Ergodic Properties of Microcanonical Observables

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Abstract: The problem of the existence of a Strong Stochasticity Threshold in the FPU-β model is reconsidered, using suitable microcanonical observables of thermodynamic nature, like the temperature and the specific heat. Explicit expressions for these observables are obtained by exploiting rigorous methods of differential geometry. Measurements of the corresponding temporal autocorrelation functions locate the threshold at a finite value of the energy density, that results to be independent of the number of degrees of freedom.

Keywords: Strong stochasticity threshold, ergodic hypotesis, microcanonical ensemble

I. INTRODUCTION

Models of interest for applications in plasma and condensed matter physics as well as in molecular biology and chemistry are described by many degrees of freedom Hamiltonians of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(\{q_i\}) \tag{1}$$

where $V(\{q_i\})$ is a nonlinear interaction potential among the N particles of mass m, located on a regular lattice, whose sites are labelled by the integer index i. The displacement and momentum canonical coordinates of the i-th particle are denoted by q_i and p_i, respectively. Apart ramarkable exceptions like the Toda chain [1], a generic choice for V yields a chaotic dynamics. One of the main issues in this field is the existence of different levels of chaos that typically occur when some control parameter (e.g. energy or energy density) is varied. Fermi, Pasta and Ulam in their pioneeering numerical experiment [2], first observed the strong rigidity of low-k excitations that prevented equipartion of the energy among the Fourier modes over exceedingly large time scales. Izrailev and Chirikov provided an explanation of this fact in terms of the resonance-overlap criterion [3], while more refined numerical experiments showed that, for sufficiently high energies, equipartition among the Fourier modes sets in very rapidly [4–7]. In particular, already Bocchieri et al. [5] raised the question of the existence of an energy threshold separating a quasi-regular dynamics from a highly chaotic phase. Nowadays, there is theoretical and numerical evidence that such a threshold does exist for large values of N. In this respect, it is worth stressing the following points:

- this threshold in general occurs at energy values that prevent any possibility of quantitative explanation in terms of the canonical perturbation theory;
- in the strongly chaotic phase the time needed to reach equipartition is almost independent of energy and N; just beyond the threshold it suddenly increases, while the dynamics results to be very weakly chaotic.

These remarks point out that the equipartition threshold (ET) separates definitely different dynamical regimes, in such a way that for sufficiently small energies the time needed for approaching equilibrium properties may become so long that the dynamics maintains an ordered structure over any practically available time scale. [8]. On the other hand, it should be stressed that ET does not seem to exhibit analogies with the standard scenario of equilibrium phase transitions: for instance, it is not at all clear which kind of symmetry breaking mechanism, if any, could be responsible for the slowing down of energy equipartition among the Fourier modes.

A further crucial problem concerns the persistence of ET in the thermodynamic limit. This is a key point that recently led various authors to reconsider this problem, by exploiting different approaches and techniques. Let us briefly summarize the state of the art. Some investigations have refined the original approach based on the study of energy equipartition among the Fourier modes: the so-called spectral entropy was first introduced as a global observable able to quantify the amount of energy equipartition [9,10]. The scaling properties of this quantity have been carefully analyzed in ref.s [11,12], yielding the conclusion that the time needed to reach energy equipartition scales in a nontrivial way with both the energy and N. Further numerical investigations and theoretical arguments based on an improved treatment of the Chrikov's resonance overlap criterion [12–14] indicate that, at least for low-k modes excitations, ET should vanish in the thermodynamic limit.

An alternative approach to the characterization of the different dynamical regimes occurring in models like (1) has been pursued by directly investigating proper geometrical features of the phase space. Concepts and tools taken from Riemannian geometry were translated in Hamiltonian language in [15–17]. By exploiting such techniques it has been possible to obtain an analytic estimate in the thermodynamic limit of the maximum Lyapunov exponent as a function of the energy density for the FPU β-model [18]. It exhibits a crossover between a weak and a strong chaotic regime when the energy density is increased beyond a threshold value, that has been identified as the Strong Stochasticity Threshold (SST) [19]. Similar conclusions in favour of the existence of SST in the thermodynamic limit have been drawn by considering other specific geometrical indicators, like generalized curvatures of the phase space, whose reliability has been tested for various models [20–22]. By the way, theese studies also indicate that in the strongly chaotic regime these models may still be far from ergodic.

Upon all of these remarks, one might wonder if the existence of a threshold (either ET or SST) may have some influence on the equilibrium statistical properties of many degrees of freedom hamiltonian models. Beyond the evident interest of such a question for the foundations of Statistical Mechanics, this is a crucial point for molecular dynamics applications, that usually assume the validity of the ergodic hypothesis, i.e. the equivalence of time and ensemble averages. Such a problem would be solved from the very beginning if one could prove ergodicity for a model like (1). Unfortunately, this is possible only in a few special cases. On the other hand, it is commonly accepted that chaoticity should be sufficient for reproducing reliable statistical predictions for most of the observables of physical interest. A partial disproval of this assumption was obtained in [23], where it has been shown that the equivalence between time and ensemble averages for canonical thermodynamic observables (e.g. internal energy and specific heat) mainly depend on the model and on the nature of the observable, rather than on the degree of chaoticity of the dynamics.

In this paper we aim to clarify most of these open points by tackling the problem through the direct comparison of statistical and dynamical properties of microcanonical thermodynamic observables. The general formalism yielding explicit dynamical expressions for such observables is introduced in Section II, where we also comment on their geometrical nature. The results obtained by molecular dynamics calculations for the FPU β-model are reported in Section III. We show that SST is predicted by the decay rate of the temporal autocorrelation function associated with the microcanonical temperature and specific heat, while ergodic-like properties are found to depend mainly on the observable at hand, irrespectively of the degree of chaoticity of the dynamics. Conclusions and perspectives are contained in Section IV.

II. MICROCANONICAL THERMODYNAMIC QUANTITIES

The equivalence in the thermodynamic limit of the predictions obtained from different statistical ensembles (μ-canonical, canonical and G-canonical) is a widely accepted and partially proved fact [24]. Explicit expressions for thermodynamic observables are usually computed by canonical averages. Their relation with the corresponding microcanonical averages was established in a celebrated paper by Lebowitz, Percus and Verlet [25]. Only recently H.H. Rugh, assuming ergodicity of the phase space, obtained a general rigorous expression for the temperature of the microcanonical ensemble, that results to be strictly related to the geometrical structure of the phase space [26]. Analogously, an explicit formula for the specific heat at constant volume has been also obtained [27].

In what follows we are going to reproduce the expressions of these microcanonical thermodynamic quantities, by exploiting a different approach, based on standard tools of differential geometry (see the Appendix). We find that any of these quantities is an explicit, even if in some cases complicate, function of the canonical coordinates. As a consequence, this geometrical approach provides a natural bridge between a dynamical and a thermodynamical description of the microcanonical ensemble. Upon the remarks of the previous Section, we are interested in understanding what can be inferred about thermodynamics by molecular dynamics experiments performed on hamiltonian models of the form (1). As we have already stressed, in general such models are known not to be ergodic in a strictly mathematical sense. In this perspective, it could be hard to find out more appropriate probes for testing ergodicity, than such microcanonical thermodynamic observables.

In analogy with the rigorous approach of Rugh, we assume ergodicity in order to guarantee that the microcanonical entropy S is a well defined quantity associated to some hypervolume in phase space, equipped with a uniform undecomposable probability measure. In the μ-canonical ensemble S plays the role of a generalized thermodynamic potential from which any thermodynamic quantity can be obtained by derivations w.r.t. the physical parameters energy E and volume V:

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_V \qquad\qquad \frac{1}{C_V} = \left(\frac{\partial T}{\partial E}\right)_V \tag{2}$$

$$\frac{P}{T} = \left(\frac{\partial S}{\partial V}\right)_E \qquad\qquad \frac{1}{V\alpha_E} = \left(\frac{\partial T}{\partial V}\right)_E \tag{3}$$

where α_E is defined as the thermal expansion coefficient in the μ-ensemble. In order to be correctly defined S_μ must fulfill the following properties:

- additivity;
- invariance under adiabatic reversible transformations;
- it must be a non-decreasing function for irreversible adiabatic transformations.

Two choices are possible for the μ-ensemble:

$$\begin{aligned} \text{A)}\quad S(E,N,V) &= \ln(c_N \omega(E,N,V)) = \ln\left(c_N \int dq\, dp\, \delta(E - H(q,p))\right) \\ &= \ln\left(c_N \int_{H=E} \frac{d\sigma}{\parallel \nabla H \parallel}\right) \end{aligned}$$

$$\begin{aligned} \text{B)}\quad S(E,N,V) &= \ln(c'_N \Omega(E,N,V)) = \ln\left(c'_N \int dq\, dp\, \theta(E - H(q,p))\right) \\ &= \ln\left(c'_N \int_{H\leq E} d\Gamma\right) \end{aligned}$$

In these formulae we have set the Boltzmann constant $K_B = 1$, while c_N and c'_N are arbitrary constants to make the argument of the logarithm dimensionless.

Definition A includes all the microstates compatible with the constrain $H = E$, i.e. those microstates belonging to the constant energy surface $\Sigma_E = \{(q,p) \in \Gamma \mid H(q,p) = E\}$. Alternatively, definition B considers as microstates all those contained inside the hypervolume $V_E = \{(q,p) \in \Gamma \mid H(q,p) \leq E\}$ limited by Σ_E. Both definitions should be equivalent in the thermodynamic limit.

Let us recall that the phase-space $\Gamma = R^{2N}$ is given the structure of a sympletic manifold by the fundamental symplectic two-form $\omega_2 = \sum_{i=1}^N dq_i \wedge dp_i$. The Hamiltonian $H : \Gamma \to R$ generates a vector field $I \cdot dH$ (where I is the fundamental symplectic matrix) and an associated flux that preserves the Liouville measure. For smooth potentials $V(\{q_i\})$ it seems reasonable to assume that V_E is limited and that Σ_E is smooth and connected.

Taking into account case A, one can easily obtain an expression for the microcanonical temperature, that from here on we shall denote with T_μ, through the relation

$$\frac{1}{T_\mu} = \frac{\partial S}{\partial E} = \frac{\frac{\partial \omega}{\partial E}}{\omega} \tag{4}$$

Making use of a simple theorem of differential geometry one has

$$\frac{1}{T_\mu} = \frac{\int_{H=E} \nabla \cdot \left(\frac{\nabla H}{||\nabla H||^2}\right) \frac{d\sigma}{||\nabla H||}}{\int_{H=E} \frac{d\sigma}{||\nabla H||}} = \langle \nabla \cdot \left(\frac{\nabla H}{\parallel \nabla H \parallel^2}\right)\rangle_\mu \tag{5}$$

The derivation and the full expression of this formula are reported in the Appendix.

Analogously one can obtain an explicit formula for the specific heat per particle at constant volume

$$c_A = \frac{1}{N}\left(\frac{\partial T}{\partial E}\right)^{-1} = \frac{1}{N}\left(1 - \frac{\omega^2}{\left(\frac{\partial \omega}{\partial E}\right)^2} \cdot \frac{\frac{\partial^2 \omega}{\partial E^2}}{\omega}\right)^{-1} \tag{6}$$

By applying the differential geometry theorems reported in the Appendix the following expression is obtained

$$\begin{aligned} c_A &= \frac{1}{N}\left(1 - \frac{\left(\int_{H=E}\frac{d\sigma}{||\nabla H||}\right)^2}{\left(\int_{H=E}\nabla\cdot\left(\frac{\nabla H}{||\nabla H||^2}\right)\frac{d\sigma}{||\nabla H||}\right)^2} \cdot \frac{\left(\int_{H=E}\nabla\cdot\left[\nabla\cdot\left(\frac{\nabla H}{||\nabla H||^2}\right)\frac{\nabla H}{||\nabla H||^2}\right]\frac{d\sigma}{||\nabla H||}\right)}{\left(\int_{H=E}\frac{d\sigma}{||\nabla H||}\right)}\right)^{-1} \\ &= \frac{1}{N}\left(1 - \frac{\langle\nabla\cdot\left[\nabla\cdot\left(\frac{\nabla H}{||\nabla H||^2}\right)\frac{\nabla H}{||\nabla H||^2}\right]\rangle_\mu}{\langle\nabla\cdot\left(\frac{\nabla H}{||\nabla H||^2}\right)\rangle_\mu^2}\right)^{-1} \end{aligned} \tag{7}$$

Similarly, one can treat case B.

The temperature (that from here on we denote T_{kin}, for reasons that will be clear in a moment) can be obtained by introducing a vector $\eta = (0,\ldots,0,x_i,0\ldots,0)$, that has the property $\nabla\cdot\eta = 1$, and using the divergence theorem:

$$\frac{1}{T_{kin}} = \frac{\partial S}{\partial E} = \frac{\omega}{\Omega} = \frac{\int_{H=E}\frac{d\sigma}{||\nabla H||}}{\int_{H<E}\nabla\cdot\eta dx} = \frac{\int_{H=E}\frac{d\sigma}{||\nabla H||}}{\int_{H=E}\frac{\nabla H}{||\nabla H||}\cdot\eta d\sigma} = \frac{\int_{H=E}\frac{d\sigma}{||\nabla H||}}{\int_{H=E}x_i\frac{\partial H}{\partial x_i}\frac{d\sigma}{||\nabla H||}} \tag{8}$$

This is the usual expression deriving form the virial theorem

$$T_{kin} = \langle x_i \frac{\partial H}{\partial x_i}\rangle_\mu \tag{9}$$

that, for Hamiltonian (1) and for $\eta = 1/N\ (0,\ldots,0,p_1,\ldots,p_N)$, simplifies to

$$T_{kin} =< \frac{\sum_{i=1}^N p_i^2}{N} >_\mu$$

i.e. the same expression that is obtained in the canonical ensemble. One could naively conclude that case B should correspond to the canonical ensemble for any explicit expression of thermodynamic variables. Clearly this is not the case, as one can easily conclude from the expression of the specific heat per particle

$$c_B = \frac{1}{N}\left(1 - \frac{\Omega}{\omega}\cdot\frac{\frac{\partial\omega}{\partial E}}{\omega}\right)^{-1} = \frac{1}{N}\left(1 - \langle x_i\frac{\partial H}{x_i}\rangle_\mu \cdot \langle\nabla\cdot\left(\frac{\nabla H}{||\ \nabla H\ ||^2}\right)\rangle_\mu\right)^{-1} \tag{10}$$

Notice that c_B depends on the ratio between T_{kin} and T_μ, that is quite a different expression w.r.t. the corresponding canonical observable.

III. NUMERICAL ANALYSIS

In this Section we study the dynamical and statistical properties of the microcanonical observables introduced in Section II. We consider the so-called FPU β-model, whose Hamiltonian is of the form (1) with

$$V(\{q_i\}) = \frac{1}{2}\sum_{i=0}^{N}(q_{i+1}-q_i)^2 + \frac{\beta}{4}\sum_{i=0}^{N}(q_{i+1}-q_i)^4 \tag{11}$$

We impose fixed boundary conditions, in such a way that the total energy E is the only conserved quantity. All numerical experiments hereafter reported were performed with $\beta = 0.1$. (Notice that this is not a prejudice of generality, since rescaling β amounts to rescale E). The integration of the equations of motion has been performed by a bilateral symplectic algorithm [28] in double precision, with a time step $\Delta t = 0.005$, that guarantees the conservation of the energy at least on the sixth significative figure, for the considered range of energies. The running time average for an observable f and the corresponding variance, computed over the whole time span, are defined as follows:

$$\langle f\rangle_t = \frac{1}{t}\int_0^t f(p(t'), q(t'))dt' \tag{12}$$

$$\mathcal{V}(f) = \frac{\langle f^2\rangle - \langle f\rangle^2}{\langle f\rangle^2} \tag{13}$$

Numerical simulations typically have been performed over $O(10^8)$ time steps, after a transient of 10^5 time steps. Since in the bilateral symplectic algorithm each time step amounts to $2\cdot\Delta t$, the total integration time in natural units is $O(10^6)$, that corresponds approximately to $O(10^5)$ minimum harmonic periods of oscillations. We have considered different values of the energy density $\varepsilon = E/N$ and, at fixed ε, different values of N. Let us first analyze the strongly chaotic regime that, according to the results of ref.s [18,20–22], should extend above $\varepsilon \sim O(1)$. For the sake of space we report here only the running time averages of T_μ and T_{kin} for $\varepsilon = 10$ and for $N = 2^n, n = 5, \cdots, 9$ (see Fig. 1). Notice that both $\langle T_{kin}\rangle_t$ and $\langle T_\mu\rangle_t$ approach an asymptotic value depending on N: the former observable exhibits a fast convergence irrespectively of N, while the latter is characterized by wild fluctuations that tend to weaken for increasing values of N. Averaging over many different initial conditions allows one for reducing such wild fluctuations and to extract more reliable estimates of the asymptotic values attained by $\langle T_\mu\rangle_t$. Both "temperatures" are found to converge (from below and from above, respectively) to the same thermodynamic limit value ($T_\infty \approx 11.61$) with corrections of $O(1/N)$, as it should be expected on the basis of the ergodic theory (see Fig. 2). We have also checked that the corresponding variances $\mathcal{V}(T_{kin})$ and $\mathcal{V}(T_\mu)$ scale both like $1/N$ thus showing that they are characterized by robust statistical properties. It is worth stressing that even for such a high value of ε the model is far from ergodic in a strictly mathematical sense [21]. On the other hand, both temperatures seem to provide equally reliable thermodynamic predictions. We have verified that the same qualitative behaviour is observed for values of ε ranging in the interval (1, 100). On this basis one can state that, at least for high values of ε, the two definitions of temperature are thermodinamically (even if not dynamically) equivalent, while remarking that measurements of T_{kin} are much more efficient for any practical purpose.

A very different scenario is obtained for $\varepsilon \ll O(1)$, i.e. in the weakly chaotic regime. As an example, the running time averages of T_μ and T_{kin} for $\varepsilon = 0.01$ and $N = 128$ are shown in Fig. 3, for three different initial conditions. T_{kin} still fastly relaxes to an asymptotic value independently of the initial condition. Conversely, T_μ exhibits a dramatic dependence on the initial condition, despite its fluctuations are much less wild than in the strongly chaotic regime. The comparison between the two temperatures is quite illuminating. T_{kin} appears as a "good" thermodynamic observable that converges to its equilibrium value, irrespectively of ergodicity. In the perspective of the weak ergodic theorem by Khinchin [29] one would expect that at least the temporal autocorrelation function of T_{kin} decays to zero. The behaviour of T_μ clearly excludes this possibility, since its dependence on the initial conditions shows that the trajectories over which both quantities have been measured remain "trapped" for extremely long integration times in different regions of the phase space. As an illustration, in Fig.s 4 a,b we show the normalized temporal autocorrelation functions $C_\mu(t)$ and $C_{kin}(t)$ of the dynamical observables defining the two temperatures, for $\varepsilon = 0.01$ and $N = 128$. The corresponding power spectra clearly indicate that the dynamics amounts to a quasi-periodic motion with a few dominating harmonic components, whose frequencies and amplitudes depend on the initial conditions. If one looks at the explicit expressions for T_μ and T_{kin} this result appears much less mysterious: the former observable is sensitive to the geometry of the phase space (mainly depending on V) through its explicit dipendence on the q_i's, while the latter is sampled over the submanifold of the momenta p_i's that makes it insensitive to any geometrical intricacy of the phase space (a straightforward calculation shows that averaging T_{kin} over a quasiperiodic orbit yields the same prediction of equilibrium statistical mechanics).

The measurement of $C_\mu(t)$ and $C_{kin}(t)$ in the strongly chaotic regime provides additional elements of information, that confirm the previous conclusions and allow one for obtaining a quantitative characterization of the typical relaxation times of both temperatures to their equilibrium values. In all numerical simulations hereafter reported $C_\mu(t)$ and $C_{kin}(t)$ have been averaged over $5\cdot 10^5$ initial conditions. Typical results are shown in Fig.s 4 c,d for $\varepsilon = 10$ and $N = 256$. Both autocorrelation functions exhibit a fast exponential decay modulated by an oscillation that is rapidly damped for large times. At variance with $C_{kin}(t)$, $C_\mu(t)$ presents also a typical "hydrodynamic tail" that superposes to the exponential decay at large values of t. This shows that, even in the strongly chaotic regime, the two temperatures still exhibit quite different dynamical features that originate from their different geometrical nature, making them sensitive or insensitive to the geometrical structure of the phase space.

A systematic inspection in a wide range of ε in the strongly chaotic regime and for $N = 2^n, n = 5, \cdots, 9$ yields the following conclusions. The hull of the autocorrelation functions can be confidently fitted by the following laws

$$C_{kin}(t) = e^{-t/\tau_1} \tag{14}$$

$$C_\mu(t) = Ae^{-t/\tau_1} + \frac{1-A}{1+t/\tau_2} \tag{15}$$

where τ_1 is the same for both quantities and results to be independent of N, as well as τ_2, and A is just a normalization constant. The main outcome of this analysis is that, when varying ε in the strongly chaotic regime, τ_1 is found to obey the following remarkable scaling law

$$\tau_1 \propto (\varepsilon - \varepsilon_c)^{-1/2} \tag{16}$$

with $\varepsilon_c \approx 0.8$ (see Fig. 5). It is worth stressing that this result allows to locate unambigously the SST of the FPU β-model at a specific value of the energy density that agrees with all the estimates obtained by the methods mentioned in the Introduction. We want to observe that also τ_2 is found to diverge at ε_c, altough the poor numerical accuracy in fitting the "hydrodynamic" decay of $C_\mu(t)$ does not allow, in this case, to extract a clean scaling law.

The same analysis has been performed for the observables c_A, c_B and for the canonical specific heat per particle obtained in [25] as a function of the microcanonical fluctuations of the total kinetic energy K

$$c_{can} \simeq \left(2 - N\frac{\langle K^2\rangle - \langle K\rangle^2}{\langle K\rangle^2}\right)^{-1} \tag{17}$$

The running time averages of c_A and c_{can} exhibit behaviours very similar to those reported in Fig. 1 for T_μ and T_{kin}, respectively. For the sake of space, in Fig. 6 we simply report the scaling with N of the asymptotic values attained by c_A and c_{can}, that are found to converge to the same thermodynamic limit value c_∞. We have also looked at the temporal autocorrelation function of those observables, whose averages determine the expressions of the specific heats per particle. In practice, the only new interesting quantity, with respect to those already considered in the study of the temperatures, is the numerator of the fraction in eq.(7). We have verified that its autocorrelation functions coincide with those of T_μ for each value of ε. All these results indicate that these specific heats provide a scenario fully consistent with the temperatures analysis.

On the contrary, the running time averages of c_B are characterized by extremely wild fluctuations, that do not show any tendency to a smooth approach to the expected thermodynamic limit value over available time spans. This fact definitely enforce the conclusion that relaxation mechanisms may strongly depend on the very nature of the observable at hand.

IV. CONCLUSIONS AND PERSPECTIVES

Upon assuming ergodicity, thermodynamic variables in the microcanonical ensemble can be explicitly written as dynamical quantities, by exploiting standard methods of differential geometry. In the thermodynamic limit they can be shown to coincide with the corresponding quantities obtained in the canonical and gran-canonical ensembles (this can be easily checked at least for some basic quantities like temperature, specific heat etc.).

On the other hand, many degrees of freedom hamiltonian systems are known not to be ergodic even at high energies [21]. In particular, for sufficiently small energy densities such models exhibit quasi-periodic evolution along trajectories, that remain trapped inside some submanifold of the phase space for extremely long integration times. This peculiar dynamical feature is at the basis of the long-standing problem of “ergodicity threshold” raised by the celebrated paper of FPU [2] . An up to date summary of this problem is contained in the introduction.

In this paper we have pointed our attention on the FPU β-model, providing an unambiguous description of the Strong Stochasticity Threshold. This was obtained using the previously mentioned microcanonical observables as probes of ergodicity. In particular, this analysis allowed us for locating the SST at a finite value of the energy density $\varepsilon_c \simeq 0.8$, that results to be independent of N. It is worth stressing that this value agrees with rougher estimates still originating from the study of “geometrical” observables [18,22].

Moreover, the comparison with the corresponding canonical observables allows us for concluding that the crucial point about the ergodic hypothesis concerns the very nature of the observable and not just the features of the dynamics. Such a point of view was already raised by Khinchin [29], although we have shown that it may exist thermodynamic observables (like T_{kin} and c_{can}) that converge to the predictions of equilibrium statistical mechanics even when time averages are performed over highly non-chaotic evolutions, where the “weak ergodic theorem” by Khinchin does not certainly apply.

Let us finally observe that one can obtain other different dynamical expression for microcanonical observables by proper choices of the coordinates space representation. The only constraint for such a choice is to maintain invariant the flux through the constant energy surface. For instance, in case B, one could choose the vector $\eta = 1/2N(q_1, \cdots, q_N, p_1, \cdots, p_N)$, in such a way that the temperature depends also on the q_i coordinates. This arbitrariness, obviously, does not affect thermodynamic limit properties, since all expressions for the same observables coincide, while, dynamically, the scenario should not change significantly with respect to the one described in Section III.

Nonetheless a detailed investigation of these different choices can provide a deeper insight on the way "statistical fluctuations" can be consistently introduced in the microcanonical ensemble. This point goes beyond the aims of this paper and will be discussed elsewhere.

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APPENDIX A:

In this appendix we report a simple theorem of differential geometry that allows to express the derivatives of the entropy w.r.t. the energy E. Moreover, we give the explicit expressions for the temperature and of the quantities defining the specific heat of standard Hamiltonian (1).

Theorem: Consider Σ_E as a $(2N-1)$-dimensional hypersurface of R^{2N} parametrized by $H(x) = E$, where $H(x) : R^{2N} \to R$ is the Hamiltonian function in the Γ-space. Given a function $f(x) : R^{2N} \to R$, that is $C^{2N}(R^{2N})$, we let

$$\omega(E) = \int_{H=E} f(x) d\sigma \tag{A1}$$

where $d\sigma$ denotes the $(2N-1)$-dimensional measure. Suppose that it exists a constant $c > 0$ such that $||\nabla H|| = \langle \nabla H, \nabla H \rangle^{1/2} \geq c$. Then the following formula holds for the n-th derivative of $\omega(E)$:

$$\frac{d^n \omega}{dE^n} = \int_{H=E} A^n f(x) d\sigma \tag{A2}$$

where A^n denotes the n-th iterate of the operator A, defined by

$$Af(x) = \nabla \cdot \left(f(x) \frac{\nabla H}{||\nabla H||} \right) \frac{1}{||\nabla H||} \tag{A3}$$

Proof: It clearly sufficies to prove the result for $n = 1$. We assume, without loss of generality, that ∇H points towards the inside of the hypersurfaces parametrized by $H(x) = E$. Consider the difference quotient for $\omega(E)$

$$\frac{\omega(E+h) - \omega(E)}{h} = \frac{1}{h} \left[\int_{E+h} f(x) d\sigma - \int_E f(x) d\sigma \right] \tag{A4}$$

Exploiting the identity

$$1 = \frac{\nabla H \cdot \nabla H}{||\nabla H||^2}$$

and, remembering that $n(x) = \frac{\nabla H}{||\nabla H||}$ is the unit inner normal to Σ_E at point x, one can write

$$\begin{aligned} \frac{\omega(E+h) - \omega(E)}{h} &= \frac{1}{h} \left[\int_{E+h} f(x) \frac{\nabla H}{||\nabla H||} n d\sigma - \int_E f(x) \frac{\nabla H}{||\nabla H||} n d\sigma \right] \\ &= \frac{1}{h} \left[\int_{E+h} f(x) \frac{\nabla H}{||\nabla H||} n_e d\sigma + \int_E f(x) \frac{\nabla H}{||\nabla H||} n_e d\sigma \right] \end{aligned} \tag{A5}$$

where n_e is the unit normal pointing toward the exteriors of the annular region $\{x \in R^{2N} : E < H(x) < E + h\}$. We may now applay the divergence theorem to obtain

$$\frac{\omega(E+h)-\omega(E)}{h} = \frac{1}{h}\int_E^{E+h} \nabla \cdot \left(f(x)\frac{\nabla H}{||\nabla H||}\right) dx \tag{A6}$$

Finally, using the co-area formula (see [29]), we have

$$\frac{\omega(E+h)-\omega(E)}{h} = \frac{1}{h}\int_E^{E+h} dE' \int_{H=E'} \nabla \cdot \left(f(x)\frac{\nabla H}{||\nabla H||}\right) \frac{d\sigma}{\| \nabla H \|} \tag{A7}$$

and, taking the limit for $h \to 0$, we conclude that

$$\omega'(E) = \int_{H=E} \nabla \cdot \left(f(x)\frac{\nabla H}{||\nabla H||}\right) \frac{1}{||\nabla H||} d\sigma \qquad\qquad q.e.d. \tag{A8}$$

If we consider the theorem with

$$f(x) = \frac{1}{||\nabla H||}$$

and the cases $n = 1, 2$ we obtain the expressions that enter in the formula for temperature and specific heat given in the previous Sections. In particular:

$$\frac{\partial \omega}{\partial E} = \int_{H=E} \nabla \cdot \left(\frac{\nabla H}{\| \nabla H \|^2}\right) \frac{d\sigma}{\| \nabla H \|} \tag{A9}$$

$$\frac{\partial^2 \omega}{\partial E^2} = \int_{H=E} \nabla \cdot \left[\nabla \cdot \left(\frac{\nabla H}{\| \nabla H \|^2}\right) \frac{\nabla H}{\| \nabla H \|^2}\right] \frac{d\sigma}{\| \nabla H \|} \tag{A10}$$

In the case of standard Hamiltonian (1), for which one has $\partial H/\partial p_i = \partial V/\partial q_i = -F_i$ and $\partial H/\partial p_i = p_i$, the explicit dynamical expressions are:

$$\begin{aligned}\nabla \cdot \left(\frac{\nabla H}{\| \nabla H \|^2}\right) &= \frac{\triangle H}{||\nabla H||^2} + \nabla\left(\frac{1}{||\nabla H||^2}\right)\cdot \nabla H \\ &= \frac{N - \sum_{i=1}^N \frac{\partial F_i}{\partial q_i}}{\sum_{i=1}^N p_i^2 + F_i^2} + 2 \cdot \frac{\sum_{k=1}^N \sum_{i=1}^N F_k F_i \frac{\partial F_i}{\partial q_k} - \sum_{k=1}^N p_k^2}{(\sum_{i=1}^N p_i^2 + F_i^2)^2}\end{aligned} \tag{A11}$$

$$\nabla \cdot \left[\nabla \cdot \left(\frac{\nabla H}{\| \nabla H \|^2}\right) \frac{\nabla H}{\| \nabla H \|^2}\right] = \frac{(\triangle H)^2}{||\nabla H||^4} + \nabla\left(\frac{\triangle H}{||\nabla H||^4}\right)\cdot \nabla H + \triangle\left(\frac{1}{||\nabla H||^2}\right) \tag{A12}$$

$$\frac{(\triangle H)^2}{||\nabla H||^4} = \frac{\left(N - \sum_{i=1}^N \frac{\partial F_i}{\partial q_i}\right)^2}{\left(\sum_{i=1}^N p_i^2 + F_i^2\right)^2}$$

$$\begin{aligned}\nabla\left(\frac{\triangle H}{||\nabla H||^4}\right)\nabla H = &\frac{\left(\sum_{k=1}^N \sum_{i=1}^N F_k \frac{\partial^2 F_i}{\partial q_k \partial q_i}\right)}{\left(\sum_{i=1}^N p_i^2 + F_i^2\right)^2} \\ &+ 4 \cdot \frac{\left(N - \sum_{i=1}^N \frac{\partial F_i}{\partial q_i}\right)\left(\sum_{k=1}^N \sum_{i=1}^N F_k F_i \frac{\partial F_i}{\partial q_k} - \sum_{k=1}^N p_k^2\right)}{\left(\sum_{i=1}^N p_i^2 + F_i^2\right)^3}\end{aligned}$$

$$\begin{aligned}\triangle\left(\frac{1}{||\nabla H||^2}\right) &= -2 \cdot \frac{\left(N + \sum_{k=1}^N \sum_{i=1}^N (\frac{\partial F_i}{\partial q_k})^2 + (F_i \frac{\partial^2 F_i}{\partial q_k^2})\right)}{\left(\sum_{i=1}^N p_i^2 + F_i^2\right)^2} \\ &+ 8 \cdot \frac{\left(\sum_{k=1}^N p_k^2 + \sum_{k=1}^N \left(\sum_{i=1}^N F_i \frac{\partial F_i}{\partial q_k}\right)^2\right)}{\left(\sum_{i=1}^N p_i^2 + F_i^2\right)^3}\end{aligned}$$

Figure Captions

FIG. 1. Running time averages for the temperatures T_{kin} (solid lines) and T_{μ} (dot-dashed lines) for $\varepsilon = 10$ and $N = 2^n$, $n = 5, \cdots, 9$. Increasing N, T_{kin} (T_{μ}) better and better approximates the equilibrium expectation from below (above).

FIG. 2. The inverse reduced temperature IRT=$|T(N) - T_{\infty}|^{-1}$ versus N for $T_{\mu}(N)$ (circles) and $T_{kin}(N)$ (triangles). Solid lines are best fits.

FIG. 3. Running time averages for the temperatures T_{kin} (solid lines) and T_{μ} (dot-dashed lines) for $\varepsilon = 10^{-2}$, $N = 128$ and for three different initial conditions.

FIG. 4. The temporal autocorrelation functions of T_{kin} and T_{μ} for $N = 256$ and $\varepsilon = 10^{-2}$ (a and b, respectively) and for $\varepsilon = 10$ (c and d , respectively)

FIG. 5. Log-log plot of τ_1^{-2} versus $(\varepsilon - \varepsilon_c)$. The solid line is the best fit obtained assuming the otimal exstimate $\varepsilon_c = 0.79$.

FIG. 6. The inverse reduced specific heat IRC = $|c(N) - c_{\infty}|^{-1}$ versus N for $c_A(N)$ (circles) and $c_{can}(N)$ (triangles). Solid lines are best fits.

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