A theory for the Lyapunov exponent of a many-particle system

Raúl O. Vallejos & Celia Anteneodo

CBPF, Rio de Janeiro

C. Anteneodo & ROV, PRE 65, 016210 (2001)
ROV & C. Anteneodo, PRE 66, 021110 (2002)
C. Anteneodo, R. N. P. Maia & ROV, PRE 68, 036120 (2003)

Presented at NEXT2003,
Villasimius (Sardinia), September 22, 2003
http://www.ca.infn.it/~lissia/next2003/main.html

Abstract

First-principles theory for estimating the largest Lyapunov exponent of a many-particle system having a smooth Hamiltonian, possibly long-range

Based on cumulant expansion (van Kampen et al)

Application to the disordered phases of the infinite-range XY Hamiltonian (aka HMF)

"Recover" the geometric method (alternative approach) as a special limit.

Introduction

Hamilton equations

$$\frac{dx}{dt} = J \nabla H(x)$$

$$J = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{1}} & \underline{\underline{0}} \end{pmatrix}$$

$2N \times 2N$ symplectic matrix

$$x = (q_1, \ldots, q_N; p_1, \ldots, p_N)$$

Tangent dynamics

$$\frac{d\xi}{dt} = A(t)\,\xi$$

$\xi \equiv \delta x$ distance vector

linear system

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q_1, \ldots q_N) \quad \Rightarrow \quad A(t) = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{V}}(t) & \underline{\underline{0}} \end{pmatrix}$$

$\underline{\underline{V}}$: $N \times N$ Hessian of $V(q)$

First steps

$$\lambda = \lim_{t\to\infty} \frac{1}{2t} \ln |\xi|^2$$

Definition of Lyapunov exponent : rate of exponential growth

Simplification : Lyapunov exponent does not depend on initial conditions, add averages in phase space (and tangent space)

$$\lambda = \lim_{t\to\infty} \frac{1}{2t} \left\langle \ln |\xi|^2 \right\rangle_{x_0,\xi_0}$$

$\left\langle \cdots \right\rangle_{x_0}$ microcanonical average

Aproximation # 1 : exchange average and logarithm

$$\lambda \approx \lim_{t\to\infty} \frac{1}{2t} \ln \left\langle |\xi|^2 \right\rangle_{x_0,\xi_0}$$

(weak intermittency) may be tested a posteriori

A theory for $\left\langle |\xi|^2 \right\rangle$

ROV & C. Anteneodo, 2002
D. M. Barnett et al, 1996

Introduce a "density matrix" $\xi\xi^T$ so that $Tr\left\langle \xi\xi^T \right\rangle = \left\langle |\xi|^2 \right\rangle$

The equation for $\xi\xi^T$ is also linear :

using $\dfrac{d\xi}{dt} = A(t)\xi$

$$\frac{d}{dt}\xi\xi^T = \hat{A}\xi\xi^T$$

where $\hat{A}\xi\xi^T \equiv A\xi\xi^T + \xi\xi^T A^T$

Solution :

$$\left\langle \xi\xi^T(t) \right\rangle = \left\langle T\, e^{\int_0^t \hat{A}(t_1;x_0)\,dt_1} \right\rangle_{x_0} \underline{\underline{1}}$$

The cumulant expansion (van Kampen)

Perturbative expansion : average + fluctuations

$$A(t) = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\langle \underline{\underline{\mathrm{V}}} \rangle & \underline{\underline{0}} \end{pmatrix} + \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{0}} \\ -\delta \underline{\underline{\mathrm{V}}}(t) & \underline{\underline{0}} \end{pmatrix} \quad \Rightarrow \quad \hat{A} = \langle \hat{A} \rangle + \delta \hat{A}$$

Fluctuations of small amplitude and/or short correlation time

$$\left\langle T\ e^{\int_0^t \hat{A}(t_1;x_0)\,dt_1} \right\rangle = e^{\hat{O}t}$$

$\hat{O}$ is time-independent

$$\hat{O} = \langle \hat{A} \rangle + \int_0^\infty d\tau \left\langle \delta\hat{A}(t) e^{\tau \langle \hat{A} \rangle} \delta\hat{A}(t-\tau) e^{-\tau \langle \hat{A} \rangle} \right\rangle + \cdots$$

average + integrated autocorrelation function + ...

Once $\hat{O}$ is known …

Recalling that $$\left\langle \left|\xi\right|^2 \right\rangle = Tr\left\langle \xi\xi^T(t)\right\rangle = Tr\; e^{\hat{O}t}\,\underline{\underline{1}}$$

The Lyapunov exponent is given by

$$\lambda = \tfrac{1}{2}\Re\left(L_{\max}\right)$$

$L_{\max}$ is the eigenvalue of Ô with the largest real part

Next steps : calculate and diagonalize Ô

Calculation of $\hat{O}$

Truncate cumulant expansion at second order :

$$\hat{O} \approx \left\langle \hat{A} \right\rangle + \int_0^\infty d\tau \left\langle \delta\hat{A}(t) e^{\tau\left\langle \hat{A} \right\rangle} \delta\hat{A}(t-\tau) e^{-\tau\left\langle \hat{A} \right\rangle} \right\rangle$$

Approximation # 2

In the case of quasi-ballistic dynamics (e.g. high energy HMF) we can use the interaction representation associated to the free propagator :

$$e^{\tau\left\langle \hat{A} \right\rangle} \approx e^{\tau \hat{A}_0}$$

Approximation # 3

$$\underbrace{\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\left\langle \underline{\underline{\mathrm{V}}} \right\rangle & \underline{\underline{0}} \end{pmatrix}}_{\langle A \rangle} \rightarrow \underbrace{\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ \underline{\underline{0}} & \underline{\underline{0}} \end{pmatrix}}_{A_0}$$

Explicit expression for Ô

μ-canonical averages

$$\hat{O}\underline{\underline{M}} \approx \begin{pmatrix} 0 & 1 \\ -\langle \underline{\underline{V}} \rangle & 0 \end{pmatrix} \underline{\underline{M}} +$$

$$+\int_0^\infty d\tau \begin{pmatrix} 0 & 0 \\ \tau & -\tau^2 \end{pmatrix} \begin{pmatrix} \langle \delta\underline{\underline{V}} \cdot \delta\underline{\underline{V}}' \rangle & 0 \\ 0 & \langle \delta\underline{\underline{V}} \cdot \delta\underline{\underline{V}}' \rangle \end{pmatrix} \underline{\underline{M}} +$$

$$+\int_0^\infty d\tau \left\langle \begin{pmatrix} 0 & 0 \\ \delta\underline{\underline{V}} & 0 \end{pmatrix} \underline{\underline{M}} \begin{pmatrix} \delta\underline{\underline{V}}' & 0 \\ 0 & \delta\underline{\underline{V}}' \end{pmatrix} \right\rangle \begin{pmatrix} \tau & 1 \\ -\tau^2 & 0 \end{pmatrix} + (\dots)^T$$

$$\delta\underline{\underline{V}} \equiv \delta\underline{\underline{V}}(t)$$

$$\delta\underline{\underline{V}}' \equiv \delta\underline{\underline{V}}(t-\tau)$$

Now we must identify the relevant subspace for diagonalization : <u>system dependent</u>

Diagonalizing HMF

$$H=\sum_i \frac{p_i^2}{2}+\frac{1}{2N}\sum_{i,j}\left[1-\cos\left(\theta_i-\theta_j\right)\right]$$

For HMF one can prove that the relevant subspace is 3-dimensional, spanned by the matrices

$$\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix},\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

This “isotropic” basis amounts to a mean field approximation in tangent space, *i.e.*, the problem becomes equivalent to a one-degree-of-freedom problem:

$$\frac{d}{dt}\begin{pmatrix}\xi_q\\ \xi_p\end{pmatrix}=\begin{pmatrix}0 & 1\\ -\kappa(t) & 0\end{pmatrix}\begin{pmatrix}\xi_q\\ \xi_p\end{pmatrix}$$

$\kappa(t)$ scalar stochastic process

The mean field approximation is exact for HMF.

Second-order + mean-field diagonalization …

$$\left\| \hat{O} \right\| = \begin{pmatrix} 0 & 0 & 2 \\ 2\sigma^2\tau_c^{(1)} & -2\sigma^2\tau_c^{(3)} & -2\mu \\ -\mu + 2\sigma^2\tau_c^{(2)} & 1 & -2\sigma^2\tau_c^{(3)} \end{pmatrix}$$

3x3 matrix

Definitions :

$$\mu = \frac{1}{N}\mathrm{Tr}\left\langle \underline{\underline{V}} \right\rangle$$

$$\sigma^2 = \frac{1}{N}\mathrm{Tr}\left\langle \left(\delta \underline{\underline{V}}\right)^2 \right\rangle$$

normalized autocorrelation function

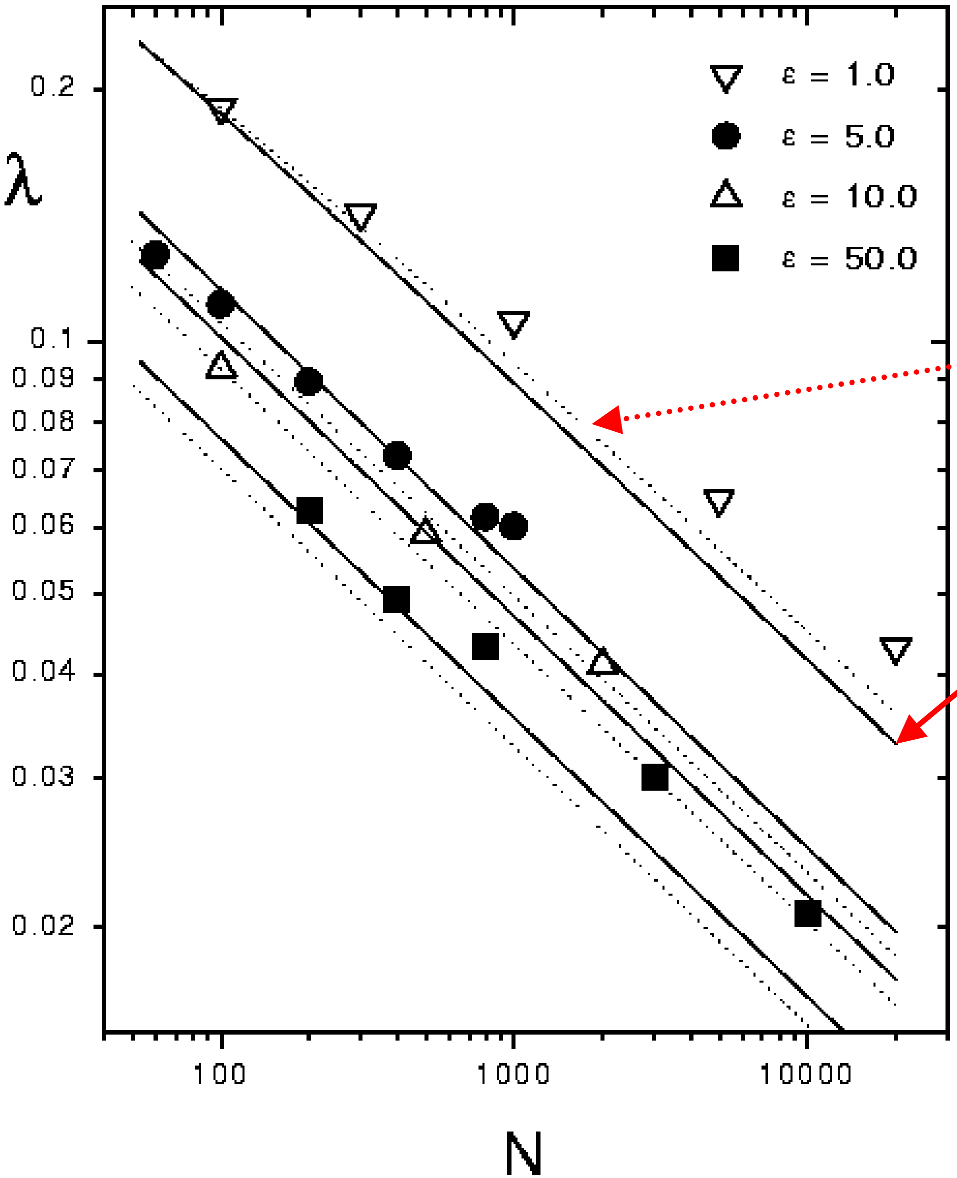
$$f(\tau) = \frac{1}{N\sigma^2}\mathrm{Tr}\left\langle \delta \underline{\underline{V}}(0) \cdot \delta \underline{\underline{V}}(\tau) \right\rangle$$

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

$\tau_c^{(1)}$ correlation time

Test : high-energy phase of the infinite-range XY

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2}+\frac{1}{2N}\sum_{i,j=1}^{N}\left[1-\cos\left(\theta_i-\theta_j\right)\right]$$



simulations
Latora, Rapisarda & Ruffo, 1998
Anteneodo & Tsallis, 1998

geometric method
M.-C. Firpo, 1998

perturbative + mean field,
Anteneodo, Maia & ROV, 2003

good agreement,
especially for N < 500

correct scaling law $\lambda \approx N^{-1/3}$

Summary

Constructed a theory for the Lyapunov exponent of a many particle system. Approximations :

1 : $\langle \ln(\cdots) \rangle \approx \ln\langle \cdots \rangle$ weak intermittency

2 : truncation at second cumulant $\sigma\tau_c << 1$

basic

3 : $e^{\tau\langle \hat{A} \rangle} \approx e^{\tau \hat{A}_0}$ weak interactions

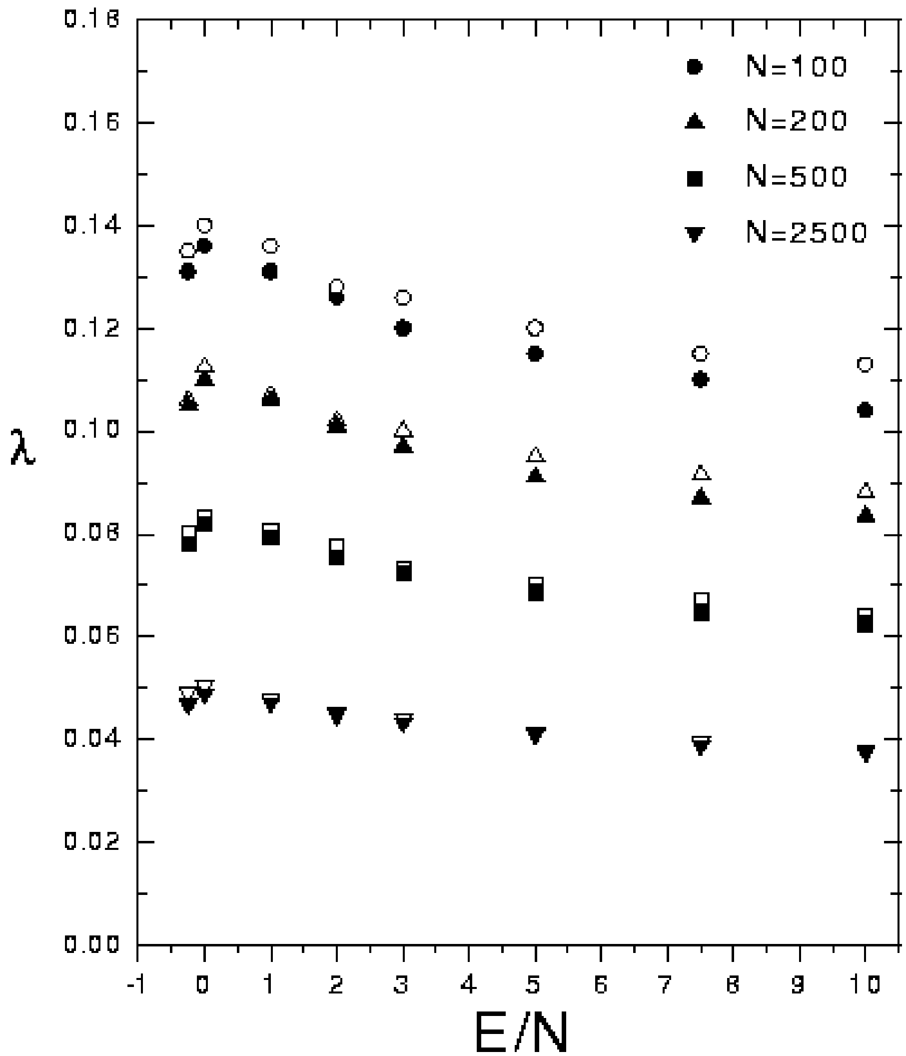
4 : mean-field diagonalization : lower bound !

specific of HMF

Results : theoretical $\rightarrow$ satisfactory
practical $\rightarrow$ just beginnning

Comparison λ vs λ’

“quenched *vs* annealed”



$$J = -1$$

○ $$\lim_{t\to\infty} \frac{1}{2t} \ln\left\langle \xi^2 \right\rangle$$

● $$\lim_{t\to\infty} \frac{1}{2t} \left\langle \ln \xi^2 \right\rangle$$

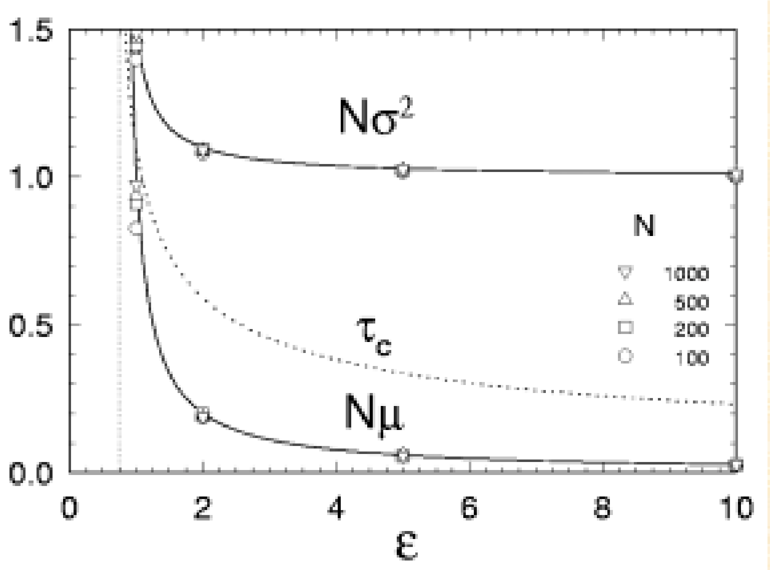
Weak intermittency (!?)

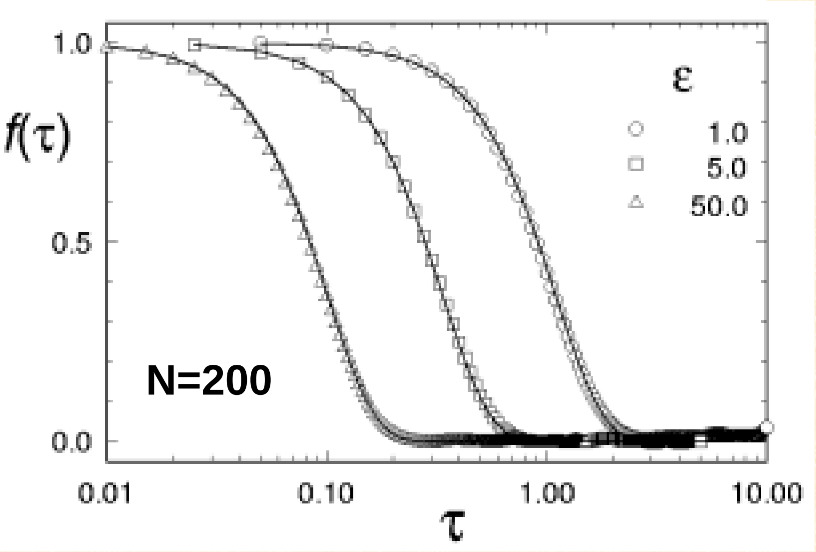
Anteneodo, Maia & ROV, 2003

Application to HMF

$$J=1, \quad E/N>3/4$$

Ingredients : microcanonical averages $\mu, \sigma, f(\tau)$





μ, σ

microcanonical averages
(analytical calculations)
vs simulations

the correlation function is gaussian !

τ_c thermal time, independent of N