Equipartition threshold in nonlinear large Hamiltonian systems: The Fermi-Pasta-Ulam model

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The Fermi-Pasta-Ulam β model has been studied by integrating numerically the equations of motion for a system of N nonlinearly coupled oscillators with N ranging from 64 to 512. Multimode excitations have been considered as initial conditions; the number Δn of initially excited modes is such that the ratio $\Delta n/N$ is kept constant. We can consider the system as a gas of weakly coupled phonons (normal modes), so that if we keep the ratio $\Delta n / N$ constant we find an analogy with the thermodynamical limit of statistical mechanics where the ratio M/V is constant when both the volume V and the number of particles M are increased up to infinity. The relaxation towards stationary states is followed through the time evolution of a suitably defined "spectral entropy" which depends on the shape of the space Fourier spectrum; this spectral entropy is a good equipartition indicator: Strong evidence is reported in favor of the existence of an equipartition threshold. Its persistence at very different values of N is also clearly shown. The main result concerns the occurrence of the threshold at the same value of the energy density (i.e., of the "control parameter") when the number of degrees of freedom is changed. More general initial conditions are also considered and the same result is found using as a control parameter a pseudo-Reynolds-number R: The threshold occurs at the same critical value R_c when N is varied. It turns out that a fully chaotic regime (equipartition) is obtained with an "average nonlinearity" of the system of about 3%.

I. INTRODUCTION

The relation between the Boltzmann-Ehrenfest statistical mechanics ("kinetic-dynamical" approach) and the Gibbs-Einstein statistical mechanics ("static" approach via ensemble theory) relies upon the ergodic hypothesis,¹ i.e., the equivalence of time averages and ensemble averages. There are several general results on the equivalence of ergodicity with other properties (e.g., metrical indecomposability of a system, nonexistence of prime integrals other than energy). Unfortunately no general constructive criterion for ergodicity exists, given the form of the Hamiltonian; there are some exceptions, which are—as far as we know—the trivial case of a system with one degree of freedom and the free particle which bounces elastically on the walls of a billiard.

For a long time, up to the 1950s, the community of physicists has considered the problem of ergodicity sub-

stantially solved. From a fundamental theorem of Poincaré (generalized by Fermi),² which proves the nonexistence of prime integrals independent from the energy in generic nonlinear Hamiltonian systems (apart from some particular cases), Fermi himself concluded (erroneously) that a generic Hamiltonian system must be ergodic. Such a belief fell through because of two basic results: (i) the Kolmogorov-Arnol'd-Moser (KAM) theorem,³ which showed that even without other prime integrals the phase space of a nonlinear Hamiltonian system can present open set bounded by nonsmooth invariant invariant manifolds-the set of invariant tori;⁴ (ii) the famous (at least among physicists) numerical experiment of Fermi, Pasta, and Ulam⁵ (FPU) which proved, for the first time, that a weak nonlinearity is not sufficient to lead a Hamiltonian system to equipartition of the energy among the degrees of freedom. For Hamiltonian systems with a small number N of degrees of freedom $(N \sim 2-5)$ there exists a huge amount of numerical simulations (beginning with the famous Henòn-Heiles model),⁶ showing the existence of a stochasticity threshold—at a fixed value of the nonlinear coupling constant λ there is a critical energy E_c such that at $E < E_c$ we observe a prevalence of ordered orbits, while at $E > E_c$ the trajectories with chaotic motion are dominant. The term "chaotic" is very vague and usually stands for exponential divergence of initially close orbits (or, equivalently, Kolmogorov-Sinai entropy different from zero), the Poincaré map presenting scattered "spots" of points rather than "lines," as in periodic or quasiperiodic motions.

The persistence of ordered motions or nearly integrability in the thermodynamic limit $(N \rightarrow \infty)$ is far from being understood: The KAM theorem holds for any finite N but unfortunately no estimate of the dependence of E_c on N exists. One of the main problems in the foundations of classical statistical mechanics concerns the evaluation of $\lim_{N\to\infty} E_c/N$: Is it zero or finite?

There are on this fundamental question different and diverging viewpoints. Some scholars support the impossibility of a dynamical construction of ensemble theory in statistical mechanics and therefore the irrelevance of the ergodic problem (Landau).⁷ Others think that an equivalence between time and ensemble averages must hold only for a few physically relevant functions (Khinchin).⁸ In particular for any function f that can be expressed as a sum of functions f_i dependent on single-particle phase-space coordinates one can prove that, for almost every initial condition,

$$\frac{\lim_{T \to \infty} \langle f \rangle_T}{\langle f \rangle_{\text{ens}}} \xrightarrow[N \to \infty]{} \stackrel{1}{\longrightarrow} 1, \qquad (1)$$

where $\langle f \rangle_T = (1/T) \int_0^1 f \, dt$ and the brackets $\langle \rangle_{\text{ens}}$ stand for the ensemble average. Although this result is very interesting one should note that this theorem cannot be applied to many phase-space functions of some physically interesting systems. Let us consider, for instance, a chain of coupled particles whose Hamiltonian is

$$\mathscr{H} = \sum_{i=1}^{N} \left\{ \frac{1}{2} \left[\pi_i^2 + (\phi_i - \phi_{i+1})^2 \right] + \lambda V(\phi_i - \phi_{i+1}) \right\}, \quad (2)$$

where ϕ_i are the displacements about the stable positions of the particles and $V(\xi)$ is nonquadratic [in the FPU β model $V(\xi) = \beta \xi^4/4$].

The theorem (1) establishes the virialization of kinetic and potential energy in the thermodynamic limit but does not say anything about the equipartition of the total energy among the normal modes. The theorem (1) has a scarce dynamical content being substantially a probabilistic statement.

Now let us comment in more detail on the concept of critical energy E_c . One must be clear about the definition of E_c : One can introduce parameters which detect the appearance of stochastic orbits (e.g., Lyapounov exponents), thus determining a stochastic critical energy $E_c^{s,9}$ while in other cases the attention may be to the equipartition critical energy $E_c^{e,10}$ It is in general reasonable to think that $E_c^s < E_c^e$, since it is possible that the phase space is divided in two or more regions inside which the motion is chaotic,

but clearly we have not ergodicity and equipartition. This effect has been actually observed in the two-dimensional Lennard-Jones model.¹¹

There are two distinct viewpoints with respect to the dependence of E_c^e (or E_c^s) on N.

(i) $\lim_{N\to\infty} E_c^{\vec{e}}/N=0$, and the KAM theorem is irrelevant for the thermodynamic limit (Chirikov).

(ii) $\lim_{N\to\infty} E_c^e/N = \text{const} > 0$ (Galgani).

There have also been some proposals on the dependence of E_c on the initial conditions. For the FPU model and for initial conditions which consist in the excitation of Δn normal modes near to the normal mode n, whose wave number is $k_n = 2\pi n / N$ (N is the number of particles), Chirikov¹² suggests

$$\frac{E_c}{N} \sim \begin{cases} (\Delta n)^{1/2} / n\lambda, & n \ll N \\ k_n^2 / \lambda N^2, & n \sim N \end{cases}$$
(3)

using arguments based on the application of the Bogoliubov-Krylov technique.

On the contrary Galgani et al.¹³ propose

$$\frac{E_c^s}{N} \sim f(k_n) , \qquad (4)$$

where $f(k_n)$ is a monotonically increasing function of k_n . Galgani and collaborators have also proposed for this model $E_c/N \sim \omega_{exc}$, where ω_{exc} is the angular frequency of the central initially excited mode, and using this result they put forth a possible classical interpretation of Planck's law. Some indications, from numerical simulations, of the fact that E_c/N goes to a nonzero value as N increases are obtained for a chain of particles interacting with a Lennard-Jones¹⁴ potential and for the FPU model.¹⁵

In Eq. (3) we have purposely written E_c instead of E_c^e (or E_c^s), as there is some controversy between Refs. 12 and 16; in the former paper $E_c = E_c^s$ seem to be considered while in the latter $E_c = E_c^e$ is probably assumed. In this paper we will deal with the study of E_c^e as a function of N and of the initial condition.

In Sec. II we will introduce the model and the indicator of equipartition, the "spectral entropy"; in Sec. III we will discuss the numerical results on the dependence of E_c on N and on the initial condition; Sec. IV is devoted to some perspectives of future work.

II. THE MODEL AND THE SPECTRAL ENTROPY

In this paper we consider a model representing a chain of N nonlinearly coupled particles, whose Hamiltonian is given by

$$\mathscr{H} = \sum_{i=1}^{N} \left[\frac{1}{2} \pi_i^2 + \frac{1}{2} (\phi_i - \phi_{i+1})^2 + \frac{1}{4} \beta (\phi_i - \phi_{i+1})^4 \right], \quad (5)$$

where ϕ_i are the displacements with respect to the stable positions and $\pi_i = \dot{\phi}_i$ are the conjugate moments to ϕ_i . This is the well known Fermi-Pasta-Ulam β model.⁵ We have integrated the equation of motion derived by the Hamiltonian (5), which reads

$$\ddot{\phi}_{i} = (\phi_{i+1} + \phi_{i-1} - 2\phi_{i}) + \beta [(\phi_{i+1} - \phi_{i})^{3} - (\phi_{i} - \phi_{i-1})^{3}] = F_{i} \{\phi_{i}(t)\}$$
(6)

by means of the leap-frog algorithm; that is,

$$\phi_i(t + \Delta t) = 2\phi_i(t) - \phi_i(t - \Delta t) + (\Delta t)^2 F_i\{\phi_i(t)\} .$$
(7)

In our numerical experiments we have chosen periodic boundary conditions, i.e., $\phi_1 = \phi_{N+1}$. It is evident that the $\beta = 0$ model can be integrated by the Fourier transformation, which reduces it to a system of decoupled harmonic oscillators in the wave-number space. Since we are interested in the mechanism of energy sharing among the many degrees of freedom at small β , or small nonlinear energy, it is sensible to choose the Fourier basis even at $\beta \neq 0$.

In formula the displacements $\phi_i(t)$ can be expanded in Fourier components $A_n(t)$, $B_n(t)$ as follows:

$$\phi_{i}(t) = (2\pi)^{-1/2} \sum_{n=0}^{N/2} \left[A_{n}(t) \cos\left[\frac{2\pi n}{N}(i-1)\right] + B_{n}(t) \sin\left[\frac{2\pi n}{N}(i-1)\right] \right].$$
 (8)

In all our numerical experiments we take $N = 2^m$ so that it is possible to perform the Fourier transformation to compute A_n, B_n by using the fast Fourier transformation algorithm.

The quantity of interest here is the power spectrum

$$W_n(t) = \langle A_n^2(t) \rangle_{\rm sm} + \langle B_n^2(t) \rangle_{\rm sm} , \qquad (9)$$

where $\langle \rangle_{sm}$ means a smoothing operation centered around the time *t*:

$$\langle A_n^2(t) \rangle_{\rm sm} = \frac{1}{\Delta T} \int_{t-\Delta T/2}^{t+\Delta T/2} dt' A_n^2(t') . \tag{10}$$

We shall see that the smoothing does not change sensitively with ΔT if ΔT is much greater than the typical time of the system which is O(1).

If the equipartition of energy between all the normal modes is finally reached we have

$$W_n(t) \underset{t \to \infty}{\sim} \omega_n^{-2} , \qquad (11)$$

where $\omega_n = 2 \sin(\pi n / N)$ is the pulsation of the mode with wave vector $k_n = 2\pi n / N$ in the limit $\beta = 0$. The problem is to find an "equipartition energy indicator" which measures the "degree" of equipartition. We are interested in the study of the sharing of the energy among all the normal modes when at the initial time the energy is distributed only on a few of them.

We therefore need a very sensitive probe of the powerlaw behavior (11) (i.e., the energy equipartition), with the following properties.

(i) It must be very stable for a long time and independent of the intermediate shapes assumed by the spectrum.

(ii) It must be reliable and well defined with different choices of initial conditions. In a previous paper¹⁷ the slope $\alpha(t)$ of the exponential spectrum $W_n \sim e^{-n\alpha(t)}$, when only one mode was initially excited, was chosen as the equipartition parameter. This choice is not possible any more for excitations involving initially many modes.

(iii) It must select the inverse square law, denoting the equipartition of energy. The fact that the "slope" of the

spectrum for initial one-mode excitations goes to zero, while detecting correctly the onset of a generic power law, it does not necessarily select the desired behavior (11), which can be observed only by looking directly at the evolution of the spectrum.

Let us introduce the quantity

$$H(t) = -\sum_{n=1}^{N/2} p_n(t) \ln p_n(t) \ge 0 , \qquad (12)$$

where $p_n(t) = E_n / \sum_i E_i$; E_n is the harmonic energy of the normal mode with wave vector $k_n = 2\pi n / N$. In our practical computations we set $p_n(t) = \omega_n^2 W_n(t) / \sum_i \omega_i^2 W_i(t)$; this choice is possible because there is a virialization of kinetic and potential energies for each normal mode and then $E_n \propto \omega_n^2 W_n$.

This spectral entropy reaches zero when $p_s = 1$, $p_n = 0 \forall n \neq s$, i.e., only one normal mode is excited. Its maximum value $H_{\max} = \ln(N/2)$, is obtained when $p_n = 2/N \forall n$, i.e., the power spectrum W_n shows the power law (11). The value of H diminishes the more the spectrum is concentrated or lumped, while the maximum is obtained at the equipartition of the energy per mode— $E_n \propto \omega_n^2 W_n = \text{const.}$

There is still a drawback for the quantity just introduced, i.e., its maximum depends on N which we are going to vary in our simulations. To avoid this undesired feature we have introduced the *normalized* quantity

$$\eta = \frac{H_{\max} - H_{\infty}}{H_{\max} - H(0)} , \qquad (13)$$

where H_{∞} is the maximum value reached by H(t) during the integration of the equation of motion; in some sense it is the "asymptotic" value of H(t), since the tendency of the spectrum is towards a spreading of the energy among the modes. Let us notice that η is bounded between zero and one, which correspond, respectively, to the equipartition of energy and to a situation which does not differ a great deal from the initial condition; in the latter case there is not a substantial spreading of energy among the modes.

III. PERSISTENCE OF THE THRESHOLD AT LARGE N: NUMERICAL RESULTS

In this section we show our numerical results obtained using the numerical methods previously mentioned and the parameter η , which measures the degree of equipartition, with different initial conditions and different numbers N of degrees of freedom.

The characteristic time of our system is given by the period of the fastest mode, i.e., π ; in all our computations we have used $\Delta t = 10^{-1}$, which ensures a good time sampling. A relevant problem, as was discussed in Sec. I, is the existence of the equipartition threshold and the dependence of $\epsilon_c^e = E_c^e / N$ on the number of degrees of freedom N.

The numerical experiment has been performed with different values of N ranging from N=64 to 512 $(N=2^m, m=6,7,8,9)$ and initial conditions of the type

$$\phi_i(0) = \sum_{n=1}^{N/2} \left[A_n \cos\left[\frac{2\pi n}{N}(i-1)\right] + B_n \sin\left[\frac{2\pi n}{N}(i-1)\right] \right], \quad (14)$$

with A_n and B_n different from zero only for $n \in [\overline{n}, \overline{n} + \overline{\Delta n} - 1]$, where the overbars indicate a certain fixed value of n and of a range of n. The values of $k_{\overline{n}}$ and $\Delta k_{\overline{n}}$ do not change when N is varied and A_n , B_n are chosen so that the energy at the initial time is equally shared in the range $[\overline{n}, \overline{n} + \overline{\Delta n} - 1]$; clearly the number of modes contained in this range grows linearly with N. We think that this choice is a natural one to study the trend towards the thermodynamic limit; indeed, we are considering a system which describes a gas of weakly coupled phonons and increasing the number of initially excited modes ("quasiparticles") with N (which is the "volume" of the system). This procedure resembles the limit of $N \rightarrow \infty$ and $V \rightarrow \infty$ when the density N/V is left unchanged. With the initial conditions (14) we perform the numerical integration to compute H(t) from $W_n(t)$ and we choose the value $\beta = 0.1$.

We find that at $t \sim 2000$ (ΔT ranging from 100 to 1000) $\eta(t)$ has already reached its asymptotic value, we have followed in some cases the evolution of $\eta(t)$ up to a time $t \sim 10\,000$ ($\Delta T \sim 100-2000$) and we did not observe any difference. In Fig. 1 η is plotted versus the energy density $\epsilon = E/N$ with the above-mentioned value of N and two different choices of \overline{n} .

We can observe that ϵ_c^e does not change significantly with increasing N. This suggests the relevance of the existence of an equipartition threshold also when the thermodynamic limit is approached. We remark that the experimental points lie on a "universal curve" $\eta(\epsilon)$ within the numerical errors. This behavior is, by the way, an indication that η is a good equipartition probe. In Fig. 2 we have reported some of the results shown in Fig. 1 together with those referring to more general excitations, i.e., without the restriction of a fixed Δk_n and this time η is plotted versus the asymptotic Reynolds number R of the system, i.e., the asymptotic space average of the ratio between the nonlinear (NL) and linear (L) terms in the equation of motion (6):

$$\left\langle \frac{O(\mathrm{NL})}{O(L)} \right\rangle_{\mathrm{space}} = \frac{\beta}{N} \sum_{i=1}^{N-1} (\phi_{i+1} - \phi_i)^2 \underset{\mathrm{large } t}{\longrightarrow} R , \qquad (15)$$

where $\langle \rangle_{\text{space}}$ stands for space average.

In the particular case of the FPU β model $R \sim \beta \epsilon_L \sim \beta \epsilon$ when β is small, where ϵ_L is the density of the linear energy.

As usual in hydrodynamic estimates there is some arbitrariness in the definition of R with the constraint that it must reproduce correctly the competition between the nonlinear and linear term.

The dependence of η on R turns out to be very similar to the previously mentioned $\eta(\epsilon)$, thus defining a critical value R_c . We have found the value $R_c \cong 0.03$ which is consistent with $\epsilon_c \cong 0.35$ (remember that $\beta = 0.1$) so we can remark that even with only few percent of "nonlinearity" one obtains the energy equipartition. This is a relevant point. With such a small value of R it is still meaningful to consider the energy of a single normal mode because the total amount of the interaction energy is only a few percent of the total energy.

It is interesting to note that H_{∞} gives a rough estimate of the number of the "excited" degrees of freedom, i.e., the number of normal modes which significantly ex-



FIG. 1. η vs ϵ ; $\bar{k} = 2\pi\bar{n}/N$, $\Delta \bar{k} = 2\pi\bar{\Delta n}/N$, $\bar{\Delta n} = N/16$, $\bar{n} = N/32$; $\frac{5}{32}N$; with N = 64, 128, 256, 512. Dashed line is a free-hand smoothing of the experimental results.



FIG. 2. η vs R with different N and kind of initial conditions. \Box indicates N=256 and an initial condition so that the energy is distributed on normal modes with wave vector $k_n = (2\pi/N)n$ with $8 \le n \le 24$ or $40 \le n \le 56$.

change their energies with the others. One can assume that, in a first rough approximation, $H_{\infty} \sim \ln(N_{\rm eff}/2)$ where $N_{\rm eff}$ is the asymptotic number of the "effective" degrees of freedom of the system. Loosely speaking we could consider an equivalent spectrum E(k) made by a dichotomic choice: If E(k), for any given k, is greater than a fixed reference value the corresponding normal mode is considered excited; on the contrary, it is "frozen." Considering H_{∞} as an information entropy, one can infer that $N_{\rm eff} = 2 H_{\infty}$ is an estimate of the number of the relevant degrees of freedom. This definition is similar to that of the number of different \mathcal{N} messages contained in a sequence of symbols, and $\mathcal{N} \sim e^S$ where S is the information entropy of the sequence of symbols (Shannon's theorem).¹⁸ This is clearly a very rough estimate but it gives us an idea of the volume of the phase space effectively accessible at different energy densities.

In Fig. 3 we have plotted $N_{\rm eff}$ versus ϵ in the case N=128 and $N_{\rm eff}=16$ in the limit $\epsilon \rightarrow 0$ corresponding to the initial condition. Again the figure shows a threshold effect at $\epsilon \approx 0.3$.

Another relevant problem is the dependence of ϵ_c on ω_{exc} where $\omega_{\text{exc}}/2\pi$ is the frequency of the normal mode corresponding to \overline{n} in the limit of a very small $\overline{\Delta n}$. As was mentioned in the Introduction there is a disagreement among the theoretical predictions and numerical experiments. It is possible to give a naive prediction of $\epsilon_c = \epsilon_c(\omega_{\text{exc}})$ with a dimensional argument and a reasonable hypothesis. The hypothesis is that no matter what the initial condition is the energy equipartition occurs when the nonlinear term is "dominant," i.e., when R is greater than a certain critical value R_c which is independent of ω_{exc} . Since $R \sim \beta \epsilon$, it follows that $\epsilon_c(\omega_{\text{exc}}) \simeq \text{const}$. We have performed numerical simulations to compute $\epsilon_c = \epsilon_c(\omega_{\text{exc}})$. In these computations we have fixed

N = 128, $\overline{\Delta k} = 2\pi/128$ changing \overline{n} ; at any value of \overline{n} we obtained H_{∞} as a function of E and from these curves the critical values E_c are obtained (see Fig. 4 as an example). In Fig. 5 the dependence $E_c = E_c(\omega_{\text{exc}})$ is reported. We have found $E_c \simeq \text{const} \simeq 128\epsilon_c$.

After these results concerning the energy equipartition threshold we wonder whether this phenomenon is really related to the competition between the linear and nonlinear terms, or could it be due to some "hidden" symmetry of the system which, for instance, is related to the space-translation invariance of the model. In other words the problem is to understand if the system is generic or not.¹⁹

For this reason we change the Hamiltonian (5) in



FIG. 3. N_{eff} vs ϵ for N=128 and initial condition $\overline{n}=4$, $\overline{\Delta n}=8$.



FIG. 4. H_{∞} vs *E* for N = 128, $\omega_{\text{exc}} \approx 0.4$, 0.6.

$$\mathscr{H} = \sum_{i=1}^{N} \left[\frac{1}{2} \pi_i^2 + \frac{1}{2} (\phi_i - \phi_{i+1})^2 + \frac{1}{4} \beta_i (\phi_i - \phi_{i+1})^4 \right],$$
(16)

where β_i are quenched random variables; $\beta_i = \beta + \delta_i$, where δ_i is a random variable uniformly distributed in the interval $[-0.1\beta, 0.1\beta]$, and such that $\langle \delta_i \delta_i \rangle = 0$ if $i \neq j$.

If some hidden conservation law exists, then the phenomenology associated to the system described by the Hamiltonian (12) should be very different from that observed for system (5). Figure 6, where H_{∞} versus *E* is shown for both systems (5) and (16) shows evidence that the quenched randomness of the nonlinear coupling constant does not affect the phenomenology. This strongly supports the idea that the energy equipartition threshold is still present when we explicitly break some symmetry of the model. All our computations have been performed on a CDC 7600 in double precision; the overall simulation required about 8 h of CPU time.





FIG. 6. H_{∞} vs *E* for N = 128, (**•**) $\beta = 0.1$, (\triangle) $\beta_i = 0.1 + \delta_i$, δ_i quenched random variables uniformly distributed in [-0.01, +0.01]. Each run is performed with different realizations of $\{\delta_i\}$.

IV. PERSPECTIVES AND OUTLOOKS

In this paper we have reported strong evidence in favor of the existence of an equipartition threshold for a nonlinear Hamiltonian system with a large number of degrees of freedom and its persistence as this number is increased. The main result is that this threshold occurs at the same value of the "control parameter," i.e., the energy density, when the number of degrees of freedom varies. This result has been worked out for large enough integration times ($\sim 10^4$ characteristic times) of the equation of motion and it seems to suggest that we have actually reached a frozen situation. For the N dependence our results seem to be unquestionable and in contrast with the existing theoretical predictions¹² but as far as the time dependence is concerned we cannot conclude that the threshold does not vanish as t approaches ∞ . Moreover, an N dependence could be present at much larger times. This situation can be likened to the very slow relaxation behavior in disordered systems, where the evolution towards "equilibrium" takes place through metastable states, approached at different time scales. Such a phenomenology could be conjectured by applying similar arguments to those discussed in Ref. 20. Let us suppose that the energy transfer among the normal modes, after the "frozen state" has been approached, can take place only when in some part of the system the nonlinear term is sufficiently strong so that the local Reynolds number R(x) is such that $R(x) > R_c$. Thus, following a standard argument based on the central limit theorem, in the thermodynamic limit one could also expect that if $R < R_c$ then there is always some time interval when in some part of the system $R(x) > R_c$ and, therefore, energy transfer takes place. If this were the case this energy transfer would be highly inefficient and very slow, and therefore difficult to detect numerically.²¹ In any case the equipartition threshold observed for the integration time discussed in this paper is physically sensible when we are interested in the behavior of a system for long but finite times.

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