limit, it is possible to derive the evolution for the observable $\langle a_{k_i} a_{k_j}^* \rangle = n_i \delta_i^j$, that is a *kinetic equation* [18,19,23],

$$\begin{aligned} \dot{n}_1 = g^2 \int_{-\pi}^{\pi} \delta_{2\pi}(k_1 + k_2 - k_3 - k_4)\delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \\ \times \left(V_{1234}\right)^2 n_1 n_2 n_3 n_4 \left(\frac{1}{n_1} + \frac{1}{n_2} - \frac{1}{n_3} - \frac{1}{n_4}\right) \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4, \end{aligned} \tag{9}$$

where δ is now the Dirac δ-function, $\delta_{2\pi}(k) \equiv \delta(2\pi j + k)$ with $j \in \mathbb{Z}$, and $\omega_k = \sqrt{m + 4\sin(k/2)^2}$, with now $k \in [-\pi, \pi)$. It is interesting to note that the time scale of the evolution of the spectrum via the collision integral (9) is proportional to $1/g^2$. The δ-functions in eq. (9) define the conditions under which the collision integral does not vanish; these *resonance conditions* are in the following form:

$$k_1 + k_2 - k_3 - k_4 = 0, \mod 2\pi, \quad \omega_1 + \omega_2 - \omega_3 - \omega_4 = 0. \tag{10}$$

As can be shown numerically, nontrivial solutions of the above equations for $k \in [-\pi, \pi)$ and $\omega_k = \sqrt{m + 4\sin(k/2)^2}$ can be found for each value of m, while other scattering processes are forbidden because of the shape of the dispersion relation (6). For this reason, only $2 \to 2$ processes have been explicitly included in eq. (9).

The importance of eq. (9) relies on the fact that it is possible to define an entropy function,

$$S = \int_{-\pi}^{\pi} \log(n_k) \mathrm{d}k, \tag{11}$$

such that $\mathrm{d}S/\mathrm{d}t \geq 0$, *i.e.*, the resonant interactions lead to irreversible dynamics. Moreover, the entropy is maximized by the Rayleigh-Jeans (RJ) distribution,

$$n_k = \frac{T}{\omega_k + \mu}, \tag{12}$$

where T and μ are constants (that can be calculated from initial conditions) associated to the conserved quantities of the kinetic equation: energy and number of particles. Essentially, the prediction in the large-box limit is that n_k relaxes to the RJ distribution, eq. (12), and if $\mu \sim 0$ then the energy per mode $e_k \equiv n_k \omega_k = \text{const}$. Note that with respect to continuous wave turbulence, because of the presence of periodic Dirac delta functions the total momentum is not conserved.

The picture outlined above is valid in the limit of infinitely many modes and small nonlinearity. We expect

that in regimes close to this limit, the predictions should apply with some degree of accuracy. In any numerical simulation, the number of modes is always finite, therefore, the resonances in principle may take place only for integer values of wave numbers. However, in nonlinear dispersive wave systems, another effect comes into play, that is the broadening of frequencies [24]: the frequency of the modes becomes stochastic around the value described by the dispersion relation. The implication of this phenomenon is that if N or ϵ are sufficiently large, the resonance conditions, eqs. (10), do not need to be satisfied exactly in the computational grid and *quasi-resonances* may become important [10]. On the other hand, in the weakly nonlinear regime and when the number of modes is low, we assume that exact resonant interactions in a discrete system may lead on average to an irreversible process just like in the large-box limit, even though a statistical description, *i.e.*, a kinetic equation, with discrete wave numbers has not been developed. This case is considered hereafter.

Exact resonances in the DNKG for small number of masses. –

Four-wave exact resonances. We now consider the finite-size system and study whether eqs. (10) can hold for the dispersion relation eq. (6). We will indicate the l.h.s. of the equation for the resonance condition on frequencies for a process $X \to Y$ as $\Delta\omega_X^Y$. Processes of the kind $4 \to 0$ are obviously excluded because $\Delta\omega_X^0 > 0$ for $m > 0$. Processes of the type $3 \to 1$ can be decomposed into the sum of two $2 \to 1$ processes, $\omega_1 + \omega_2 - \omega_{1+2} + (\omega_{1+2} + \omega_3 - \omega_{1+2+3}) = 0$. For $m = 0$ it can be shown that $\Delta\omega_{12}^{1+2} > 0$ (except for $k = 0$, but the mode a_0 is not well defined for $m = 0$ and it is effectively excluded from the dynamics): furthermore, assuming $\Delta\omega_{12}^{1+2} = 0$, then $\partial\Delta\omega_{12}^{1+2}/\partial m > 0$, and, therefore, for continuity in m (for $m > 0$) of both $\Delta\omega_{12}^{1+2}$ and $\partial\Delta\omega_{12}^{1+2}/\partial m$ no new solution can appear by increasing m. Consequently, no processes of the type $3 \to 1$ are present in the system. Let us consider now the resonance condition on frequencies for a process $2 \to 2$, $\Delta\omega_{12}^{34}$. After successively squaring the equation and renaming $s_i \equiv \sin(k_i\pi/N)$ one gets to

$$m \prod \left(s_1^2 \pm s_2^2 \pm s_3^2 \pm s_4^2\right) = \frac{1}{2} \prod \left(s_1 \pm s_2 \pm s_3 \pm s_4\right), \tag{13}$$

where the first product is intended between all combinations of the plus-minus signs with a total of two minus signs (*e.g.*, $s_1^2 + s_2^2 - s_3^2 - s_4^2$), while the second product is intended between all possible combinations of plus-minus signs without any constraint. Equation (13) can be used to find solutions for $\Delta\omega_{12}^{34} = 0$ both dependent on and independent of m. The independent solutions can be found by requiring that the product on the left, that is the coefficient of m, is zero, and then inserting back the resulting solutions in the definition of $\Delta\omega_{12}^{34}$ with $m = 0$. Using $k_4 = k_1 + k_2 - k_3 + jN$ with $j \in \mathbb{Z}$ arbitrary, after some algebra, one finds that the only solutions are the trivial process $\{k_1, k_2, k_1, k_2\}$, and the so-called Umklapp scattering process

$$\{k_1, k_2, -k_1, -k_2\} \quad \text{with} \quad k_1 + k_2 = N/2, \tag{14}$$

which is only possible when N is even; such solutions are related to the periodicity of the dispersion relation and are the same for the standard α and β-FPU chain [17]. The trivial processes do not contribute to the dynamics but for a nonlinear correction to the frequencies, [10]. The Umklapp scattering process, on the other hand, does contribute to the dynamics, but since all quartets are disconnected (*i.e.*, there is no common mode between the quartets), their dynamics cannot lead the system to equipartition.

Six-wave exact resonant interactions. Since the only m-independent four-waves resonances permitted are due to the Umklapp scattering mechanism, and they are not connected, it is necessary to perform a quasi-linear change of variables and remove the nonresonant four-waves terms in eq. (7) and obtain a Hamiltonian with higher-order wave-wave interactions to predict the evolution of the system at large times (see, for example, [8]). This change of variables is canonical, up to the order in consideration, and in our case the transformation reads

$$\begin{aligned} a_1 \;=\; b_1 - g \sum_{234} V_{1234} \big(& 3b_2^* b_3^* b_4 / \Delta\omega_{123}^4 + 3b_2^* b_3 b_4 / \Delta\omega_{12}^{34} \\ & + b_2 b_3 b_4 / \Delta\omega_1^{234} + b_2^* b_3^* b_4^* / \Delta\omega^{1234} \big) + (\text{h.o.t}), \end{aligned} \tag{15}$$

where h.o.t means higher-order terms. Due to this transformation the equation of motion in the new variables b_k gains new terms corresponding to six-wave interactions, and after examination they turn out to be all proportional to factors of the type $g^2 V_{1234} V_{5678}$. Note also that, for interactions of the type $2 \to 2$, the sum is made only over nonresonant terms because otherwise such transformation would be singular. In the new variables it would be formally possible to derive a six-wave kinetic equation [10], and obtain resonance conditions analogous to eqs. (10), but with six wave numbers and frequencies. However, in doing so one would need to take again the thermodynamic limit first, in which, as explained later, the m-dependent exact four-wave interactions would dominate the dynamics. In the following we conjecture that, in practice, there exists a regime with finite N and small nonlinearity ϵ such that six-wave resonance dynamics are dominant, even though, as far as we are aware, a WT formalism with finite N has not been developed yet.

Six-waves resonances. As for the $4 \to 0$ and $3 \to 1$ cases, also $6 \to 0$ and $5 \to 1$ resonances are not allowed. Resonances of the type $3 \to 3$ can be trivially constructed by analogy from eq. (14) using an arbitrary wave number k_3,

$$\{k_1, k_2, k_3, -k_1, -k_2, -k_3\},\ k_1 + k_2 + k_3 = 0 \mod (N). \tag{16}$$

These resonant sextuplets are interconnected, and they provide a way to exchange energy among all the modes

of the system. Note that eq. (16) is valid also for odd values N. For even N, eq. (16) is also valid for $k_1+k_2+k_3 = 0 \mod (N/2)$, and finally it is also possible to construct again from eq. (14) these additional resonances,

$$\{k_1, k_2, k_3, -k_1, -k_2, k_3\}, \quad k_1 + k_2 = N/2. \tag{17}$$

As in the case of four-waves interactions, there also exist the trivial resonances $\{k_1, k_2, k_3, k_1, k_2, k_3\}$ but they only contribute to the nonlinear frequency shift.

The previous analysis of the resonances in the KG system is limited to resonances that are independent of the value of m, *i.e.*, they are valid for any value of m. One may ask if, for specific values of m, new resonances appear. Such analysis if far more difficult. For the four-waves case, it is possible to solve for m in eq. (13), and then to find values of m that connect arbitrary wave numbers. These solutions however appear to have little significance in the dynamics: in fact, we could not find numerically for $N = 32$ and $N = 64$ cases in which for a specific value of m there are more than two connected quartets. For the six-waves resonances it is possible, just as in the case of four-waves resonances, to successively square $\Delta\omega^{456}_{123}$ and obtain an equation for m. However, this turns out to be of the sixth order in m. Furthermore, it is possible to show that resonances of the type $4 \to 2$ can only exist if $m < 4/3$, in particular we have obtained the relation

$$m \leq \frac{4Y^2}{X^2 - Y^2} \tag{18}$$

which leads to $m < 4/3$ for a $4 \to 2$ resonance.

No special solutions of the exact resonances conditions for the four- and six-waves resonances were numerically found for the chosen value of $m = 1$ with N finite, and only the resonances of the Umklapp type were satisfied exactly in our simulations. Numerical simulations of the equation of motion show that, for the specific values of m for which new resonances appear, there is no appreciable effect on the dynamics, as will be shown shortly.

Estimation of the scaling of $T_{eq}(\epsilon)$. – From the previous discussion we understand the following. A WT formalism can be developed from the equation of motion (7) in the weakly nonlinear regime and in the large-box limits. The latter implies that wave numbers are dense in the domain $[-\pi, \pi)$. In these limits the expected time scale of thermalization is $T_{eq} \sim \epsilon^{-2}$. When the number of modes is not sufficiently large for the system to be considered as in the thermodynamic limit, wave numbers are discrete; in such condition four-wave exact resonant interactions exist but cannot bring the system to equipartition because they are not interconnected. However, if the frequency gaps between the modes are sufficiently low (a condition attained by having either N or ϵ sufficiently large), we conjecture that the frequency broadening (Chirikov's argument) can allow "quasi-resonaces" effectively bridging between the disconnected Umklapp-type four-waves resonances in the system, and hence bringing the system to equipartition with typical times $T_{eq} \sim \epsilon^{-2}$, as per eq. (9). If both N and ϵ are small, the dynamics is intrinsically discrete both in physical and spectral space and we assume that in the weakly nonlinear regime discrete six-wave exact resonances lead, as in the continuous case, to an irreversible dynamics, although the WT has not been developed for such discrete case.

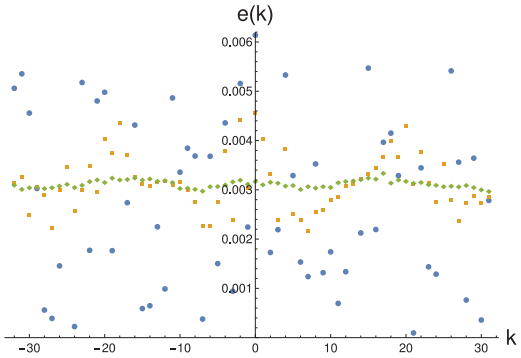

Fig. 1: (Colour online) A typical process of thermalization, for $N = 64$, $m = 1$, $E = 0.2$, $g = 5$ ($\epsilon \simeq 0.002$). The three datasets are $s(0) \simeq 14$ (●), $s(100000) \simeq 1$ (■), $s(2000000) \simeq 0$ (♦).

The leading-order nontrivial wave-wave interaction process displayed by the DNKG equation is the six-wave one, as it turns out from using the standard procedure of removing the nonresonant four-waves interactions through eq. (15). The time scale associated to the dynamical equation for the six-wave interactions is ϵ^{-2} and, even though there is no formal derivation of the wave kinetic equation, we expect, just as for the standard WT, that the spectrum evolves on a time scale which is given by the square of the coupling coefficient, *i.e.*, we expect to observe $T_{eq} \sim \epsilon^{-4}$ (see also [17]).

Numerical simulations. – In order to verify the predictions, a number of simulations have been run with different values of N and g. The numerical integration of eq. (1) has been implemented with a symplectic integrator of the sixth order [25], and the marching timestep was set to $\delta t = 0.1$, a value that has been found to conserve the Hamiltonian at least up to the sixth digit in all simulations. The number of realizations in the ensemble is 4096 for all the following simulations. The initial ensemble of eq. (1) consists of a fixed random choice of amplitudes of the normal modes, all with random and different phases for each realization. The scheme ensures that all the realizations have the same initial linear energy. The initial random amplitudes are also adjusted in order to cancel the chemical potential in eq. (12), in order to better observe the equipartition. The equations of motion are then integrated, and the approach to equipartition is monitored with the following indicator function [26]:

$$s(t) \equiv \sum_k f_k \log(f_k), \qquad f_k = \frac{N}{E} e_k(t), \tag{19}$$

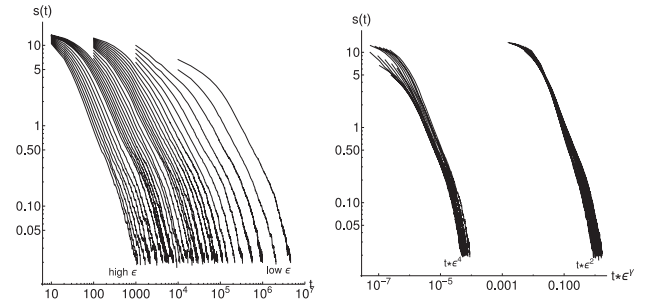

Fig. 2: Left: the entropy curves for the same parameters as fig. 1. The entropy curves are naturally ordered from left to right for decreasing ϵ, with values in the range 0.002–0.03 for $N = 64$. Right: the same curves with rescaled time: the two regimes $T_{eq} \propto \epsilon^{-2}$ and $T_{eq} \propto \epsilon^{-4}$ are highlighted by scaling the time either by ϵ^2 or by ϵ^4 (transition occurs at $\epsilon \simeq 0.007$).

with $e_k(t) = n_k(t)\omega_k$, the energy per mode, and $E = \sum e_k$. While the fundamental entropy function in WT is defined in eq. (11), it is common to refer to $s(t)$ just as "entropy", (because it is proportional to a Shannon entropy [14]). At equipartition, $s(t) = 0$, otherwise $s(t) > 0$. During evolution, $s(t)$ will decrease, and T_{eq} is defined as the time when $s(t)$ goes under some threshold value that depends in general on the number of realizations in the ensemble. The parameter ϵ is calculated *a posteriori*, that is inspecting the Hamiltonian at thermalization. A typical initial condition and its thermalization can be seen in fig. 1. The parameters are $N = 64$, $m = 1$, $E = 0.2$, $g = 5$ ($\epsilon \simeq 0.002$). The system goes to thermalization, although approximatively, as the size of the ensemble is finite. The difference between ϵ calculated from the initial and final (equipartition) states was found to be in the few percent points for the lowest values of ϵ, and larger (up to 20%) for large values of ϵ. In the left panel of fig. 2 we show the approach to equipartition for different values of $\epsilon = 0.002$–0.03 and $N = 64$. For large times the indicator function $s(t)$ settles and fluctuates to some value right below the chosen threshold (not shown here). The two predicted scaling laws can be highlighted by rescaling the time properly (fig. 2, right). We see that all the results now collapse into two separated curves with ϵ^{-2} and ϵ^{-4}, respectively. This indicates that the whole dynamics depends only on ϵ. Furthermore, two distinct regimes appear for ϵ lower and higher of a given critical ϵ_c. In fig. 3 we show $T_{eq}(\epsilon)$ in a log-log plot for $N = 64$ for the same simulations of fig. 2. The change of the dynamics between the ϵ^{-4} and ϵ^{-2} scalings is evident. In the same figure we also show the dependence of the thermalization dynamics on different values of $m = \{0.1, 0.5, 1\}$. There is no substantial difference between the runs, as the two different scalings are clearly visible, and the threshold of ϵ that determines the crossover between them is roughly the same for the cases $m = \{0.5, 1\}$, and slightly displaced to higher nonlinearity values for $m = 0.1$. The larger span of the steeper ϵ^{-4} scaling for the lower values of m is due to the larger average spacing between frequencies, and

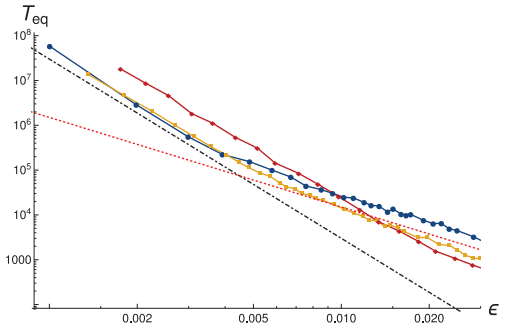

Fig. 3: (Colour online) The scaling of T_{eq} on ϵ for $N = 64$ and $m = 1$ (■), $m = 0.5$ (●) and $m = 0.1$ (♦). Scaling laws ϵ^{-2} and ϵ^{-4} in red dotted and black dash-dotted lines.

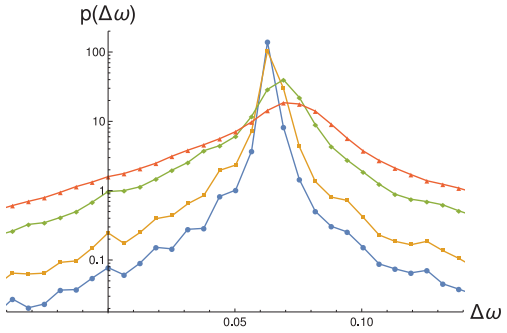

Fig. 4: (Colour online) The dispersion of the frequency mismatch $\Delta\omega$, for a $2 \to 2$ resonance with $N = 32$ and $k = \{1, -15, -11, -3\}$, calculated numerically with an accuracy of $\delta\omega = 2\pi/1000 \simeq 0.00628$. The product $a_1 a_{-15} a^*_{-11} a^*_{-3}$ is sampled in time, and the square amplitude of the Fourier coefficients of this time series is plotted after averaging and normalizing as a probability. $\epsilon \simeq 0.0026$ (●), 0.0052 (■), 0.0144 (♦), 0.023 (▲).

consequently the suppression of quasi-resonances. Indeed, as mentioned, the nonlinearity causes a broadening of the frequencies which, for a sufficiently strong nonlinearity, can lead to a frequency overlap phenomenon. In this case quasi-resonances can take place. This mechanism is qualitatively supported in fig. 4 for $N = 32$, where the probability density function of the mismatch frequency $\Delta\omega^{34}_{12}$ for a generic $k = \{1, -15, -11, -3\}$ (this is not an exact resonance) is computed from the simulations. If one considers frequencies from the very weakly nonlinear regime, one will obtain a function peaked at $\Delta^{34}_{12} \simeq 0.0626$, that is the waves are not in resonance ($\Delta^{34}_{12} \neq 0$); because of the nonlinearity, the value of Δ^{34}_{12} is actually stochastic, and a numerical evaluation of its probability distribution leads to the broad functions displayed in fig. 4. It is seen that with the increase of the nonlinearity over the range of the numerical studies reported in this letter, the probability of $\Delta^{34}_{12} \simeq 0$ increases by an order of magnitude, showing that four-waves quasi-resonances are not possible for small nonlinearities but become probable for larger nonlinearity.

We have then investigated the robustness of the predictions in the thermodynamic limit increasing N. The dependence of T_{eq} on N is shown in fig. 5. The transition

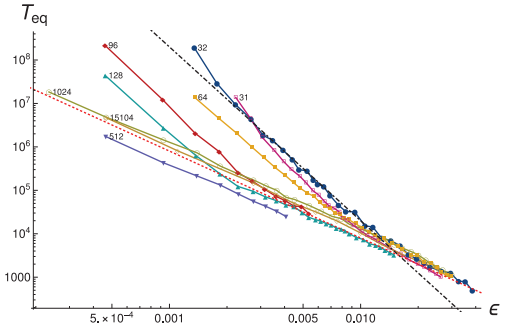

Fig. 5: (Colour online) The scaling of T_{eq} on ϵ for multiple values of N, with $m = 1$ and $E = 0.1N/32$. Scaling laws ϵ^{-2} and ϵ^{-4} are shown in red dotted and black dash-dotted lines.

between the two scalings is still well visible for the cases $N = 32$, $N = 64$ and $N = 96$, $N = 128$. As expected, there is no qualitative difference between even and odd N (see dataset with $N = 31$). For larger N the transition turns out to manifest always later until it disappears for $N \geq 512$, meaning that four-waves dominate the thermodynamic limit. It has been checked that no new dynamics appear even for a larger number of modes, up to $N = 15104$. The behavior in the thermodynamics limit is consistent with the WT analysis.

We conclude this section with a short discussion about the issue of averages in statistical mechanics [27,28]. While we have performed ensemble averages in order to evaluate accurately $T_{eq}(\epsilon)$ suppressing the entropy fluctuations, the behavior of the single realization appears always "typical", in the sense that eventually it fluctuates around the thermalized irreversible final state. We have indeed verified numerically that thermalization is observed if a suitable time average is performed over the energy per mode of a single system. It is remarkable that it is true even for a rather small number of degrees of freedom.

Conclusions and discussion. – In this letter we have studied the problem of the thermalization of the discrete nonlinear Klein-Gordon chain. In this framework, we understand the dynamics toward equipartition of energy through the mechanism of exchange of energy between resonant wave-wave interactions. Our prediction are the following: i) for generic weakly nonlinear initial conditions and a large enough number of modes (large-box limit), the system always thermalizes according to the WT theory (resonant four-wave interactions) on a time scale ϵ^{-2}; ii) when the number of modes and the nonlinearity are small, then exact resonances over a discrete regular grid of wave numbers become relevant. The six-wave interactions are dominant and the time scale for equipartition is ϵ^{-4} (this is the same scaling observed for the α-FPU, [17] and β-FPU [29]; iii) by increasing the nonlinearity in the discrete regime a crossover from ϵ^{-4} to a scaling ϵ^{-2} is observed. The transition takes place at different threshold values of ϵ depending on the number of modes; this is due to the phenomenon of frequency overlap. Interestingly, the scaling is the same as the one predicted in the large-box limit, implying that the frequency overlap has the role of reactivating exact four-wave resonances.

All the results have been verified by extensive numerical simulations, for different values of N, m and ϵ.

* * *

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