Analytic estimation of the Lyapunov exponent in a mean-field model undergoing a phase transition

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The parametric instability contribution to the largest Lyapunov exponent λ_1 is derived for a mean-field Hamiltonian model, with attractive long-range interactions. This uses a recent Riemannian approach to describe Hamiltonian chaos with a large number N of degrees of freedom. Through microcanonical estimates of suitable geometrical observables, the mean-field behavior of λ_1 is analytically computed and related to the second-order phase transition undergone by the system. It predicts that chaoticity drops to zero at the critical temperature and remains vanishing above it, with λ_1 scaling as $N^{-(1/3)}$ to the leading order in N. [S1063-651X(98)03506-5]

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I. INTRODUCTION

The largest Lyapunov exponent λ_1 is a good quantity to measure the degree of chaoticity of a generic nonintegrable Hamiltonian system. However, its numerical computation requires computing also the microscopic dynamics for a, sometimes, very long and, theoretically, infinite time. This may obviously turn rapidly difficult to tackle and much effort has been devoted to deriving some asymptotic scaling laws [1] and, more recently, to getting analytic estimates by relating microscopic dynamics with statistical averages, provided the number N of degrees of freedom is large enough [2–4]. This latter way of analytically computing λ_1 as a function of $\varepsilon = E/N$, the energy per degree of freedom, has proved to be remarkably efficient. It reformulates Hamiltonian dynamics in the language of Riemannian geometry, using the fact that the natural motions can be viewed as geodesics of a suitable Riemannian manifold [5]. Chaotic motion then reflects into the instability of the geodesic flow, which depends on curvature properties of the manifold. This geometric formulation of the dynamics has long been known and has led to fundamental results in abstract ergodic theory when the ergodicity of geodesic flows on compact manifolds of negative curvature was demonstrated by Hedlund and Hopf in 1939, and later exploited by Krylov [6]. However, when more physical Hamiltonian systems come into play, such as coupled nonlinear oscillators, a major source of chaos appears to be parametric instability activated by a fluctuating curvature along the geodesics, even when curvature is always positive [7,8]. This has been exploited in the theoretical model proposed by M. Pettini and co-workers. Modeling the effective curvature felt by a geodesic by a Gaussian stochastic process, with the mean the average Ricci curvature and variance its fluctuations, and under the ergodic hypothesis replacing the previous geometrical quantities with their averages κ_0 and σ_κ^2 according to the natural ergodic measure, i.e., in the microcanonical ensemble, they derive the following expression for λ_1 [2,3]:

$$\lambda_1 = \frac{\Lambda}{2} - \frac{2\kappa_0}{3\Lambda} \tag{1}$$

with

$$\Lambda = \left(2\sigma_\kappa^2 \tau + \sqrt{\frac{64}{27}\kappa_0^3 + 4\sigma_\kappa^4 \tau^2} \right)^{1/3} \tag{2}$$

and τ, a time scale for the stochastic process estimated as

$$\tau = \frac{\pi\sqrt{\kappa_0}}{2\sqrt{\kappa_0}\sqrt{\kappa_0 + \sigma_\kappa} + \pi\sigma_\kappa}. \tag{3}$$

In this article, we apply these geometrical tools to a mean-field Hamiltonian system of globally coupled rotators exhibiting a second-order phase transition at a certain critical energy ε_c. We analytically estimate the parametric instability contribution to $\lambda_1(\varepsilon)$ and predict a neat distinction between the two cases: $\varepsilon < \varepsilon_c$ and $\varepsilon > \varepsilon_c$. Numerical simulations [9,10] seem to qualitatively support the analytical conclusions. The remarkable behavior of the Lyapunov exponent in the mean-field limit, as a consequence of the simple expressions of relevant geometrical quantities as functions of the order parameter, could then be a dynamical signature of the phase transition.

The model at hand will be described in Sec. II and some useful geometric expressions derived there. A detailed derivation of the largest Lyapunov exponent λ_1 as a function of the energy density ε will be exposed in Sec. III, Sec. IV being devoted to comments and conclusions.

II. MEAN-FIELD MODEL AND FIRST USEFUL GEOMETRIC EXPRESSIONS

Here we study the so-called mean-field Hamiltonian X-Y model, which can be considered as a toy model for investigating long-range interactions in Coulomb systems [11,12]. The dynamics of N interacting particles moving on the unit circle $\Pi = [0;2\pi]$ derives from the following Hamiltonian:

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$$H=\sum_{l=1}^{N}\frac{p_l^2}{2}+\frac{c}{2N}\sum_{l,r=1}^{N}[1-\cos(q_l-q_r)]=K+V(q), \quad (4)$$

where K and V stand for the kinetic and the potential energy, respectively. Constant c may be rescaled to $+1$, 0, or -1 by a change of variables. The scaling factor $1/N$ for the potential energy ensures that the interaction energy is extensive and emphasizes its mean-field nature. Thus, in the following, we would not deal with the usual thermodynamic limit with fixed density, but rather with the mean-field limit $N\to\infty$, $H/N\to\varepsilon$, ε finite. Note that the total momentum is also a constant of the motion. However, this will not affect the following calculation since the potential only depends on positions.

The equilibrium statistical mechanics of this model can be exactly derived [13]. In the case of an attractive potential (i.e., $c>0$), which will be assumed in the following, that is, in the ferromagneticlike case, it predicts a second-order phase transition with order parameter $\|\mathbf{M}\|$ where $\mathbf{M}$ is the mean-field magnetizationlike variable defined as

$$\mathbf{M}=\left(\frac{1}{N}\sum_{l=1}^{N}\cos(q_l),\frac{1}{N}\sum_{l=1}^{N}\sin(q_l)\right). \quad (5)$$

This phase transition can be easily conjectured by observing that at small energy $\|\mathbf{M}\|=O(1)$ with a clustered phase, whereas at large energy, the central limit theorem predicts that $\|\mathbf{M}\|=O(N^{-(1/2)})$ with particles having random ballistic motions. It is also interesting to note that introducing the global variable $\mathbf{M}$ enables us to reexpress the equation of motion of any particle as

$$\ddot{q}_i=-c\|\mathbf{M}\|\sin(q_i-\phi) \quad \text{where} \quad \phi=\arg(\mathbf{M}), \quad (6)$$

that is, the equation of a perturbed pendulum, the full system being closed by adding the evolution equations for $\|\mathbf{M}\|$ and ϕ.

Let us now first express in the framework of the Eisenhart metric the Ricci curvature associated to this system, then derive the microcanonical averages of the geometrical quantities involved, via the canonical ensemble, which leads to simpler calculations. Recall here that in the limit of infinite size, that is, $N\to\infty$, the averages of thermodynamic observables in different ensembles coincide [14], but not their fluctuations [15]. Therefore, in order to get the fluctuations of an observable f in the microcanonical ensemble, it will be necessary to add a corrective term according to the formula derived in [16], which is not valid at the critical point:

$$\langle\delta^2 f\rangle_\mu=\langle\delta^2 f\rangle_c+\left(\frac{\partial\langle\varepsilon\rangle_c}{\partial\beta}\right)^{-1}\left[\frac{\partial\langle f\rangle_c}{\partial\beta}\right]^2, \quad (7)$$

where [17]

$$\langle\delta^2 f\rangle\equiv\frac{1}{N}\langle(f-\langle f\rangle)^2\rangle. \quad (8)$$

So, with the Eisenhart metric, the Ricci curvature reads $K_R(q)=\Delta V$, where Δ stands for the Euclidian Laplace operator in the configuration space, so that the average Ricci curvature [3], defined as $k_R(q)\equiv[K_R(q)/N-1]$, is

$$k_R(q)=\frac{1}{N-1}\sum_{i=1}^{N}\frac{\partial^2 V(q)}{\partial q_i^2}=c-\frac{2}{N-1}V(q). \quad (9)$$

Moreover, a straightforward calculation gives

$$V(q)=\frac{cN}{2}(1-\|\mathbf{M}\|^2). \quad (10)$$

Thus we obtain the key expression that the mean Ricci curvature reads simply in terms of the order parameter, the mean-field magnetization $\mathbf{M}$ as

$$k_R=c\|\mathbf{M}\|^2 \quad (11)$$

up to a $O(N^{-1})$ term, which, as far as the mean-field limit is concerned, gives a vanishing contribution and will be ignored. It will only play a part in corrections above the transition. It should be pointed out that this expression for the mean Ricci curvature as a smooth function of the natural order parameter, the magnetization, is not claimed here (since not proved) to be a generic property of, for instance, some class of mean-field Hamiltonian systems. At present we should thus consider the results obtained in this article as peculiar features of the model at hand. As only positions-involving quantities come into play, let us now focus on the contribution of the potential energy to the partition function in the canonical ensemble at temperature $T=\beta^{-1}$ (with $k_B=1$):

$$\begin{aligned}Z_c(\beta)&=\int_{\Pi^N}\exp[-\beta V(q)]d^N q\\&=\exp\left(-\beta\frac{cN}{2}\right)\int_{\Pi^N}\exp\left(\beta\frac{cN}{2}\|\mathbf{M}\|^2\right)d^N q.\end{aligned}$$

Then, using the integral representation of Gaussian functions, we get

$$\begin{aligned}Z_c(\beta)&=\exp\left(-\beta\frac{cN}{2}\right)\int_{\Pi^N}\frac{1}{\pi}\\&\quad\times\left[\int_{\mathbb{R}^2}\exp(-\mathbf{u}^2+2\sqrt{\beta(cN/2)}\,\mathbf{u}\cdot\mathbf{M})d\mathbf{u}\right]d^N q\\&=\exp\left(-\beta\frac{cN}{2}\right)\frac{(2\pi)^N}{\pi}\int_{\mathbb{R}^2}\exp(-\mathbf{u}^2)\\&\quad\times[I_0(2\sqrt{\beta(c/2N)}\|\mathbf{u}\|)]^N d\mathbf{u}\\&=(2\pi)^N\frac{N}{\beta c}\int_0^\infty r\,dr\exp[-N\psi(r,\beta)]\end{aligned}$$

where $\psi(r,\beta)\equiv r^2/2\beta c-\ln[I_0(r)]+\beta c/2$ and where I_n stands for the modified Bessel function of order n.

Then, according to the saddle-point method, in the limit $N\to\infty$ the previous integral is fully dominated by the minimum of ψ obtained by solving the consistency equation $\partial_r\psi(r,\beta)=0$, that is,

$$\frac{r}{\beta c}-\frac{I_1(r)}{I_0(r)}=0. \quad (12)$$

When $\beta c<2$, ψ is minimal for $r=0$, which corresponds to a vanishing magnetization. For $\beta c>2$, Eq. (12) admits a nonvanishing solution noted $r^*(\beta)$, the phase transition taking place for $\beta c=2$, i.e., for $T_c=c/2$ and $\varepsilon_c=3c/4$.

Before examining these two cases, we establish some useful canonical relations: as $\langle V(q)\rangle_c=-\partial_\beta \ln(Z_c)$ and $\langle (V(q)-\langle V(q)\rangle)^2\rangle_c=\partial_\beta^2 \ln(Z_c)$, one obtains, respectively,

$$\langle k_R\rangle_c=c+\frac{2}{N}\partial_\beta \ln(Z_c), \tag{13}$$

$$\langle \delta^2 K_R\rangle_c\equiv\frac{1}{N}\langle (K_R-\langle K_R\rangle)^2\rangle_c=\frac{4}{N}\partial_\beta^2 \ln(Z_c). \tag{14}$$

Moreover the energy density $\varepsilon(\beta)$ is given by

$$\varepsilon(\beta)=\frac{1}{2\beta}-\frac{1}{N}\partial_\beta(\ln Z_c). \tag{15}$$

In the following, when dealing with microcanonical estimates, this expression will be implicitly systematically used to express β as a function of the energy density. We define also the two notations $\kappa_0\equiv\langle k_R\rangle_\mu$ and $\sigma_\kappa^2\equiv\langle \delta^2 K_R\rangle_\mu$.

III. ANALYTIC ESTIMATE FOR λ_1 BELOW AND ABOVE THE TRANSITION

Let us now derive the analytic estimate for λ_1 below and above the transition. Below the critical energy, the saddle-point method gives

$$Z_c(\beta)\simeq(2\pi)^N\frac{Nr^*}{\beta c}\exp[-N\psi(r^*,\beta)]\sqrt{\frac{2\pi}{N\partial_r^2\psi(r^*,\beta)}}. \tag{16}$$

As the ensemble averages $\langle k_R\rangle_c$ and $\langle k_R\rangle_\mu$ coincide in the mean-field limit, this gives

$$\langle k_R\rangle_\mu=c+\frac{2}{N}\partial_\beta \ln(Z_c)\sim c-2\partial_\beta[\psi(r^*(\beta),\beta)]$$
$$=c-2\frac{dr^*}{d\beta}\partial_r\psi|_{r*}-2\partial_\beta\psi|_{r*}=c-2\left(-\frac{r^{*2}}{2\beta^2 c}+\frac{c}{2}\right);$$

that is,

$$\langle k_R\rangle_\mu\sim\frac{r^*(\beta)^2}{c\beta^2}. \tag{17}$$

Remember that k_R is proportional to the square norm of the magnetization (11) so that we expect it to exhibit the same behavior at the transition point with twice the characteristic exponent. Actually, a straightforward expansion near the transition leads to

$$\langle k_R\rangle_\mu\sim\frac{2(\beta c-2)}{\beta}=\frac{8}{1+4c}(\varepsilon_c-\varepsilon)\quad \text{for}\quad \varepsilon_c\gtrsim\varepsilon.$$

Taking into account the correction (7) and noting that $\partial_\beta\langle k_R\rangle_c=\frac{1}{2}\langle \delta^2 K_R\rangle_c$, one finally obtains

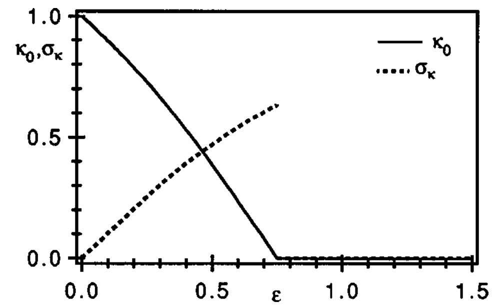

FIG. 1. Analytic expressions for the microcanonical averages of the average Ricci curvature κ_0 (solid curve) and of its fluctuations σ_κ (dot-dashed curve) in the mean-field limit, below and above the phase transition.

$$\langle \delta^2 K_R\rangle_\mu=\langle \delta^2 K_R\rangle_c\left(1+\frac{\beta^2}{2}\langle \delta^2 K_R\rangle_c\right)^{-1} \tag{18}$$

with $\langle \delta^2 K_R\rangle_c=4/N\partial_\beta^2\ln(Z_c)\sim 4r^*/\beta^2 c(\partial_\beta r^*-r^*/\beta)$.

Figure 1 displays the behaviors of both the average Ricci curvature κ_0 and fluctuations σ_κ, with the control parameter c set equal to 1 in both figures. Using Eqs. (17) and (18), one can then derive $\lambda_1(\varepsilon)$ in the clustered phase. The result, obtained through Eqs. (1–3), is reported in Fig. 2. When ε approaches ε_c, expanding the expression for the largest Lyapunov exponent $\lambda_1(\varepsilon)$ provides the scaling law

$$\lambda_1(\varepsilon)\propto(\varepsilon_c-\varepsilon)^{1/6}, \tag{19}$$

associating thereby a critical exponent, equal to 1/6, to the dynamical observable λ_1. Above the critical energy, one obtains, in the same way,

$$Z_c(\beta)\simeq(2\pi)^N\exp\left(-N\frac{\beta c}{2}\right)\left(1-\frac{\beta c}{2}\right)^{-1}. \tag{20}$$

Here, as $\|\mathbf{M}\|^2$ becomes of order $O(N^{-1})$, we shall use the full expression $k_R=c\|\mathbf{M}\|^2-c/N+O(N^{-2})$. Then

$$\langle k_R\rangle_\mu=\frac{\beta c^2}{N(2-\beta c)}+O(N^{-2}), \tag{21}$$

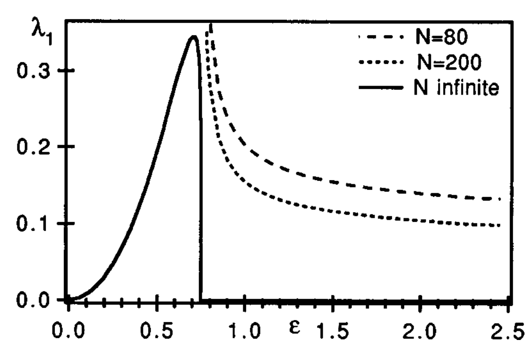

FIG. 2. Analytic expression for the largest Lyapunov exponent λ_1 in the mean-field limit (solid curve) below and above the phase transition. Analytic corrections (dot-dashed curves) to the mean-field limit for finite N with $N=80$ and $N=200$ above ε_c. Here the derivation is not restricted to the leading term (23) but computes Eqs. (1–3) up to further orders, as N is not very large. There is a nice fit with results exposed in [10] apart from the vicinity of the critical energy.

i.e., the microcanonical average of the Ricci curvature vanishes in the mean-field limit. Similarly,

$$\langle \delta^2 K_R \rangle_c = \frac{4}{N} \partial_\beta^2 \ln(Z_c) = \frac{4c^2}{N}(2-\beta c)^{-2} = O(N^{-1}).$$

As $\varepsilon(\beta) \sim (1/2\beta) + (c/2)$, the correcting term needed to get the microcanonical fluctuations is of order N^{-2}, thus negligible. Then

$$\langle \delta^2 K_R \rangle_\mu \sim \frac{4c^2}{N}(2-\beta c)^{-2} = O(N^{-1}). \tag{22}$$

We can keep in further calculations the dominant order in N, and derive the scaling law with N for the largest Lyapunov exponent. Using expressions (1–3), in the limit $N \to \infty$, one obtains

$$\lambda_1 \sim \frac{4^{1/3} c \sqrt{\beta c}}{(2-\beta c)^{3/2}} N^{-(1/3)}. \tag{23}$$

IV. COMMENTS AND CONCLUSIONS

Let us first comment here on the reliability expected for the expressions just derived. As developed in Refs. [2–5], the geometrical approach aims at extracting information on, at least, an average degree of chaoticity of the dynamics from mean global geometrical properties of the Riemannian manifold constructed from a given Hamiltonian. This implies the crucial assumption of ergodicity as a way of bypassing the knowledge of the trajectories, i.e., the numerical integration of the equations of motion. This ergodic hypothesis is not expected to be realized in the integrable limits of small and large energy, the latter following from the boundedness of the potential energy in Eq. (4). However, it is well known that chaos is not a necessary condition for ergodicity, the most striking piece of evidence being provided by the ideal gas of point particles, for which there is no velocity mixing at all. Also, recent studies [18] have emphasized that ergodiclike properties should depend mainly on the observable at hand, irrespective of the degree of chaoticity of the dynamics. Concerning our model, Ruffo already observed in [12] a good agreement between Gibbsian predictions and numerical simulations for the observable $\|\mathbf{M}\|$. Moreover, in the mean-field limit, this happens even in the integrable limit of large energy, an explanation for this being provided by a result of Kac [12,19], so that the mean-field magnetization appears like a good observable with respect to ergodicity. Therefore it is not surprising to observe that numerical calculations of the mean Ricci curvature and its variance fit well the microcanonical predictions presented in Fig. 1 [9,20], except in the vicinity of the phase transition where finite-N effects dominate. Concerning the transition region, as noted before, the formula [16] used to get fluctuations in the microcanonical ensemble from canonical ones is not valid at the critical energy. Therefore we should exclude in our conclusions a small neighborhood of ε_c, all the smaller as N is large. So the analytic estimate for $\lambda_1(\varepsilon)$ in the mean-field limit is expected to be quite reliable except maybe for small ε and in the vicinity of ε_c. It should also be noted that the time scale τ estimated as Eq. (3), that is, the time under which the effective curvature felt by a geodesic cannot be regarded as a random process, is the less solid point of the geometrical modeling [3,4] as Eq. (3) relies mainly on phenomenological arguments. Then it can, if necessary, be slightly adjusted to fit numerical calculations. Nonetheless, that estimate for τ is also a powerful tool, as it provides a natural time scale, depending on ε, that should be taken into account to connect, for instance, results for mappings [1] to results for continuous flows as is the case here.

Keeping these remarks in mind, we can now comment on the results obtained in Sec. III. Expression (23) means that, in this mean-field model, above the critical energy, chaos does not survive to the limit $N \to \infty$. This can be conjectured straightforwardly from the equation (6) governing the time evolution of any particle, which predicts ballistic motion as $\|\mathbf{M}\|$ vanishes above ε_c. Moreover, one obtains the scaling law $N^{-(1/3)}$ for the largest Lyapunov exponent to the leading order in N. The same scaling law has been found numerically by Latora, Rapisarda, and Ruffo [9]. A rather nice fit (see Fig. 2) is also obtained with Yamaguchi's simulations [10] on a wide range of ε, except in the vicinity of ε_c, where finite size effects smooth the transition. Here strong metastability related to critical slowing down may also affect numerical results with relaxation times towards equilibrium increasing greatly with N. Besides, for a given N large enough, expression (23) rightly gives a vanishing Lyapunov exponent in the integrable limit of large energy where rotators tend to behave as free particles.

Concerning the transition region, in spite of the above mentioned remarks on the validity of our results at the critical energy, let us mention the remarkable features exhibited by Figs. 1 and 2: κ_0, σ_κ, and λ_1 display singular behaviors at the critical point. Here curvature fluctuations exhibit a discontinuity that is similar to the ''cusp'' numerically observed in [4]. In our case, this appears as a direct consequence of the second-order phase transition exhibited by the model and, following Eq. (11), of the expressions of the different parameters used in the geometrical approach in terms of smooth functions of the order parameter. Following conjectures exposed in [4], the geometrical meaning of these singular behaviors might be that a topology change of the ''mechanical'' manifold underlying the dynamics occurs at the critical energy.

Finally, as for λ_1, its maximal value would be reached slightly below the critical point and not at the critical point. Numerical simulations made in [9] for 20 000 particles show such a tendency. Moreover, when ε approaches the critical energy, calculations (19) show that λ_1 goes to 0 as $(\varepsilon_c - \varepsilon)^{1/6}$. This suggests that a critical exponent could be associated to the largest Lyapunov exponent as a dynamical observable.

Further studies should inspect more precisely the region where the amplitudes of the curvature and fluctuations are comparable, around $\varepsilon = 0.45$ (see Fig. 1). As observed in other models, for such a situation strong stochasticity may be expected. A more refined treatment may imply some corrections to the Gaussianity of the effective curvature, which would take into account further moments of the mean Ricci curvature. Also, the vicinity of the critical energy, as well as a possible extension of the results obtained in this article to a larger class of mean-field Hamiltonian systems deserve, obviously, further investigations.

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