Theoretical estimates for the largest Lyapunov exponent of many-particle systems

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The largest Lyapunov exponent of an ergodic Hamiltonian system is the rate of exponential growth of the norm of a typical vector in the tangent space. For an N-particle Hamiltonian system with a smooth Hamiltonian of the type $p^2+\mathcal{V}(q)$, the evolution of tangent vectors is governed by the Hessian matrix $\mathbf{V}$ of the potential. Ergodicity implies that the Lyapunov exponent is independent of initial conditions on the energy shell, which can then be chosen randomly according to the microcanonical distribution. In this way, a stochastic process $\mathbf{V}(t)$ is defined, and the evolution equation for tangent vectors can now be seen as a stochastic differential equation. An equation for the evolution of the *average squared norm* of a tangent vector can be obtained using the standard theory in which the average propagator is written as a cumulant expansion. We show that if cumulants higher than the second one are discarded, the Lyapunov exponent can be obtained by diagonalizing a small-dimension matrix that in some cases can be as small as 3×3. In all cases, the matrix elements of the propagator are expressed in terms of correlation functions of the stochastic process. We discuss the connection between our approach and an alternative theory, the so-called geometric method.

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I. INTRODUCTION

The largest Lyapunov exponent measures the sensitivity to initial conditions in a dynamical system. In low-dimensional models, the Lyapunov exponent sets a limit to the prediction of the time evolution of a given state of the system. In the high-dimensional systems encountered in thermodynamics, one abandons from the start a description in terms of single (microscopic) states, and resorts to a statistical approach. In these cases a positive Lyapunov exponent is usually welcome, as it is a necessary condition for the validity of the Boltzmann-Gibbs scenario. A Lyapunov exponent that becomes null in the thermodynamic limit is a signal of anomalous behaviors. For instance, metastable phases of some long-range interacting systems, where the Lyapunov exponent vanishes in the large N limit, exhibit breakdown of ergodicity, anomalous diffusion, and non-Maxwell velocity distributions [1]. An extension of standard statistical mechanics is required for the theoretical explanation of such phenomena [2].

In many-particle systems, the Lyapunov exponent is also an indicator (order parameter) of phase transitions [3–5] and may be related to transport coefficients [6,7].

In practice, for a given system, the largest Lyapunov exponent must be obtained through numerical simulations, typically using the method developed by Benettin *et al.* [8] (a proof that this method gives the Lyapunov exponent of Oseledec's theorem [9] can be found in Ref. [10]). For some special cases, e.g., hard-sphere systems, the theory of Lyapunov exponents is remarkably developed [11]. This contrasts with the situation in smooth Hamiltonian systems, where comprehensive analytical estimates are scarce. In 1984, when studying two-dimensional billiards, Benettin made the first step towards the construction of random matrix methods for modeling *universal* features of Lyapunov spectra [12]. These methods were further developed by other authors and applied to many-particle smooth Hamiltonians [13].

To our knowledge, the first theory for estimating the largest Lyapunov exponent of a specific Hamiltonian system, and its dependence on the system parameters, was formulated by Pettini and co-workers some years ago [14,15]. In this approach, the dynamics is geometrized by absorbing the force terms into a suitable metric, thus mapping the Hamiltonian problem onto a geodesic motion on a curved manifold. After making the ''quasi-isotropy'' approximation, the Hamilton equations for the tangent vectors become decoupled. As a consequence, the initial system of $2N$ differential equations has been reduced to only two equations. While the original problem was governed by the Hessian matrix of the potential, of size $N\times N$, the new (reduced) one is controlled by the Laplacian of the potential, $\triangle\mathcal{V}(t)$, a scalar function of time. Thereafter, $\triangle\mathcal{V}(t)$ is treated as Gaussian white noise and the 2×2 system of differential equations is solved using the methods developed by van Kampen and others [16]. See Ref. [15] for a review.

When applied to a Fermi-Pasta-Ulam chain [17], the so-called ''geometric method'' was extremely successful in reproducing the largest Lyapunov exponent over the entire energy range [15]. However, in other cases the agreement is not so good. For instance, in a chain of rotators with first-neighbor (bounded) interactions, the method works well only in the low- and high-energy regimes, where the dynamics is weakly chaotic (integrable in the limits $E\to0,\infty$). In the intermediate region of stronger chaos, the theory has to be amended to obtain a good agreement with simulations [15]. This and other examples [5,18] raise several questions concerning the domain of validity of the theory. What is the nature of the quasi-isotropic approximation? Or, what are the parameters that control the quality of the estimates of the theory? Is the geometric method perturbative? If so, what are the next leading corrections?

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In this paper we present an alternative theoretical approach in which the validity domains of the successive approximations can be precisely delimited. The basic idea is to employ van Kampen's methods [16] to solve the *original* system of $2N$ differential equations for the evolution of tangent vectors. By applying this scheme to a three-dimensional dilute gas, Barnett *et al.* [7] established a link between the Lyapunov exponent and the self-diffusion coefficient (see also Ref. [19]). We show that this approach can be extended to reach other systems, such as the Fermi-Pasta-Ulam chains and lattices of classical spins, either with short- or long-range interactions. By doing so, we shall settle down a connection with the results of the geometric method and suggest some answers to the above-mentioned questions.

The paper has been organized as follows. Section II presents the theory that leads to an estimate of the largest Lyapunov exponent. This is a perturbative theory that rests on a cumulant expansion. We argue that the general (perturbative) solution can be obtained by diagonalizing a small-dimension matrix. In Sec. III we analyze an approximation that reduces the problem to diagonalizing a 3×3 matrix. Section IV discusses some examples that illustrate the working of the theory. The connection between our results and those obtained by the geometric method is discussed in Sec. V. Finally, Sec. VI contains the concluding remarks.

II. THEORY

The theory we present in this section can, in principle, be applied to any smooth Hamiltonian system. For simplicity, and for the sake of comparisons with the geometric method, we restrict ourselves to the ''natural'' Hamiltonians

$$\mathcal{H}=\sum_{i=1}^{N}\frac{p_i^2}{2m}+\mathcal{V}(q_1,\ldots,q_N), \tag{1}$$

where q_i and p_i are conjugate position-momentum coordinates. Other Hamiltonians can be considered but they may require modifications of the theory.

The Hamilton equations can be written in the compact form

$$\dot{x}=\mathbf{J}\frac{\partial\mathcal{H}}{\partial x}, \tag{2}$$

where we have introduced the $2N$-dimensional column vector x, $x=(q_1,\ldots,q_N,p_1,\ldots,p_N)^T$, the superscript meaning ''transposed,'' and the symplectic matrix $\mathbf{J}$ being

$$\mathbf{J}=\begin{pmatrix}0 & \mathbb{1}\\ -\mathbb{1} & 0\end{pmatrix} \tag{3}$$

with $\mathbb{1}$ being the $N\times N$ identity matrix. Differentiating the Hamilton equations, one obtains the evolution equations for tangent vectors $\xi=(\delta q_1,\ldots,\delta q_N,\delta p_1,\ldots,\delta p_N)^T$,

$$\dot{\xi}=\mathbf{A}(t)\xi. \tag{4}$$

For a Hamiltonian of the special form (1), and setting $m=1$, the operator $\mathbf{A}$ has the simple structure

$$\mathbf{A}(t)=\begin{pmatrix}0 & \mathbb{1}\\ -\mathbf{V}(t) & 0\end{pmatrix}. \tag{5}$$

Here $\mathbf{V}$ is the Hessian matrix of the potential $\mathcal{V}$, namely,

$$V_{ij}=\frac{\partial^2\mathcal{V}}{\partial q_i\partial q_j}. \tag{6}$$

Once initial conditions x_0 and ξ_0 have been specified, Eqs. (2) and (4) allow one to find the Lyapunov exponent λ by calculating the limit [8]

$$\lambda=\lim_{t\to\infty}\frac{1}{2t}\ln|\xi(t;x_0,\xi_0)|^2. \tag{7}$$

We will assume that for any initial condition x_0, the phase-space trajectory $x(t;x_0)$ is ergodic on its energy shell. This implies that λ is independent of initial conditions x_0, which can then be chosen randomly according to the microcanonical distribution. There will also be no dependence on initial tangent vectors, because if ξ_0 is also chosen randomly, it will have a nonzero component along the most expanding direction.

If the corrections to the exponential law in Eq. (7) go to zero fast enough as $t\to\infty$, one can also write

$$\langle|\xi(t;x_0,\xi_0)|^2\rangle\propto e^{2\lambda t}, \tag{8}$$

where the brackets mean microcanonical averages over x_0. We will prefer the estimate of Eq. (8) because the averaging procedure is crucial for finding an analytical expression for the Lyapunov exponent. In case of doubt, the equality of the exponents defined by Eqs. (7) and (8) can be tested numerically, e.g., using the data generated by Benettin's algorithm.

By letting x_0 be a random variable, a stochastic process $\mathbf{V}(t;x_0)$ is defined, and Eq. (4) can be thought as a stochastic differential equation. However, the quantity we are interested in is the square of the norm of ξ, which can be written as the trace of the ''density matrix'' $\xi\xi^T$. Thus, we must focus on the equation for the evolution of $\xi\xi^T$:

$$\frac{d}{dt}(\xi\xi^T)=\mathbf{A}\xi\xi^T+\xi\xi^T\mathbf{A}^T\equiv\hat{\mathbf{A}}\xi\xi^T, \tag{9}$$

the rightmost identity defining the linear superoperator $\hat{\mathbf{A}}$. Except for the fact that we must deal now with a superoperator, Eq. (9) is not different from Eq. (4), and can be handled with the same techniques. For the purpose of the perturbative approximations that will follow, the operator $\hat{\mathbf{A}}$ is split into two parts:

$$\hat{\mathbf{A}}=\hat{\mathbf{A}}_0+\hat{\mathbf{A}}_1(t), \tag{10}$$

where $\hat{\mathbf{A}}_0$ corresponds to the evolution in the absence of interactions. In our case, $\hat{\mathbf{A}}_0$ and $\hat{\mathbf{A}}_1$ are associated with

$$\mathbf{A}_0=\begin{pmatrix}0 & \mathbb{1}\\ 0 & 0\end{pmatrix} \quad \text{and} \quad \mathbf{A}_1=\begin{pmatrix}0 & 0\\ -\mathbf{V}(t) & 0\end{pmatrix}, \tag{11}$$

respectively. Whenever $\mathbf{A}_1(t)$ is small (in a sense that will be discussed below), it is possible to manipulate Eq. (9) to derive an explicit expression for the evolution of the *average* of $\xi\xi^T$. A clear exposition of this derivation, together with a very detailed discussion of its domain of validity has been given by van Kampen [16]. We just outline the basic steps: (a) Rewrite Eq. (9) in the interaction representation associated with $\hat{\mathbf{A}}_0$. (b) Write the propagator as a time ordered exponential. (c) Expand its average in a series of cumulants. (d) Go back to the original representation. The final result is

$$\langle \xi\xi^T\rangle(t)=e^{t\hat{\mathbf{\Lambda}}}\xi_0\xi_0^T, \tag{12}$$

where $\hat{\mathbf{\Lambda}}$ is a time-independent superoperator given by the perturbative expansion

$$\hat{\mathbf{\Lambda}}\equiv\hat{\mathbf{A}}_0+\langle\hat{\mathbf{A}}_1\rangle+\int_0^\infty d\tau\langle\delta\hat{\mathbf{A}}_1(t)e^{\tau\hat{\mathbf{A}}_0}\delta\hat{\mathbf{A}}_1(t-\tau)e^{-\tau\hat{\mathbf{A}}_0}\rangle+\cdots \tag{13}$$

with

$$\delta\hat{\mathbf{A}}_1(t)=\hat{\mathbf{A}}_1(t)-\langle\hat{\mathbf{A}}_1\rangle. \tag{14}$$

Let $L_{\max}$ be the eigenvalue of $\hat{\mathbf{\Lambda}}$ which has the largest real part. We find that the largest Lyapunov exponent λ is related to the real part of $L_{\max}$:

$$\lambda=\tfrac{1}{2}\mathrm{Re}(L_{\max}). \tag{15}$$

In Eq. (13) we give explicitly only the first two cumulants, the dots stand for third cumulants and higher-order ones. The perturbative parameter can be understood as the product of two quantities. The first one, let us call it σ, characterizes the amplitude of the fluctuations of $\delta\hat{\mathbf{A}}_1(t)$. The second, τ_c, is a typical (the largest relevant) correlation time of $\delta\hat{\mathbf{A}}_1(t)$. Thus, the second cumulant is of the order of $\sigma^2\tau_c$, the third one is of the order of $\sigma^3\tau_c^2$, and so on. If all cumulants were summed up, Eq. (12) would be exact in the long-time regime $t\gg\tau_c$ [16].

From now on, we restrict our analysis to the propagator $\hat{\mathbf{\Lambda}}$ truncated at the second order, i.e., Eq. (13) without the dots. This approximation will be better for smaller values of $\sigma\tau_c$. However, if $\hat{\mathbf{A}}_1(t)$ is not far from a Gaussian process, the validity of the second-order approximation may extend outside the perturbative region $\sigma\tau_c\ll 1$. In the exceptional case that $\hat{\mathbf{A}}_1(t)$ is a Gaussian process, cumulants higher than the second one will be strictly zero and the truncation will introduce no error.

To proceed further, one needs the matrix of $\hat{\mathbf{\Lambda}}$ in some basis. So, let us calculate $\hat{\mathbf{\Lambda}}\mathbf{M}$, $\mathbf{M}$ being a symmetric matrix (it is easy to see that the truncation has not spoiled the symmetry of the density matrix). First, notice that the exponentials of $\hat{\mathbf{A}}_0$ represent no problem as they are finite polynomials,

$$e^{\tau\hat{\mathbf{A}}_0}\mathbf{Q}=[\mathbb{1}+\tau\mathbf{A}_0]\mathbf{Q}[\mathbb{1}+\tau\mathbf{A}_0^T] \tag{16}$$

for any matrix $\mathbf{Q}$. Inserting this expression into Eq. (13), we arrive at

$$\hat{\mathbf{\Lambda}}\mathbf{M}=(\mathbf{A}_0+\langle\mathbf{A}_1\rangle)\mathbf{M}+\int_0^\infty d\tau\langle\delta\mathbf{A}_1(t)[\delta\tilde{\mathbf{A}}_1(t-\tau)\mathbf{M}+\mathbf{M}\delta\tilde{\mathbf{A}}_1^T(t-\tau)]\rangle+(\cdots)^T, \tag{17}$$

where $(\cdots)^T$ means "the previous terms transposed," and

$$\delta\tilde{\mathbf{A}}_1(t-\tau)=[\mathbb{1}+\tau\mathbf{A}_0]\delta\mathbf{A}_1(t-\tau)[\mathbb{1}-\tau\mathbf{A}_0]. \tag{18}$$

Substituting Eq. (11) into Eq. (17), we arrive at the final result of the second-order perturbative approach,

$$\begin{aligned}\hat{\mathbf{\Lambda}}\mathbf{M}=&\begin{pmatrix}0 & \mathbb{1}\\ -\langle\mathbf{V}\rangle & 0\end{pmatrix}\mathbf{M}+\int_0^\infty d\tau\begin{pmatrix}0 & 0\\ \tau & -\tau^2\end{pmatrix}\\ &\times\begin{pmatrix}\langle\delta\mathbf{V}\delta\mathbf{V}'\rangle & 0\\ 0 & \langle\delta\mathbf{V}\delta\mathbf{V}'\rangle\end{pmatrix}\mathbf{M}\\ &+\int_0^\infty d\tau\left\langle\begin{pmatrix}0 & 0\\ \delta\mathbf{V} & 0\end{pmatrix}\mathbf{M}\begin{pmatrix}\delta\mathbf{V}' & 0\\ 0 & \delta\mathbf{V}'\end{pmatrix}\right\rangle\begin{pmatrix}\tau & \mathbb{1}\\ -\tau^2 & -\tau\end{pmatrix}\\ &+(\cdots)^T.\end{aligned} \tag{19}$$

To abbreviate the notation, we have written τ^n instead of $\tau^n\mathbb{1}$; $\delta\mathbf{V}$ and $\delta\mathbf{V}'$ substitute $\delta\mathbf{V}(t)$ and $\delta\mathbf{V}(t-\tau)$, respectively.

The largest Lyapunov exponent is buried into Eq. (19). To get an explicit expression, one must diagonalize the matrix of $\hat{\mathbf{\Lambda}}$. The outcome will be λ as a function of the first two cumulants of the stochastic process $\mathbf{V}(t)$, i.e., averages and (integrated) two-time correlation functions:

$$\langle V_{ij}\rangle;\ \int_0^\infty d\tau\,\tau^n\langle\delta V_{ij}(0)\delta V_{kl}(\tau)\rangle,\quad n=0,1,2. \tag{20}$$

At first sight it may be thought that as $\hat{\mathbf{\Lambda}}$ is a superoperator, the matrix one should diagonalize is of the order of $N^2\times N^2$, then straightforward diagonalization would be out of the question for large N. Notwithstanding, $\hat{\mathbf{\Lambda}}$ is an averaged object, and as such, it possesses some symmetries that can be exploited to reduce the dimensionality of the problem to tractable levels, say $N\times N$. This will be illustrated with an example in Sec. IV. So, if desired, the largest Lyapunov exponent could be found by numerical diagonalization, at least for systems with $N\approx 1000$ degrees of freedom (provided one can estimate the correlation functions).

An alternative to exact diagonalization is the approximate diagonalization, i.e., the diagonalization of the restriction of $\hat{\mathbf{\Lambda}}$ to some small-dimension subspace. Notice that the problem we are dealing with is not very different from finding the

ground-state energy of a quantum system. However, in the quantum problem, the operator one must diagonalize is Hermitian, and it is well known that diagonalization in a truncated basis produces an upper bound to the exact ground-state energy. It frequently happens that this bound is close to the exact result, even if the ground-state wave function is not. In spite of the operator $\hat{\mathbf{\Lambda}}$ not being Hermitian (see Sec. III), we still expect that diagonalization in a small basis will give a lower bound for the Lyapunov exponent. If the basis is suitably chosen, this estimate may be close to the result of the exact diagonalization.

To proceed with the construction of a basis for $\hat{\mathbf{\Lambda}}$, we take advantage of the fact that λ is independent of ξ_0, and simplify Eq. (12) further by averaging over an orthonormal set of initial tangent vectors, obtaining

$$\langle\langle \xi\xi^T\rangle\rangle(t)=\frac{1}{2N}e^{t\hat{\Lambda}}\mathbb{1}. \tag{21}$$

This second averaging allows us to consider, instead of $\hat{\mathbf{\Lambda}}$ itself, the restriction of $\hat{\mathbf{\Lambda}}$ to the subspace spanned by the matrices $\hat{\mathbf{\Lambda}}^k\mathbb{1}$, $k=0,1,2,\ldots$. A look at the first terms of this sequence gives a hint for constructing an appropriate basis. The first term is the identity, the second one is

$$\hat{\mathbf{\Lambda}}\mathbb{1}=\begin{pmatrix} 0 & \mathbb{1}-\langle\mathbf{V}\rangle \\ \mathbb{1}-\langle\mathbf{V}\rangle & 0 \end{pmatrix} + 2\int_0^\infty d\tau \begin{pmatrix} 0 & \tau\langle\delta\mathbf{V}\delta\mathbf{V}'\rangle \\ \tau\langle\delta\mathbf{V}\delta\mathbf{V}'\rangle & (1-\tau^2)\langle\delta\mathbf{V}\delta\mathbf{V}'\rangle \end{pmatrix}, \tag{22}$$

and so on.

III. THE ISOTROPIC APPROXIMATION

Typically, the diagonal elements of $\mathbf{V}(t)$ will be larger than the off-diagonal ones. This is evident in the case of translational invariance, where one has the property

$$V_{ii}=-\sum_{j\neq i} V_{ij}. \tag{23}$$

Introducing a matrix $\mathbf{Y}$ having all entries equal to one, i.e.,

$$\mathrm{Y}_{ij}=1, \quad \forall \ \ i,j \tag{24}$$

we can rewrite Eq. (23) as

$$\mathbf{YV}=\mathbf{VY}=0. \tag{25}$$

Then it is clear that Eq. (23) is also satisfied by $\langle\mathbf{V}\rangle$, $\langle\delta\mathbf{V}\delta\mathbf{V}'\rangle$, and by the higher moments of $\mathbf{V}$ that will appear in the blocks of $\hat{\mathbf{\Lambda}}^k\mathbb{1}$ for $k>1$. So, in a first (crude) approximation one may be tempted to discard the off-diagonal elements of the moments of $\mathbf{V}$. If we also assume that all coordinates q_i are statistically equivalent, and remind that the matrices $\hat{\mathbf{\Lambda}}^k\mathbb{1}$ are symmetric, we arrive at the simplest approximation for diagonalizing $\hat{\mathbf{\Lambda}}$. We call this approximation "isotropic," and it consists in restricting $\hat{\mathbf{\Lambda}}$ to the subspace spanned by the following three matrices:

$$\mathbf{I}_1=\begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{I}_2=\begin{pmatrix} 0 & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \quad \mathbf{I}_3=\begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \tag{26}$$

These matrices are mutually orthogonal with respect to the standard Euclidean scalar product, i.e.,

$$\mathrm{Tr}(\mathbf{I}_i\mathbf{I}_j^T)\propto\delta_{ij}. \tag{27}$$

Then the matrix elements of $\hat{\mathbf{\Lambda}}$ with respect to the basis $\{\mathbf{I}_1,\mathbf{I}_2,\mathbf{I}_3\}$ are

$$\Lambda_{ij}^{II}=\frac{\mathrm{Tr}([\hat{\mathbf{\Lambda}}\mathbf{I}_j]\mathbf{I}_i^T)}{\mathrm{Tr}(\mathbf{I}_i\mathbf{I}_i^T)}. \tag{28}$$

Using Eq. (19) and skipping some simple algebra, we arrive at the 3×3 matrix

$$\mathbf{\Lambda}^{II}=\begin{pmatrix} 0 & 0 & 2 \\ 2\sigma^2\tau_c^{(1)} & -2\sigma^2\tau_c^{(3)} & -2\mu \\ -\mu+2\sigma^2\tau_c^{(2)} & 1 & -2\sigma^2\tau_c^{(3)} \end{pmatrix} \tag{29}$$

with the definitions

$$\mu=\frac{1}{N}\mathrm{Tr}\langle\mathbf{V}\rangle, \tag{30}$$

$$\sigma^2=\frac{1}{N}\mathrm{Tr}\langle(\delta\mathbf{V})^2\rangle, \tag{31}$$

$$\tau_c^{(k+1)}=\int_0^\infty d\tau\tau^k f(\tau), \tag{32}$$

where we have introduced the normalized correlation function $f(\tau)$

$$f(\tau)=\frac{1}{N\sigma^2}\mathrm{Tr}\langle\delta\mathbf{V}(0)\delta\mathbf{V}(\tau)\rangle = \frac{1}{N\sigma^2}\sum_{i,j=1}^{N}\langle\delta V_{ij}(0)\delta V_{ij}(\tau)\rangle. \tag{33}$$

It is evident from Eq. (29) that the operator $\hat{\mathbf{\Lambda}}$ is not Hermitian. Normalization of the basis $\mathbf{I}_j$ will not make $\mathbf{\Lambda}^{II}$ symmetric.

In the isotropic approximation, the Lyapunov exponent is expressed in terms of the set of four parameters, μ and $\sigma^2\tau_c^{(k+1)}$, $k=0,1,2$. The parameters μ and σ are, respectively, the mean and variance of the stochastic process $\mathbf{V}(t)$, and can in principle be obtained analytically by calculating the corresponding microcanonical averages. (In practice, the calculations can be done in the canonical ensemble, and then

connected with the microcanonical results by the formula of Lebowitz, Percus and Verlet [20].)

The characteristic time $\tau_c^{(1)}$ is naturally interpreted as the correlation time of the process $\mathbf{V}(t)$. Its calculation requires the knowledge of the autocorrelation functions of $V_{ij}(t)$, which are system dependent. Moreover, the correlation functions of a given system will, in general, depend on energy. However, if the functional form of the correlation function $f(\tau)$ is known (or conjectured), its parameters can also be calculated as thermal averages. For instance, if $f(\tau)$ is approximately Gaussian,

$$f(\tau) \approx e^{-\gamma \tau^2}, \tag{34}$$

the expansion of $\langle \mathbf{V}(0)\mathbf{V}(\tau)\rangle$ around $\tau=0$ gives an explicit formula for the correlation time, namely,

$$\frac{1}{\tau_c^{(1)}} = \left[\frac{2}{\pi \sigma^2 N} \mathrm{Tr} \left\langle \left(\frac{d\mathbf{V}}{dt} \right)^2 \right\rangle \right]^{1/2}. \tag{35}$$

In this case $\tau_c^{(2)}$ and $\tau_c^{(3)}$ are trivially related to $\tau_c^{(1)}$:

$$\tau_c^{(2)} = \frac{2}{\pi} [\tau_c^{(1)}]^2, \tag{36}$$

$$\tau_c^{(3)} = \frac{2}{\pi} [\tau_c^{(1)}]^3. \tag{37}$$

A purely numerical calculation of $\tau_c^{(k)}$ may be very difficult, if not impossible, because correlation functions estimated from finite-length time series usually fail to damp as expected [21]. Perhaps, a more sensible approach to the estimation of $\tau_c^{(k)}$ should start with a numerical study of the correlation functions; then a functional form for $f(\tau)$ could be proposed, based on the short-time behavior of the numerical correlation functions; finally, the parameters defining $f(\tau)$ would be calculated as suitable thermal averages. An alternative, more powerful approach involves the use of ''memory functions'' [22]. They are related in a one-to-one way to correlation functions and seem to be more amenable to simple approximations (see, e.g., Ref. [23]).

IV. EXAMPLES

In this section, we analyze the application of the perturbative theory of Sec. II to some simple models. We remark that, in principle, the theory is expected to be successful only in regimes where the Lyapunov exponent is very small. All the systems considered below exhibit regimes with vanishingly small Lyapunov exponents. It is understood that our discussion will be restricted to such regimes.

A. Mean field *XY* Hamiltonian

Let us begin by analyzing one special case in which the isotropic approximation of Sec. III is exact. Consider the one-dimensional Hamiltonian [24–26]

$$H_1 = \frac{1}{2} \sum_{i=1}^{N} L_i^2 + \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)]. \tag{38}$$

This is the so-called mean-field XY Hamiltonian. It represents a lattice of classical spins with infinite-range interactions. Each rotator is restricted to the unit circle and it is therefore described by an angle $0 < \theta_i \leqslant 2\pi$ and its conjugate angular momentum L_i, with $i=1,\ldots,N$. At the critical energy $E_c = 3N/4$, there is a second-order phase transition separating a disordered regime ($E > E_c$) from an ordered one ($E < E_c$).

In both limits $E \to 0,\infty$, the Lyapunov exponent goes to zero. For a fixed energy $E > E_c$, λ also goes to zero when $N \to \infty$. This behavior has also been observed in a metastable disordered phase with $E < E_c$. The perturbative approach should be a good approximation in these regimes. Moreover, we argue that the infinite-range interactions justify the isotropic approximation.

All single-particle averages are equal, and, given that the forces are independent of the distances between spins, all two-particle averages must also be equal. So, one has

$$\langle V_{ii} \rangle = c_1, \quad \forall \ i, \tag{39}$$

$$\langle V_{ij} \rangle = c_2, \quad \forall \ i \neq j. \tag{40}$$

Notice that translational symmetry, Eq. (23), implies that

$$c_2 = -\frac{c_1}{N-1}. \tag{41}$$

This is the reason why the isotropic approximation will work in this case, i.e., off-diagonal matrix elements are indeed smaller than diagonal ones [18]. But let us keep the discussion quantitative, and rewrite Eq. (39) as

$$\langle \mathbf{V} \rangle = c_1 \mathbb{1} + c_2 (\mathbf{Y} - \mathbb{1}) \tag{42}$$

with $\mathbf{Y}$ defined in Eq. (24). Using the time-reversal symmetry of the stochastic process $\mathbf{V}(t)$, one can also show that

$$\langle \delta \mathbf{V}(0)\, \delta \mathbf{V}(\tau) \rangle = c_1' \mathbb{1} + c_2' (\mathbf{Y} - \mathbb{1}). \tag{43}$$

Then all blocks of $\hat{\mathbf{\Lambda}}\mathbb{1}$ [Eq. (22)] belong to the subspace spanned by $\mathbb{1}$ and $\mathbf{Y}$. Taking into account Eq. (25) and

$$\mathbf{Y}^2 = N\mathbf{Y}, \tag{44}$$

we conclude that the blocks of all the sequence $\hat{\mathbf{\Lambda}}^k \mathbb{1}$ belong to the subspace $\{\mathbb{1}, \mathbf{Y}\}$. Thus, the relevant subspace for diagonalizing $\hat{\mathbf{\Lambda}}$ is six dimensional. It is spanned by $\mathbf{I}_1, \mathbf{I}_2, \mathbf{I}_3$ [Eq. (26)] and $\mathbf{Y}_1, \mathbf{Y}_2, \mathbf{Y}_3$, with the definitions

$$\mathbf{Y}_1 = \begin{pmatrix} \mathbf{Y} & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{Y}_2 = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{Y} \end{pmatrix}, \quad \mathbf{Y}_3 = \begin{pmatrix} 0 & \mathbf{Y} \\ \mathbf{Y} & 0 \end{pmatrix}. \tag{45}$$

However, it can be shown (see the Appendix) that the largest eigenvalue of the corresponding 6×6 matrix coincides with that of the isotropic 3×3 matrix up to corrections of order

$1/N$. In this way we have proven the validity of the isotropic 3×3 approximation for one-dimensional systems with infinite-range forces.

B. Dilute gases

Consider now a one-dimensional gas with Hamiltonian

$$H_2=\frac{1}{2}\sum_{i=1}^{N} p_i^2+\sum_{i,j=1}^{N} \nu(q_i-q_j), \tag{46}$$

where q and p are linear coordinates, and we assume that the potential ν is bounded. For large enough energies, this system is disordered and weakly chaotic. All particles, and all *pairs* of particles, are statistically equivalent. Then this problem is formally equivalent to the infinite-range XY Hamiltonian: The isotropic 3×3 approximation becomes exact.

Of course, the statistical equivalence also holds for a dilute three-dimensional gas with short-range interactions. In this case, Barnett *et al.* have shown that the largest Lyapunov exponent is found by diagonalizing a 4×4 matrix [7].

C. αXY Hamiltonian

There are cases in which no strong reasons exist to believe that the isotropic approximation will work satisfactorily. Consider, for instance, the arbitrary-range analog of the XY Hamiltonian [27,28]:

$$H_3=\frac{1}{2}\sum_{i=1}^{N} L_i^2+\frac{1}{2\tilde{N}}\sum_{i,j=1\,(i\neq j)}^{N}\frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}}. \tag{47}$$

The parameter α sets the range of the interactions: $\alpha=0$ recovers the mean-field case and $\alpha=\infty$ corresponds to first-neighbor couplings. The prefactor $\tilde{N}$ (a function of N and α) is included to make the system ''pseudoextensive'' [29]. Periodic boundary conditions are assumed, and r_{ij} is the minimum between $|i-j|$ and $N-|i-j|$. For any value of α, there exist (i) a low-energy regime of harmonic oscillators weakly coupled by nonlinear forces and (ii) a high-energy disordered phase where the spins rotate almost freely. We expect our theory to produce good estimates for the largest Lyapunov exponent in both low- and high-energy regimes.

If the forces are not of infinite range but just long-ranged, the isotropic approximation will still give good estimates in weakly chaotic regimes. Evidence supporting this statement can be found in Refs. [30] (geometric method) and [31] (random matrix approach), where some kind of ''isotropic'' approximations were used to derive scaling laws for λ in the high-energy regime, in good agreement with numerical simulations [27,32].

For α not too small, it may be necessary to improve the isotropic approximation by diagonalizing $\hat{\mathbf{\Lambda}}$ in a larger basis. In this case, the statistical equivalence holds for all pairs of particles separated by the same distance. This means that the blocks of $\hat{\mathbf{\Lambda}}^k\mathbb{1}$ are symmetric and cyclical, i.e., the matrix elements only depend on the distance r_{ij}. A basis can be constructed starting from the $N\times N$ matrix $\mathbf{S}$ of a cyclical shift:

$$S_{ij}=\delta_{i,j+1}, \tag{48}$$

where it is understood that $j+1$ must be taken modulo N. Then the set of symmetrical matrices,

$$\mathbf{\Sigma}_k\equiv\mathbf{S}^k+\mathbf{S}^{-k},\quad 0\leqslant k\leqslant N/2 \tag{49}$$

is a basis for the blocks of $\hat{\mathbf{\Lambda}}^m\mathbb{1}$. A suitable basis for diagonalizing $\hat{\mathbf{\Lambda}}$ is the set

$$\begin{pmatrix}\mathbf{\Sigma}_i & 0\\ 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0\\ 0 & \mathbf{\Sigma}_j\end{pmatrix},\begin{pmatrix}0 & \mathbf{\Sigma}_k\\ \mathbf{\Sigma}_k & 0\end{pmatrix} \tag{50}$$

with $0\leqslant i,j,\ k\leqslant N/2$. The length of this basis is $3N/2$. Notwithstanding, we expect that a small subset of this basis will be enough to get a satisfactory convergence to the largest eigenvalue of $\hat{\mathbf{\Lambda}}$. Even in the worst case of no truncation at all, numerical diagonalization is possible for relatively large systems.

V. CONNECTION WITH THE GEOMETRIC METHOD

In Sec. III, we motivated the isotropic approximation by arguing that, in the first approach, one can neglect the off-diagonal matrix elements of the blocks of $\hat{\mathbf{\Lambda}}^k\mathbb{1}$. Then in Sec. IV we proved that this approximation is indeed justified in various cases. Looking back to the results of Secs. II and III, we realize that the isotropic approximation is equivalent to postulating an ''effective'' system of equations,

$$\dot{\xi}_i=\begin{pmatrix}0 & 1\\ -K(t) & 0\end{pmatrix}\xi_i, \tag{51}$$

where $\xi_i=(\delta q_i,\delta p_i)$ is the projection of the tangent vector ξ on the subspace of the ith degree of freedom. The equations above represent the evolution of a typical component of ξ. In this sense they could alternatively be called ''mean-field'' or ''single-particle'' equations. The scalar object $K(t)$ is an effective random process that substitutes the Hessian $\mathbf{V}(t)$, and is in principle unknown. However, its first two cumulants can be identified in the following way. First solve Eq. (51) for the average of ξ_i^2 by using second-order perturbation theory, as done in Sec. II [just change $\mathbf{V}$ by K, and set $N=1$ in Eq. (19)]. Notice that, as $K(t)$ is a real number, the blocks of the effective $\hat{\mathbf{\Lambda}}$ are also real numbers, and the ''isotropic approximation'' is exact now. Then the matrix one must diagonalize to obtain the Lyapunov exponent is exactly that of Eq. (29), provided one makes the identifications:

$$\langle K\rangle=\frac{1}{N}\mathrm{Tr}\langle\mathbf{V}\rangle, \tag{52}$$

$$\langle\delta K(0)\,\delta K(\tau)\rangle=\frac{1}{N}\mathrm{Tr}\langle\delta\mathbf{V}(0)\,\delta\mathbf{V}(\tau)\rangle \tag{53}$$

with $\delta K=K-\langle K\rangle$. From this point of view, the isotropic basis $\{\mathbf{I}_1,\mathbf{I}_2,\mathbf{I}_3\}$ is a single-particle basis. It is the most natural one in the sense that it treats all degrees of freedom on the same footing.

The perturbative-isotropic approximation, as presented above, is very similar to the geometric approach. In fact, in the geometric method [15] an effective equation like Eq. (51) is proposed, containing the unknown process $K'(t)$. Then, it is argued that the first two cumulants of K' are related to the Laplacian of the potential $\Delta\mathcal{V}(t)$:

$$\langle K' \rangle = \frac{1}{N}\langle \Delta\mathcal{V} \rangle, \tag{54}$$

$$\langle \delta K'(0)\,\delta K'(\tau)\rangle = \frac{1}{N}\langle (\delta\Delta\mathcal{V})^2\rangle \bar{\tau}\delta(\tau), \tag{55}$$

where $\delta\Delta\mathcal{V}=\Delta\mathcal{V}-\langle\Delta\mathcal{V}\rangle$, and $\bar{\tau}$ is the correlation time of the process $K'(t)$, which is assumed to be δ correlated.

It is obvious that the averages of both processes K and K' coincide because Tr $\mathbf{V}=\Delta\mathcal{V}$. So, the differences between the geometric method and the perturbative-isotropic approach appear only in the fluctuations. The similarity between both theories could be enhanced by relaxing the δ-correlation assumption of the geometric method, and substituting Eq. (55) by

$$\langle \delta K'(0)\,\delta K'(\tau)\rangle = \frac{1}{N}\langle \delta\Delta\mathcal{V}(0)\,\delta\Delta\mathcal{V}(\tau)\rangle. \tag{56}$$

But even so, we have not been able to find any analytical relationship between the correlation functions of K and K'. In principle, the difference between both is non-negligible, and both the effective theories will lead to different estimates for the Lyapunov exponent. We expect that numerical simulations will decide which estimate is better.

One comment about the correlation time $\bar{\tau}$ of Eq. (55) is in order; Geometric arguments lead to the estimate [15]

$$\bar{\tau} = \frac{\pi\sqrt{\bar{\mu}}}{2\sqrt{\bar{\mu}(\bar{\mu}+\bar{\sigma})}+\pi\bar{\sigma}} \tag{57}$$

with $\bar{\mu}\equiv\langle K'\rangle$ and $\bar{\sigma^2}\equiv\langle(\delta K')^2\rangle$. Some slightly different expressions have also been proposed [4,5,14]. The criterion for testing the accuracy of these estimates has been the agreement between the geometric estimate for λ and numerical simulations, i.e., the goodness of fit (which is indeed excellent in some cases). To our knowledge, there is no *independent* test of the expression (57), or others, in the literature. Accordingly, a precise definition of $\bar{\tau}$ seems to be lacking. [Is $\bar{\tau}$ equal to the integral of the normalized autocorrelation function of $\Delta\mathcal{V}(t)$?] This is a point that affects the consistency of the geometric method. Unless a definition is given, to some extent, $\bar{\tau}$ will have the status of a fitting parameter. Comparisons of the geometric method with other theories will have to take this fact into account.

VI. SUMMARY

We showed that the evolution equation in tangent space can be thought of as a stochastic differential equation with multiplicative noise. Then, an analytical estimate for the largest Lyapunov exponent of a many-particle system in equilibrium was derived by using standard perturbative techniques. Our analysis has been focused on the second-order approximation. In this case the Lyapunov exponent can be obtained by diagonalizing a matrix whose entries are calculated from the first two cumulants of the Hessian of the potential energy, i.e., the averages $\langle V_{ij}\rangle$ and the correlation functions $\langle \delta V_{ij}(0)\,\delta V_{kl}(\tau)\rangle$. The dimension of this matrix is, in principle, of the order of $N\times N$, but we have proposed the conjecture, based on an analogy with the Hermitian problem, that diagonalization in a truncated basis may be enough to obtain satisfactory results.

In the crudest approximation, which consists in choosing the three-dimensional isotropic basis of Eq. (26), the Lyapunov exponent is extracted from a 3×3 matrix. We argued that this "isotropic approximation" is equivalent to modeling the tangent dynamics of the many-particle system by an "effective" process $K(t)$ for a single degree of freedom. In this way we established a connection with the so-called geometric method, the alternative effective theory for estimating the Lyapunov exponent. Both theories are very similar, but differ at the point of the definition of the correlation function of $K(t)$. The difference is nontrivial and is expected to lead to different predictions.

In special cases, e.g., one-dimensional lattice systems with infinite-range interactions, we have been able to prove that the isotropic approximation is exact. However, in the general case, it may be necessary to consider larger bases. We have given examples where these bases are constructed by following the symmetries of the moments of $\mathbf{V}(t)$.

The theory we have presented is perturbative. Loosely speaking, we expect to obtain good estimates of Lyapunov exponents in weakly chaotic regimes. More quantitatively, the domain of validity of the theory is controlled by the "Kubo number" $\sigma\tau_c$ that quantifies the strength of the fluctuations $\delta\mathbf{V}(t)$. For a given system, it is difficult to say *a priori* in which regimes the theory will work satisfactorily. This question and others, like the validity of the isotropic approximation and its comparison with the geometric method, will be decided with the aid of forthcoming numerical simulations.

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APPENDIX: THE INFINITE-RANGE CASE

We have seen in Sec. IV that in the case of a one-dimensional system with infinite-range interactions, the subspace spanned by the matrices $\hat{\Lambda}^k\mathbb{1}$ is six dimensional. An orthogonal basis for this subspace is the set $\{\mathbf{I}_1,\mathbf{I}_2,\mathbf{I}_3,\mathbf{Z}_1,\mathbf{Z}_2,\mathbf{Z}_3\}$, where

$$\mathbf{Z}_k = \mathbf{Y}_k - \mathbf{I}_k . \tag{A1}$$

The 6×6 matrix of $\hat{\mathbf{\Lambda}}$ can be naturally split into four blocks of size 3×3. The block II has already been calculated [Eq. (29)]. Let us now calculate the block IZ, i.e.,

$$\Lambda_{ij}^{IZ} = \frac{\mathrm{Tr}(\hat{\mathbf{\Lambda}}\mathbf{Z}_j)\mathbf{I}_i}{\mathrm{Tr}\ \mathbf{I}_i^2}. \tag{A2}$$

By setting $\mathbf{V}=0$ in Eq. (19) we obtain the operator $\hat{\mathbf{\Lambda}}_0$ ($\hat{\mathbf{\Lambda}}$ in the absence of interactions). It has the following properties:

$$\hat{\mathbf{\Lambda}}\mathbf{Y}_j = \hat{\mathbf{\Lambda}}_0\mathbf{Y}_j , \tag{A3}$$

$$\mathrm{Tr}(\hat{\mathbf{\Lambda}}_0\mathbf{Y}_j)\mathbf{I}_i = \mathrm{Tr}(\hat{\mathbf{\Lambda}}_0\mathbf{I}_j)\mathbf{I}_i . \tag{A4}$$

Using these two properties together with Eq. (A1), one arrives at

$$\Lambda_{ij}^{IZ} = \Lambda_{0,ij}^{II} - \Lambda_{ij}^{II} . \tag{A5}$$

Analogously one obtains

$$\Lambda_{ij}^{ZI} \approx \frac{1}{N}\Lambda_{ij}^{IZ} , \tag{A6}$$

$$\Lambda_{ij}^{ZZ} \approx \Lambda_{0,ij}^{II} + \frac{1}{N}\Lambda_{ij}^{II} , \tag{A7}$$

where the symbol $\approx$ means that terms of relative size $1/N$ have been discarded. The 6×6 matrix reads

$$\mathbf{\Lambda} \approx \begin{pmatrix} \mathbf{\Lambda}^{II} & -\mathbf{\Lambda}_1^{II} \\ -\frac{1}{N}\mathbf{\Lambda}_1^{II} & \mathbf{\Lambda}_0^{II} + \frac{1}{N}\mathbf{\Lambda}_1^{II} \end{pmatrix} \tag{A8}$$

with the definition $\mathbf{\Lambda}_0^{II} + \mathbf{\Lambda}_1^{II} = \mathbf{\Lambda}^{II}$. Then it can be checked that the matrix above has three zero eigenvalues while the remaining three are the eigenvalues of the matrix

$$\mathbf{\Lambda}_0^{II} + \frac{N+1}{N}\mathbf{\Lambda}_1^{II} \approx \mathbf{\Lambda}^{II}. \tag{A9}$$

Thus the isotropic approximation is essentially exact for the infinite-range XY Hamiltonian.

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