

Fractal entropy of a chain of nonlinear oscillators

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We study the time evolution of a chain of nonlinear oscillators. We focus on the fractal features of the spectral entropy and analyze its characteristic intermediate time scales as a function of the nonlinear coupling. A Brownian motion is recognized with an analytic power-law dependence of its diffusion coefficient on the coupling.

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I. INTRODUCTION

A system composed of a large number of particles (generically) relaxes toward an equilibrium state that is independent of the details of the initial state. This is one of the fundamental hypotheses of statistical mechanics. However, from the point of view of Hamiltonian dynamics, the detailed features of the relaxation are not thoroughly understood. One of the unsolved fundamental questions is how equilibrium is approached when the underlying microscopic dynamics is sufficiently chaotic, without introducing any randomization or coarse graining “by hand.”

After the pioneering work on the time evolution of non-integrable systems [1] and ergodicity [2], it is now clear that several additional factors play a primary role in characterizing the dynamical evolution [3–6]. However, for a large number of particles the Kolmogorov-Arnold-Moser (KAM) argument becomes less effective [6,7] and the Nekhoroshev bound [4] for the equilibrium time appears too weak in comparison with numerical results. This scenario has motivated a number of numerical studies of Fermi-Pasta-Ulam-like models, in the attempt to clarify the dependence of the equilibrium time (defined in terms of suitable indicators) on the strength of the nonlinear terms and the number of particles [8]. These studies yield stretched-exponential relaxation laws, enforcing the picture that macroscopic equilibrium could be built out of local ones [9].

The aim of this paper is to investigate this issue by analyzing, both analytically and numerically, the dynamics of a chain of N coupled anharmonic oscillators at intermediate time scales (for states that are close to equilibrium). One of our main results is that at these intermediate time scales the system performs a Brownian motion with a diffusion constant that can be accurately estimated and turns out to be *analytically* diverging in the coupling constant: as a consequence, a perturbative approach to this problem appears sensible.

II. THE SYSTEM

We will study a Hamiltonian made up of an integrable part and a (small) nonlinear perturbation. This is a classical

nonintegrable system that does not possess enough integrals of motion. The conjugate variables are $(q, p) = (q_1, \dots, q_N, p_1, \dots, p_N)$, where periodic boundary conditions $q_{N+1} = q_1$, $p_{N+1} = p_1$ are understood. We take $N = 2^7 = 128$, for convenience of the numerical algorithm (we observed no significant difference for larger N). The Hamiltonian (ϕ^4 model) reads

$$H(q, p) = H_0(q, p) + gV(q) \quad (g > 0), \quad (1)$$

$$H_0(q, p) = \sum_{i=1}^N \frac{1}{2} p_i^2 + \frac{1}{2} m^2 q_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2, \quad (2)$$

$$V(q) = \sum_{i=1}^N \frac{1}{4} q_i^4. \quad (3)$$

The quadratic part H_0 is easily diagonalized by means of a discrete Fourier transform, in terms of the $2N$ normal variables q_κ , p_κ , with $\kappa = (k, a)$, where $k = 0, \dots, N/2$ and $a = 0, 1$, $a = 0$ ($a = 1$) corresponding to the cosine (sine) transform with wave number k . With this coordinate change H_0 becomes

$$H_0 = \sum_{\kappa} E_{\kappa}, \quad E_{\kappa} = \frac{1}{2} p_{\kappa}^2 + \frac{1}{2} \omega_k^2 q_{\kappa}^2, \quad (4)$$

with the frequency spectrum

$$\omega_k^2 = m^2 + 2 \left[1 - \cos \left(\frac{2\pi k}{N} \right) \right],$$

$$m = \omega_{\min} \leq \omega_k \leq \omega_{\max} = \sqrt{4 + m^2}. \quad (5)$$

In this paper, we always set $m^2 \geq 0.1$. The value of m determines the width of the spectrum and has profound consequences on the dynamics, in particular at small nonlinearities: metastable states, such as solitons and breathers, are born more easily at small m and this can have drastic consequences, both at intermediate and large time scales of the equilibration process [9].

We integrated the Hamilton equations deriving from Eq. (1) via a fourth-order Runge-Kutta algorithm in double precision. Energy conservation is verified at least up to 1 part in 10^7 during the whole running time. Such a precision is nec-

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essary in order to assure that the fluctuations due to numerical integrations be negligible with respect to the physical ones in which we are interested.

III. SPECTRAL ENTROPY

From the numerically integrated solutions we analyze the behavior of the spectral entropy [8]

$$S(t) = - \sum_{\kappa} \frac{E_{\kappa}}{E_0} \ln \frac{E_{\kappa}}{E_0}, \quad (6)$$

where $E_0 = H_0$ is the unperturbed total energy. When $g=0$ all the E_{κ} 's, and therefore S , are constant. As soon as the nonlinearity is switched on, $g>0$, the spectral entropy becomes a nontrivial function of time.

The purpose of this paper is to explore the dynamics of the system over *intermediate* time scales. Previous studies [8,10] mainly concentrated on the long-time behavior of the equilibration process, starting from states that are far to equilibrium and smoothing S over sufficiently long-time intervals. Relaxation from states that are close to equilibrium has been more seldom studied [11]. In our simulation, we always set the initial conditions with the actions (unperturbed energies) randomly picked from a microcanonical ensemble and the angles completely random. Therefore, the fluctuations of $S(t)$ will be studied *close to equilibrium*.

S displays wild time fluctuations, over a wide range of frequencies. We will show that useful, univocal information can be obtained from such an irregular function: we will first recognize a Brownian structure and then look at the characteristic time scales and study their dependence on the nonlinear coupling.

Let us first discuss some analytical properties. At equilibrium, average quantities and statistical properties should depend only on integrals of motion. For Hamiltonian (1) one argues that the only global integral of motion is the total energy $E=H$ or, equivalently, the energy per mode $\epsilon \equiv E/N$. The equations for q_i possess the following scaling symmetry: if q_i is a solution of the Hamilton equations with coupling g , then $q'_i = \sqrt{A}q_i$ is solution of the Hamilton equations with coupling $g' = g/A$. With this rescaling, the energy is changed to $E' = AE$. A function X , representing the average of some quantity at equilibrium and having dimension $[X] = \text{length}^{\nu}$, can only depend on E and g , whence

$$X(AE, g/A) = A^{\nu/2} X(E, g). \quad (7)$$

Therefore, if $\nu=0$, X depends only on the dimensionless product

$$x = g \epsilon = gE/N, \quad (8)$$

which may be considered as the effective strength of the nonlinearity. We will study the dynamical properties of our system for $10^{-4} \leq x \leq 1$.

Average quantities in the weakly nonlinear regime can be calculated by using the microcanonical distribution. The use of this distribution is motivated by the empirical observation that the total *unperturbed* energy E_0 , although not constant

in time, fluctuates less than 1% around its mean value (even smaller fluctuations are observed for very small nonlinearities). We can conclude that the primary role of the perturbation V is only to allow "collisions" between normal modes (phonon exchange), provoking in this way the transition to equilibrium,¹ without "storing" any significant energy. Therefore, we can assume $E \simeq E_0$ in the following.

For the spectral entropy at microcanonical equilibrium one finds, after a straightforward but somewhat lengthy calculation,

$$\bar{S} = \psi(N+1) - (1-\gamma) = \ln N - (1-\gamma) + O\left(\frac{1}{N}\right), \quad (9)$$

$$\begin{aligned} \delta S^2 \equiv \overline{S^2} - \bar{S}^2 &= \frac{3 + 3N + (\pi^2 - 6)N^2}{3N^2(N+1)} - \psi'(N) \\ &= \frac{0.289}{N} + O\left(\frac{1}{N^2}\right), \end{aligned} \quad (10)$$

where ψ is the Euler digamma function [12] and $\gamma \simeq 0.5772$ the Euler-Mascheroni constant. The asymptotic behavior of Eq. (9) is in agreement with previous results [6,13], obtained at canonical equilibrium. In fact, as shown in the Appendix, the microcanonical and canonical averages of any function of the spectral entropy coincide. Equations (9) and (10) are therefore valid also at canonical equilibrium. These analytical results are well confirmed by numerical simulations and provide a good test of the fact that our numerical sample was representative of an equilibrium situation and free from "trend" components.

IV. CORRELATION FUNCTION

We study the fractal dimension and the characteristic time scales of the entropy by looking at the correlation function C for the generalized Brownian process S :

$$C(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt [S(t+\tau) - S(t)]^2. \quad (11)$$

In general, one can identify a fractal, or generalized Brownian motion, by the dependence $C \propto \tau^{2H}$. The exponent H is related to the fractal dimension by $D_f = 2 - H$. When using function (11) one should take care of "detrending" S [14]. However, since the system starts at equilibrium, where S fluctuates about its constant mean value (9), no detrending is required. We emphasize, however, that we obtained the same results also in nonequilibrium situations (not too far from equilibrium), provided the trend component of $S(t)$ was suitably removed.

¹In action-angle variables, one can renormalize the free Hamiltonian with a positive, nonlinear correction of the order of x . The total Hamiltonian is accordingly split into a new free part and a new perturbation.

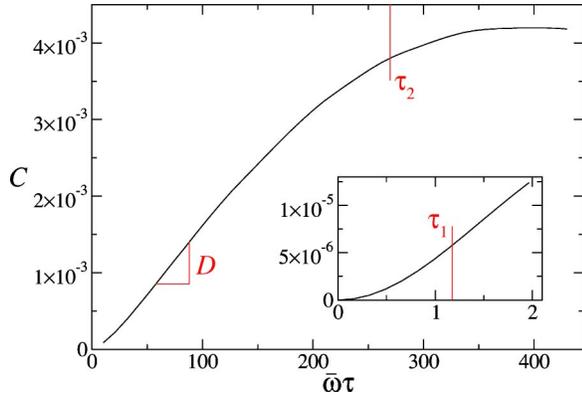


FIG. 1. C vs $\bar{\omega}\tau$. Notice the quadratic region extending up to times of the order of τ_1 (inset) and the linear region (20) in the range $\tau_1 < \tau < \tau_2$. The saturation level $C \approx 2\delta S^2 \approx 0.0044$ is in full agreement with Eq. (10) [for $N=128$]. We set $x=0.09$ and $m^2=5$, so that $\bar{\omega}=2.62$. Observe that $\tau_2 \approx 200\tau_1$ is clearly an intermediate time scale, orders of magnitude smaller than T_{relax} . Larger ratios τ_2/τ_1 are observed for smaller values of x , but the chain of inequalities (19) always remains valid.

For a Brownian process, one expects a linear dependence of C on τ [14,15], i.e., $D_f=3/2$,

$$C(\tau) \propto \tau. \quad (12)$$

Brownian motions are useful idealizations to describe physical processes in a simple and coherent mathematical way. However, in order to treat an analytic function (such as S) as a Brownian process, one must identify (at least) one time scale, say τ_1 . This time scale is such that by ‘‘observing’’ the function at time scales $\tau \lesssim \tau_1$ one obtains a smooth function, while by observing it with a time resolution $\tau \gg \tau_1$, one recognizes a Brownian process. It is possible to unambiguously identify the time scale τ_1 since $C \sim \tau^2$ for sufficiently small τ :

$$\begin{aligned} C(\tau) &\approx \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \left(\dot{S}(t)\tau + \frac{1}{2}\ddot{S}(t)\tau^2 + O(\tau^3) \right)^2 \\ &= \overline{\dot{S}(t)^2} \tau^2 + O(\tau^4). \end{aligned} \quad (13)$$

At larger τ , the quadratic dependence changes into the linear one (12): the time scale at which this change takes place is τ_1 . See inset in Fig. 1. It is important to stress that τ_1 is nothing but the linear time scale for phonons, of the order of an inverse characteristic frequency (5) of the oscillators

$$\frac{2\pi}{\bar{\omega}} = 2\pi \frac{2}{\omega_{\min} + \omega_{\max}} = \frac{4\pi}{m + \sqrt{4+m^2}}. \quad (14)$$

Up to this time scale, one is able to observe the microscopic details of the motion in phase space. At larger time scales, the motion appears very irregular and the microscopic details are lost.

For a Brownian process which is also bounded another time scale appears, since S bounded implies C bounded and

the law $C \propto \tau$ must break down at a certain time. Let us call this time scale τ_2 . It is easy to show that at equilibrium, for sufficiently large τ we have $C(\tau) \approx 2\delta S^2$, so we can interpret τ_2 as the time at which the autocorrelation of the entropy vanishes:

$$\langle S(t+\tau)S(t) \rangle - \langle S(t+\tau) \rangle \langle S(t) \rangle \approx 0 \quad \text{for } \tau > \tau_2. \quad (15)$$

This means that $S(t+\tau)$ and $S(t)$ can be considered uncorrelated random numbers chosen from a sample of mean \bar{S} and variance δS^2 . In terms of motion in phase space one can argue that the system starts at $t=0$ at (or very close to) equilibrium and at $t \sim \tau_2$ it has explored a sufficiently large part of the equilibrium region, such that the microcanonical averages (9) and (10) can be used. The theoretical predictions (10) [with $N=128$], (12), and (13) are very well verified by the numerical data shown in Fig. 1.

The relaxation of the system, when it starts from a state far to equilibrium, takes place on a time scale T_{relax} that can be defined in terms of the effective number of excited modes [8]

$$n_e \equiv \exp(S): \quad (16)$$

clearly, if the system is initially far from equilibrium,

$$\Delta n_e(T_{\text{relax}}) \equiv n_e(T_{\text{relax}}) - n_e(0) = O(N). \quad (17)$$

On the other hand, due to Eqs. (9) and (10), for a system close to equilibrium

$$\Delta n_e(\tau_2) = e^{S+\delta S} - e^S \approx \delta S e^S = O(\sqrt{N}). \quad (18)$$

In this sense, τ_2 is an intermediate time scale, characterizing, as we have seen, local fluctuations in phase space.

Finally, if one considers that only a few oscillators can exchange energy in a time τ_1 , one can summarize the above discussion by writing

$$\Delta n_e(\tau_1) = O(1) \ll \Delta n_e(\tau_2) = O(\sqrt{N}) \ll \Delta n_e(T_{\text{relax}}) = O(N). \quad (19)$$

V. DIFFUSION COEFFICIENT AND INTERMEDIATE TIME SCALES

The presence of the linear region (12) for the correlation function C is observed in the whole range of x investigated. This enables us to define a diffusion coefficient D as the rate at which C increases in its linear regime, so that in the region $\tau_1 < \tau < \tau_2$ we have

$$C = D\tau + C_0, \quad (20)$$

where D and C_0 have in general a nontrivial dependence on x . In the following, we will perform a systematic study of D , which is the physically most relevant quantity and characterizes the Brownian fluctuations. Notice that C_0 is related to the initial quadratic region (13) and therefore depends on the microscopic details of the motion.

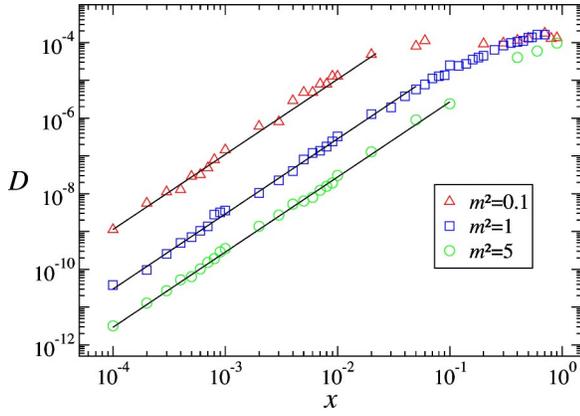


FIG. 2. D vs $x = g\epsilon = gE/N$ for different masses. The lines are the power law (21) and the error bars are included in the size of the dots.

The diffusion coefficient D has no length dimension [$\nu = 0$ in Eq. (7)] and therefore one expects it to be only a function of $x = g\epsilon = gE/N$ (at fixed N and m). This expectation is numerically confirmed with high accuracy. In particular, D is a monotonically increasing function of x , as can be seen from Fig. 2. Each point in the figure is obtained by averaging at least five numerical solutions with the same value of x . For $x \leq 0.1$, D is accurately fit by a power law

$$D = \alpha x^\beta, \quad \beta = 1.987 \pm 0.040. \quad (21)$$

This is an indication that the intermediate dynamics at these time scales can be tackled by a perturbative approach. Notice that, if one endeavors to fit the curves in Fig. 2 with a stretched-exponential law of the type $D \propto \exp(\text{const } x^{-\delta})$, one finds the very small value $\delta = 9.4 \times 10^{-4}$. In our opinion, this is a rather strong indication in support of a power-law behavior. On the other hand, for large x , D saturates to a constant (m -independent) value. Observe that the coefficient β in Eq. (21) does *not* depend on m ; the m dependence of α will be analyzed in the following (see Fig. 3).

The intermediate time scale τ_2 is strictly related to the diffusion coefficient D , via the saturation value $2\delta S^2$ in Eq.

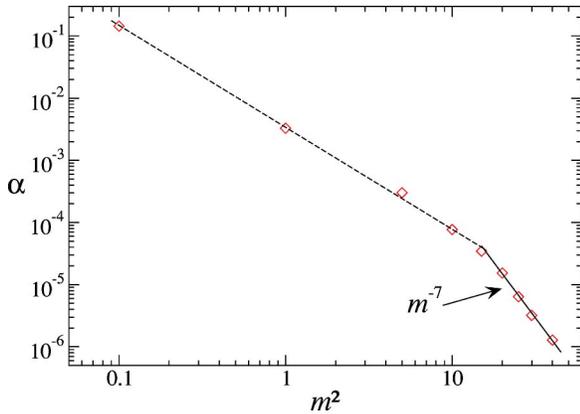


FIG. 3. $\alpha = D/x^2$ vs m^2 [in the quadratic region (21)]. The solid line is theoretical prediction for large masses $\alpha \propto m^{-7}$. The dashed line is the fit $\alpha \propto m^{-3.3}$.

(10), as discussed in connection with Fig. 1. A consistent and natural definition is $\tau_2 = 2\delta S^2/D$, so that for $x \leq 0.1$

$$\tau_2 \propto x^{-\beta} \approx x^{-2}. \quad (22)$$

Note that in order to measure τ_2 it is not even necessary to perform a numerical integration of the Hamilton equations for times of the order of τ_2 . It suffices to integrate them up to times larger than $\tau_1 (\ll \tau_2)$, get D and hence τ_2 .

The analytic dependence (22) of τ_2 on x is in full agreement with previous results and suggests the validity of a perturbative approach [11]. One expects that for sufficiently small x a sensible fraction of the phase space is covered with KAM tori, allowing only Arnol'd diffusion and yielding a consistent suppression of diffusion and a rapid divergence of the macroscopic equilibrium time. Related analytical and numerical work hints at a nonanalytic divergence (such as a stretched exponential) of the macroscopic time scales (such as T_{relax}) [4,7,8] for $x \rightarrow 0$. The fact that the intermediate time scale here analyzed diverges with a power law (22) indicates the *local* presence of a Brownian motion (in the region of parameters studied), so that diffusion should be suppressed on macroscopic regions of phase space.

The dependence of $\alpha = D/x^2$ on m is not trivial. However, in the region of validity of Eq. (21) and for large masses $m^2 \gg 1$, one expects a power-law dependence $\alpha \propto m^{-7}$. Indeed, for large m^2 we get from Eq. (2) $\epsilon \sim m^2 q^2$, so that, at fixed ϵ , q scales like $1/m$. Therefore, the strength g of the quartic potential (and hence $x = g\epsilon$) scales like m^4 . Considering that $[D] = t^{-1}$ and the characteristic oscillation time (14) scales like $1/m$, an additional factor m is obtained, yielding

$$\alpha \propto m^{-7} \quad \text{for } m^2 \geq 15. \quad (23)$$

As shown in Fig. 3, this prediction is well confirmed by our numerical data, provided $m^2 \geq 15$. For $0.1 \leq m^2 \leq 15$, we numerically found $\alpha \propto m^{-3.3}$, for which we offer no explanation. Moreover, for $m \rightarrow 0$ one expects a qualitatively different situation, since $\omega_{\text{max}}/\omega_{\text{min}} = \sqrt{4 + m^2}/m \rightarrow \infty$, such a ratio representing the available primary resonances between normal modes [6]. Actually, we observed the formation of metastable states for $m^2 \leq 0.05$ (not shown in Fig. 3): as a consequence, the correlation function showed marked oscillations of definite frequency, hindering a consistent definition of a diffusion coefficient.

VI. CONCLUSIONS

The analytic (power-law) divergence (22) of the intermediate time scales describing the Brownian motion on the constant energy surface suggests that a perturbative approach, based on a Liouville-Fokker-Planck equation [16] should apply, at least *locally*, and that an eventually nonanalytic divergence of the relaxation time from far to equilibrium should be ascribed to a nontrivial structure of the phase space at larger scales. The dependence of the intermediate time scale on the mass and the presence of long-lived metastable states indicates that the problem is very involved also at the (supposedly simpler) level of the local dynamics in phase space.

In this context, one might speculate that the relaxation from states that are not too far to equilibrium depends on the ‘‘mesoscopic’’ features of phase space. (The expression mesoscopic is not used here in its most familiar meaning, related to the interplay of classical and quantum effects, but rather in the sense of intermediate between ‘‘microscopic’’ and ‘‘macroscopic,’’ i.e., pertaining to the total system.) The approach we propose enables one to extract sensible information from the dynamics at intermediate time scales (from close to equilibrium) that are usually less studied than the longer ones, describing the relaxation from far to equilibrium. This has obvious positive spinoffs from the perspective of numerical investigations, as it requires less computing time. From a more conceptual viewpoint, we have proved the existence of a diffusive process (without introducing any randomization ‘‘by hand’’) that constitutes a building block for the global equilibration process.

APPENDIX

Let us show that, in order to compute the average of any function of the spectral entropy S , the microcanonical and the canonical ensemble are equivalent. This conclusion is a consequence of the following theorem.

In an ensemble of N noninteracting integrable classical systems, where the energies $E_i > 0$ are homogeneous functions of the action variables I_i , the average of functions of the kind $F(E_i/E)$, where $E = \sum E_i$, computed according to the Boltzmann distribution, is equal to that computed according to the microcanonical distribution. Moreover, this average is independent of the temperature β of the canonical ensemble and the energy \mathcal{E} of the microcanonical ensemble.

We prove this theorem by calculating the canonical average of a quantity F (the angle variables are trivially integrated over since they do not contribute to the energies)

$$\begin{aligned} \langle F \rangle_c &= \frac{1}{Z_c} \int d^N I e^{-\beta E} F\left(\frac{E_i}{E}\right) \\ &= \frac{1}{Z_c} \int d^N E J(E_i) e^{-\beta E} F\left(\frac{E_i}{E}\right), \end{aligned} \tag{A1}$$

where

$$Z_c = \int d^N I e^{-\beta E} \tag{A2}$$

is the canonical partition function and $J = \|\partial I_j / \partial E_i\|$ the Jacobian. Due to our hypotheses, this is a homogeneous function of the E_i 's. We obtain

$$\begin{aligned} \langle F \rangle_c &= \frac{1}{Z_c} \int d^N E \int_0^\infty d\xi \delta\left(\xi - \sum_i E_i\right) e^{-\beta E} J(E_i) F\left(\frac{E_i}{E}\right) \\ &= \frac{1}{Z_c} \int_0^\infty d\xi e^{-\beta \xi} \xi^{N-1} \int d^N x J(\xi x_i) \delta\left(1 - \sum_i x_i\right) F(x_i) \\ &= \frac{1}{Z_c} \int_0^\infty d\xi \xi^{N-1+N\alpha} e^{-\beta \xi} \\ &\quad \times \int d^N x J(x_i) \delta\left(1 - \sum_i x_i\right) F(x_i) \\ &= \frac{1}{Z_c} \beta^{-N(1+\alpha)} \Gamma[N(1+\alpha)] \\ &\quad \times \int d^N x J(x_i) \delta\left(1 - \sum_i x_i\right) F(x_i), \end{aligned} \tag{A3}$$

where Γ is the gamma function, we defined $x_i = E_i / \sum_j E_j$ and used the homogeneity of the Jacobian to write

$$J(\xi x_i) = \xi^{N\alpha} J(x_i), \tag{A4}$$

which defines the quantity α . By repeating the same derivation with $F = 1$, one readily shows that

$$\frac{Z_c}{\beta^{-N(1+\alpha)}} = \Gamma[N(1+\alpha)] \frac{Z_m}{\mathcal{E}^{N-1+N\alpha}}, \tag{A5}$$

where the Z_m is the microcanonical partition function

$$Z_m = \int d^N I \delta(\mathcal{E} - E). \tag{A6}$$

Incidentally, notice that both sides of Eq. (A5) are independent of β and \mathcal{E} . In conclusion,

$$\begin{aligned} \langle F \rangle_c &= \frac{\mathcal{E}^{N-1+N\alpha}}{Z_m} \int d^N x J(x_i) \delta\left(1 - \sum_i x_i\right) F(x_i) \\ &= \frac{1}{Z_m} \int d^N I \delta(\mathcal{E} - E) F\left(\frac{E_i}{E}\right) = \langle F \rangle_m. \end{aligned} \tag{A7}$$

This proves our assertion. Equations (9) and (10) are readily obtained by explicitly calculating the (simpler) canonical average of $F = S$ and $F = S^2$.

As a corollary, one sees that if the E_i 's are random variables distributed with e^{-E_i} , the variables $x_i = E_i / \sum_j E_j$ are distributed like $\delta(1 - \sum_j x_j)$. This provides a fast numerical recipe to generate microcanonically distributed variables.

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