Universal evolution to equipartition in oscillator chains

J. De Luca,[1,*] A. J. Lichtenberg,[2,†] and S. Ruffo[3,4,‡]
[1]*Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970, São Carlos, Brazil*
[2]*Department of Electrical Engineering and Computer Sciences and the Electronics Research Laboratory, University of California, Berkeley, CA 94720*
[3]*Dipartimento di Energetica Universitá di Firenze, 50139 Firenze, Italy*
[4]*Laboratorio Forum INFM and INFN, Firenze, Italy*
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We determine a universal evolution and time scale T to equipartition in a one-dimensional lattice of N masses coupled by quartic nonlinear (hard) springs. We consider chains made of two types of masses randomly distributed, and of random masses between limiting values. The initial energy is put in a low-frequency mode of mode number γ. T is found to be inversely proportional to the initial beat frequency between mode γ and the neighboring modes. It is also proportional to a factor $N\ln(N)/N_c^{1/2}$ where N_c is a measure of the modes quartically coupled to mode γ. [S1063-651X(96)08208-6]

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Coupled oscillator chains form good test systems for investigating energy exchange among degrees of freedom. In particular, the Fermi-Pasta-Ulam (FPU) system, consisting of a set of equal masses coupled to nearest neighbors by nonlinear springs, has been extensively studied. Fermi, Pasta and Ulam [1], in 1954, observed, for a particular initial energy distribution, that the oscillators did not relax to the equipartition state, but displayed a persistent recurrence to the initial condition, contrary to the expectations of statistical mechanics. The recurrence results were later explained in terms of beating among the system modes [2,3]. A theoretical prediction of a threshold to fast equipartition was obtained by Izrailev and Chirikov [4]. Subsequently there have been many studies of energy thresholds to give approximate equipartition among modes [5–8]. A related question of the time scale to achieve equipartition has been less extensively studied [8–10]. With initial energy in a low-frequency mode, of mode number γ, it was shown in [8], both numerically and theoretically, that energy transfer to high-frequency modes is exponentially slow in a perturbation (energy) parameter at low energy. The mechanism of a transition to more rapid energy transfer is that resonant interaction of a few low-frequency modes, in which most of the energy resides, can lead to local superperiod beat oscillations, of period $T_B \propto N^2/\gamma E$, that are stochastic. With increasing local energy, the oscillation frequency increases until the Arnold diffusion mechanism is no longer exponentially slow, transferring energy to the higher-frequency modes, at the characteristic T_B time scale. The transition was predicted to occur at a value of $E=E_c$, independent of N, which was confirmed numerically [8]. The transition with energy to fast equipartition was studied numerically in [6], finding a threshold $E_c' \propto N$, as predicted in [4]. Equipartition taking place on a slower time scale, at lower energy ($E_c<E<E_c'$), studied numerically in [7,8], was in qualitative agreement with a $T \propto N^2/\gamma E$ time scale. In subsequent work we numerically investigated the scaling of the FPU dynamics, within the normalized energy range $E_c<E<N$ [9]. Defining n_{eff} as the number of modes with significant energy (see below), we found $n_{eff}(t)/N$ to lie on a universal curve vs normalized time $\tau=t/T$, $T\propto T_B N^{1/2}$ over a range of $10<E<1000$ and $16<N<1024$, indicating that a factor $N^{1/2}$ is a reasonable approximation to the size-dependent filling-factor correction to the T_B time scale.

The FPU system with quartic coupling is not the only oscillator chain relevant to physical problems. For example, the masses need not be all the same, either in a regular [10] or in a random manner [11]. Chains with more than one type of mass and/or connecting spring are relevant to the study of finite-chain molecules [12]. In particular, considerable effort has gone into the study of *linear* (quadratic Hamiltonian) oscillator chains with random masses [13,14]. The central result of those studies is that the normal modes of the system become localized, rather than extending over the entire chain. This makes the coupling among modes more difficult and also breaks the degeneracy of the linear frequencies. Oscillator chains with a quadratic Hamiltonian are integrable, and the initial energy in each normal mode remains constant; for equipartition, nonlinearity is essential, which is our interest here. For a nonlinear chain with two types of alternating masses, where the mode frequencies split in two branches, it was shown that for small energies the energy in one branch remains decoupled from the second branch for exponentially long times [10]. Again, we expect an energy transition, above which energy may be transferred from a low-frequency group to a high-frequency group on a time scale that is not exponentially slow. We expect randomly chosen masses to have a similar transition, but one that is less distinct.

We consider chains of N atoms with most generally randomly chosen masses M_i coupled to nearest neighbors by quartic nonlinear springs. The Hamiltonian representing the chain is

*Electronic address: deluca@ifqsc.sc.usp.br
†Electronic address:ajl@eecs.berkeley.edu
‡Electronic address: ruffo@ingfi1.ing.unifi.it

$$H=\sum_{i=0}^{N}\frac{p_i^2}{2M_i}+\frac{1}{2}(q_{i+1}-q_i)^2+\frac{\beta}{4}(q_{i+1}-q_i)^4. \quad (1)$$

We consider the case of strong springs ($\beta>0$) and fixed boundaries $q_0=q_{N+1}=0$. The constant β describing the strength of the anharmonic potential can be scaled to any positive value. We vary the energy and fix β at the value 0.1 to compare with previous work on the FPU lattice [6–9].

Our results are obtained for a random mass distribution of the type $M_i=M_0\exp(\delta\chi_i)$ with $M_0=1$, δ the strength of disorder, and χ_i is a number chosen either randomly at $+1$ or -1 (the random AB system) or randomly distributed within $[-1,1]$ (the random system). The equations of motion are integrated using a fourth-order symplectic integrator [15]. The harmonic part of the Hamiltonian can be put in the form of N independent normal modes via the canonical transformation

$$q_i=\sum_{j=1}^{N}u_{ij}Q_j/\sqrt{M_i}\quad j=1,N, \quad (2)$$

with canonical variables Q_j. The columns of the matrix u_{ij} are the orthonormal eigenvectors of the positive definite Hermitian eigenvalue problem for the Q's. The frequencies w_j of the normal modes Q_j are sorted to be increasing with j. The above transformation puts the Hamiltonian (1) into the form

$$H=\sum_{i=1}^{N}\left(\frac{1}{2}P_i^2+\frac{w_i^2}{2}Q_i^2\right)+\sum_{i,j,k,\ell}G(i,j,k,\ell)Q_iQ_jQ_kQ_\ell, \quad (3)$$

where the coefficients G can be calculated numerically by substituting (2) into (1). As an approximation for early times when most of the energy is in mode γ, we consider only the quartic terms where $k=\ell=\gamma$ and define $G(\gamma,\gamma,i,j)\equiv w_\gamma^2w_iw_jC_\gamma(i,j)$ so that (3) is approximated by

$$\tilde{H}=\sum_{i=1}^{N}\frac{1}{2}(P_i^2+w_i^2Q_i^2)+w_\gamma^2Q_\gamma^2\sum_{i,j}C_\gamma(i,j)w_iw_jQ_iQ_j. \quad (4)$$

For example, in the case of the FPU lattice ($\delta=0$) the matrix $C_\gamma(i,j)$ has only $3N$ nonzero elements of the same magnitude, coupling only states where $|i-j|=0,2\gamma$, and the eigenstates are extended, including all modes.

To define a perturbation parameter for the dynamics we evaluate numerically the value of the Hamiltonian (4), at the initial time, for a given value of the linear action I_γ,

$$\tilde{H}=w_\gamma I_\gamma+f_{\gamma\delta}(w_\gamma I_\gamma)^2, \quad (5)$$

where $f_{\gamma\delta}=C_\gamma(\gamma,\gamma)$. Notice that $f_{\gamma\delta}$ is a function of δ, and also (weakly) a function of the particular stochastic realization of the mass positions along the chain. The perturbation parameter ϵ is defined as the ratio of the quartic energy to the linear energy

$$\epsilon=f_{\gamma\delta}w_\gamma I_\gamma, \quad (6)$$

where, for the FPU system, $\epsilon=0.2w_\gamma I_\gamma/N$. The nonlinear correction to $\Omega_\gamma=\partial\tilde{H}/\partial I_\gamma$, calculated from (5), is $\Omega_B\equiv 2\epsilon w_\gamma$, which approximates the beat frequency between mode γ and neighboring modes [8].

We wish to generalize our previous scaling of the time to equipartition for the FPU Hamiltonian [9] to the cases with more general mass distributions, as described above. Furthermore, we would like to obtain a time to equipartition that is absolute, rather than relative. We use the general formalism of our previous work [9] that the linear energies $E_i\equiv 1/2\,(P_i^2+w_i^2Q_i^2)$, $i=1,\ldots,N$, are calculated as a function of time. The information entropy is then given by $S=-\Sigma_{i=1}^{N}e_i\ln e_i$, where $e_i=E_i/\Sigma_{i=1}^{N}E_i$ are the normalized energies. We then define the effective number of modes sharing the energy by $n_{eff}(t)\equiv\exp S$ [6,8,9]. The scaling of the time to equipartition is obtained numerically by finding the power of N and E that brings the curves of n_{eff}/N into approximate coincidence.

Here we present a method to explicitly calculate the ''equipartition time.'' We make the approximation that the interaction of the principal driving mode γ with the other modes gives them all equal energies $E_i(t)=E_a(t)$, $i\neq\gamma$. This is justified by the numerical observations, which indicates that, after an initial transient, the result holds within a few percent, provided the initial energy E_γ is well above the critical energy $E_c\simeq 3$ for equipartition. The change in the linear energy $E_\gamma=1/2(P_\gamma^2+w_\gamma^2Q_\gamma^2)$ of the principal mode γ, calculated from (4), is

$$\frac{dE_\gamma}{dt}=-2w_\gamma f_{\gamma\delta}E_\gamma E_a\sum_{i,j}\left(\frac{C_\gamma(i,j)}{C_\gamma(\gamma,\gamma)}\right)\eta_{\gamma ij}, \quad (7)$$

where we have changed to action-angle coordinates via $w_iQ_i=\sqrt{2E_i}\cos(\phi_i)$, $P_i=\sqrt{2E_i}\sin(\phi_i)$, and defined $\eta_{\gamma ij}\equiv\sin(2\phi_\gamma)\cos(\phi_i)\cos(\phi_j)$. The exact value of the above sum depends on knowledge of the phases $\eta_{\gamma ij}$, some of which will lock because of resonances. There is a resonance frequency $\Delta\Omega\equiv|2w_\gamma-w_i-w_j|$ associated with each phase $\eta_{\gamma ij}$. As a criterion for interaction [8] we will keep a term in the sum of (7) only if $\Delta\Omega<\Omega_B$, where Ω_B is the beat frequency defined below Eq. (6). We assume the phases to be random, such that defining

$$N_c=\frac{1}{2}\sum_{\Delta\Omega<\Omega_B}|C_\gamma(i,j)/C_\gamma(\gamma,\gamma)|^2, \quad (8)$$

we can approximate the sum in (7) by $N_c^{1/2}$ For the FPU Hamiltonian ($\delta=0$), N_c can be calculated analytically, $N_c=4(N-2\gamma)$. For the more general case with random masses, the elements of the matrix $C_\gamma(i,j)$ are an integral involving the product of four normal mode eigenvectors of indices i,j,γ, and γ, which are generically all nonzero. Assuming, in analogy to the FPU system, that the phases $\eta_{\gamma ij}$ are approximately resonant and independent, we can also use (8) to calculate the interaction sum of (7) in the random-mass system. We calculated $N_c(\delta)$ numerically, for $N=128$, 256, and 512, and the result is shown in Fig. 1. In the case of finite δ, there is a localization length $l(\delta)$ [16] counting the average number of nonzero elements of the eigenvectors u_{ij} of (2) [for example, $l(0.5)=44.1$ and

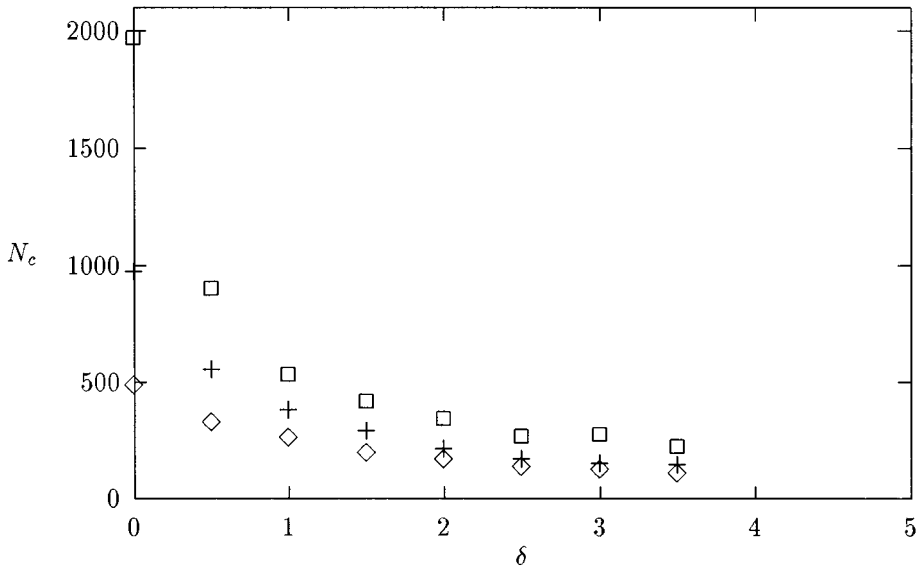

FIG. 1. N_c versus δ for a random system with $N=128$ ($\diamond$), 256 ($+$), and 512 ($\square$).

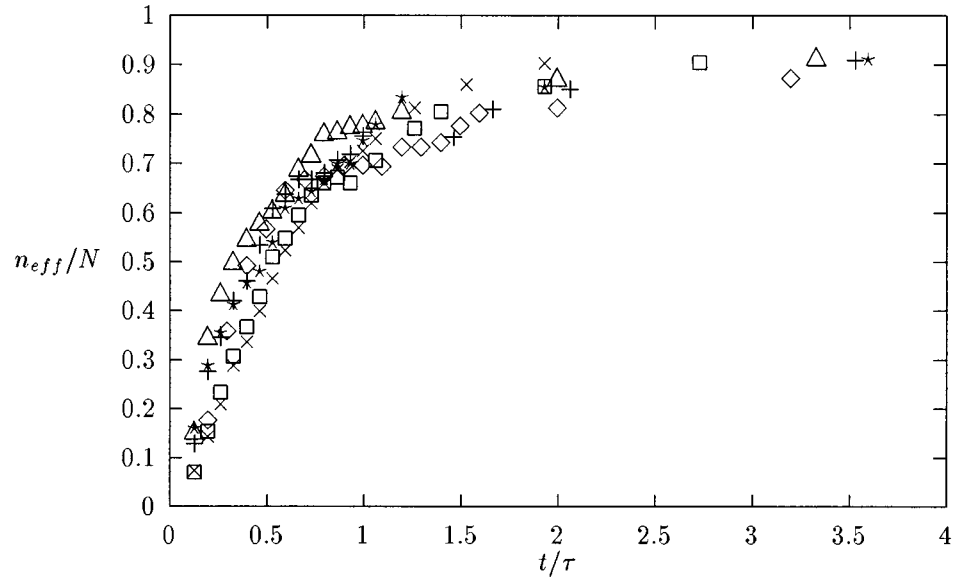

FIG. 2. n_{eff}/N versus $\tau=t/T$ for FPU system with $\epsilon=0.5$, $N=128$ ($\diamond$), 256 ($+$), 512 ($\square$), 1024 ($\times$); $\epsilon=0.35$, $N=256$ ($\triangle$); and $\epsilon=0.75$, $N=256$ ($\star$).

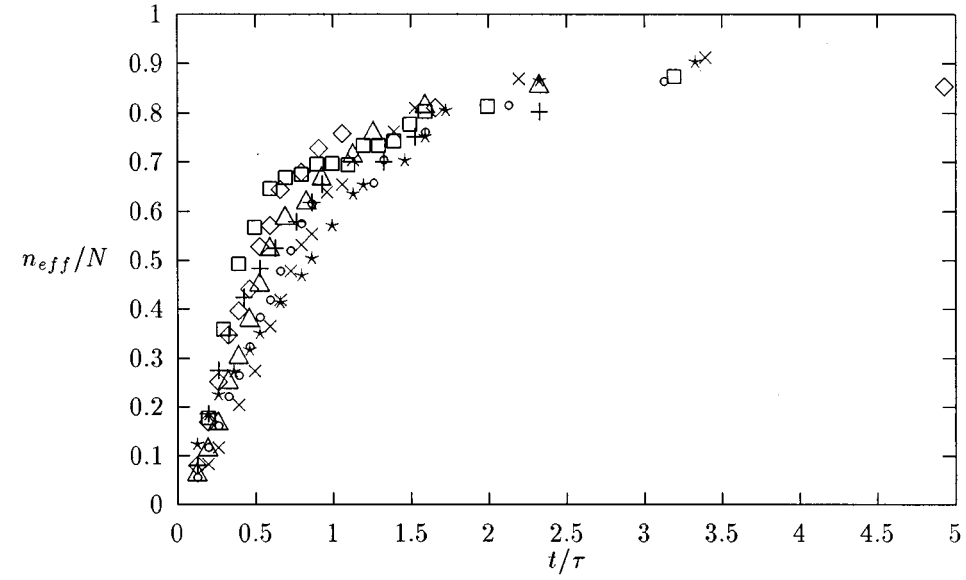

FIG. 3. n_{eff}/N versus $\tau=t/T$, for the random system at $\epsilon=0.5$: $N=128$ and $\delta=0.0$ ($\square$), $\delta=0.5$ ($\diamond$), $\delta=1.0$ ($+$); $N=256$ and $\delta=0.5$ ($\times$), $\delta=1.0$ ($\triangle$); $N=512, \delta=0.5$ ($\star$); and AB system with $N=256, \delta=0.5$ ($\bigcirc$).

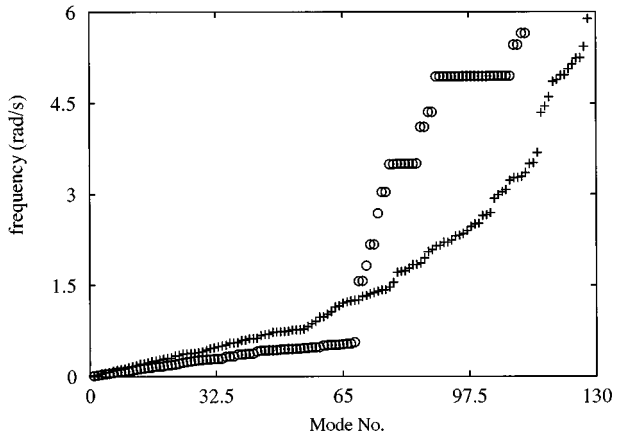

FIG. 4. Sorted frequencies of a random AB at $N=128$ system at $\delta=2.5$ ($\bigcirc$) and random system at $\delta=2.5$ ($+$).

$l(2.0)=12.2$]. If $l(\delta)$ is less than N, there will be only $l(\delta)$ modes overlapping spatially with mode γ and therefore at most $l(\delta)^2$ of $C_\gamma(i,j)$ elements could be nonzero. Together with the assumption that all the $C_\gamma(i,j)$ elements represent resonant couplings, it follows that N_c is proportional to $l(\delta)^2$ for large enough δ. In the case $\delta=0$, the modes are extended, $l(0)=N$, plus there is symmetry, as mentioned above, such that $N_c \propto N$. We see the reduction of N_c with increasing δ and the tendency of N_c to become N-independent in Fig. 1.

We substitute $\sqrt{N_c}$ for the sum in Eq. (7) and obtain the average equation

$$\frac{-dE_\gamma}{E_\gamma}=2\sqrt{N_c}w_\gamma f_{\gamma\delta}E_a(t)dt. \tag{9}$$

Integrating (9) in time with $E_\gamma(t)$ varying from E at $t=0$ to $E_\gamma(t)$ at t we get

$$\ln(E/E_\gamma)=2\sqrt{N_c}w_\gamma f_{\gamma\delta}\int_0^t E_a(t')dt'. \tag{10}$$

The final step in the approximation is to estimate the values of $E_\gamma(t)$ and $\int_0^t E_a(t')dt'$ at $t=T$, a time of ''near-equipartition.'' Although we expect E_γ to have considerably more than the average energy when our approximation breaks down, since the quantity appears in a logarithm it is sufficient to use the estimate $E_\gamma=E/N$, the value it would obtain at equipartition. On the right-hand side, the quantity $E_a(t)$ appears in an integral, so that its exact form is not required. For a diffusive process in which the amplitudes of the modes increase with $t^{1/2}$, we might expect the mode energies to increase linearly with t, $E_a(t)\simeq(t/T)(E/N)$, such that the time dependence does not depend on N. This is found to be approximately true, numerically, over most of the evolution to near-equipartition. Evaluating the integral with the above assumption and substituting $\ln(N)$ for the left-hand side, we obtain

$$T=N\ln(N)/N_c^{1/2}w_\gamma\epsilon. \tag{11}$$

In the following numerical work, as an initial condition we generally put 90% of the energy in a low-frequency mode γ (say $\gamma\simeq3$) and the remaining 10% in the two neighboring modes. We divide the characteristic time T into 15 equal segments and compute the value of $n_{eff}(t)$ at the end of each segment. In Fig. 2 we plot n_{eff}/N vs $\tau=t/T$, for $N=128$, 256, 512, 1024, with $\epsilon=0.5$, and also for $N=256$ with $\epsilon=0.35$ and 0.75. We observe good convergence to a single curve over most of the evolution. There is an initial transient for which the assumptions do not hold, and also an asymptotic behavior as $n_{eff}/N\to1$ for which (10) fails. In Fig. 3 we compare the random system for $\delta=0.5$ and 1.0, with $\epsilon=0.5$ and $N=128$,256, and 512, again finding good agreement. We averaged over five realizations, but this average differs only slightly from a single realization. We conclude that our assumptions that went into determining the factor N_c are essentially correct.

We have not considered the limitations to the universal time scale with ϵ and δ. From our previous work [7–9] there is a transition at small ϵ below which exponentially slow

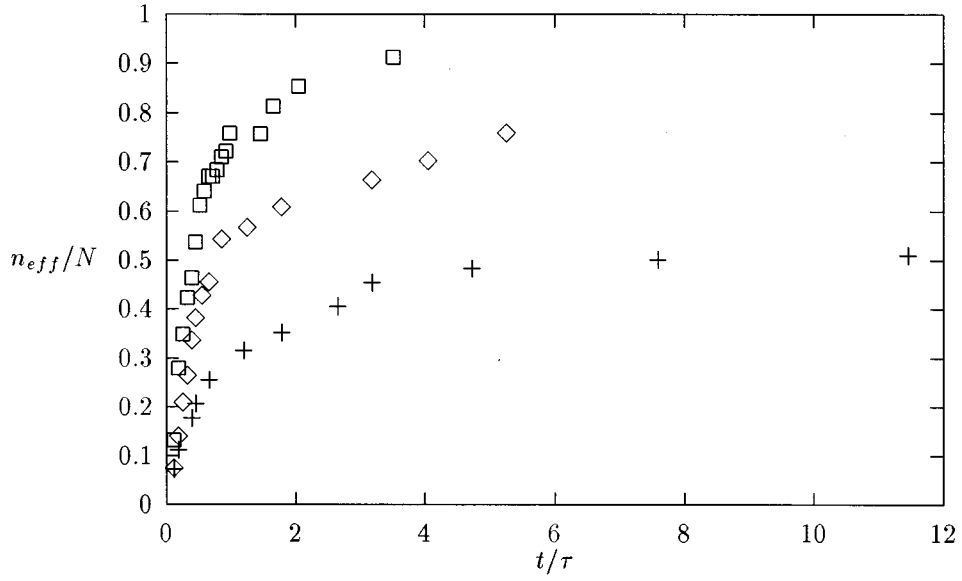

FIG. 5. n_{eff} versus $\tau=t/T$, at $\epsilon=0.5$: random system at $\delta=2.5$ ($\diamond$), AB system at $\delta=2.5$ ($+$) and FPU system ($\square$).

Arnold diffusion manifests itself. Also, for a similar model, there is a threshold energy to break the localization [17]. We would expect this threshold to be a function of δ. To illustrate this effect, we consider both the random AB system and the AB system. We indicate, in Fig. 4 the frequency separation of the modes for the random AB, and the random system, for $\delta=2.5$, at which value we find numerically that equipartition is not reached. For a random AB system with gN heavy masses and $(1-g)N$ light masses, the dispersion relation for the first gN modes is given by $\omega_i=(2/M)^{1/2}\sin[\pi i/(N+1)]$, where $M=\exp(-\delta)+g\exp(\delta)$ is the average mass, which is known as the virtual crystal approximation in solid state physics. The other $(1-g)N$ modes have a much higher frequency of order $\exp(\delta/2)$. In Fig. 5 with $N=128$ and $\epsilon=0.5$ we compare the values of $n_{eff}(\tau)/N$ for the two cases of Fig. 4 to the standard FPU. We see that the random AB case initially approximately follows the universal curve, but saturates to $n_{eff}/N\cong 0.5$, as the higher frequency modes receive very little energy. The random system exhibits this behavior but not as dramatically as the frequency separation is more continuous.

In conclusion, we see that by defining an appropriate $N_c(\delta,\epsilon)$, and, provided the frequency separation is not too large, we can calculate a time to equipartition; the evolution to equipartition lies on a universal curve of $n_{eff}(\tau)/N$.

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