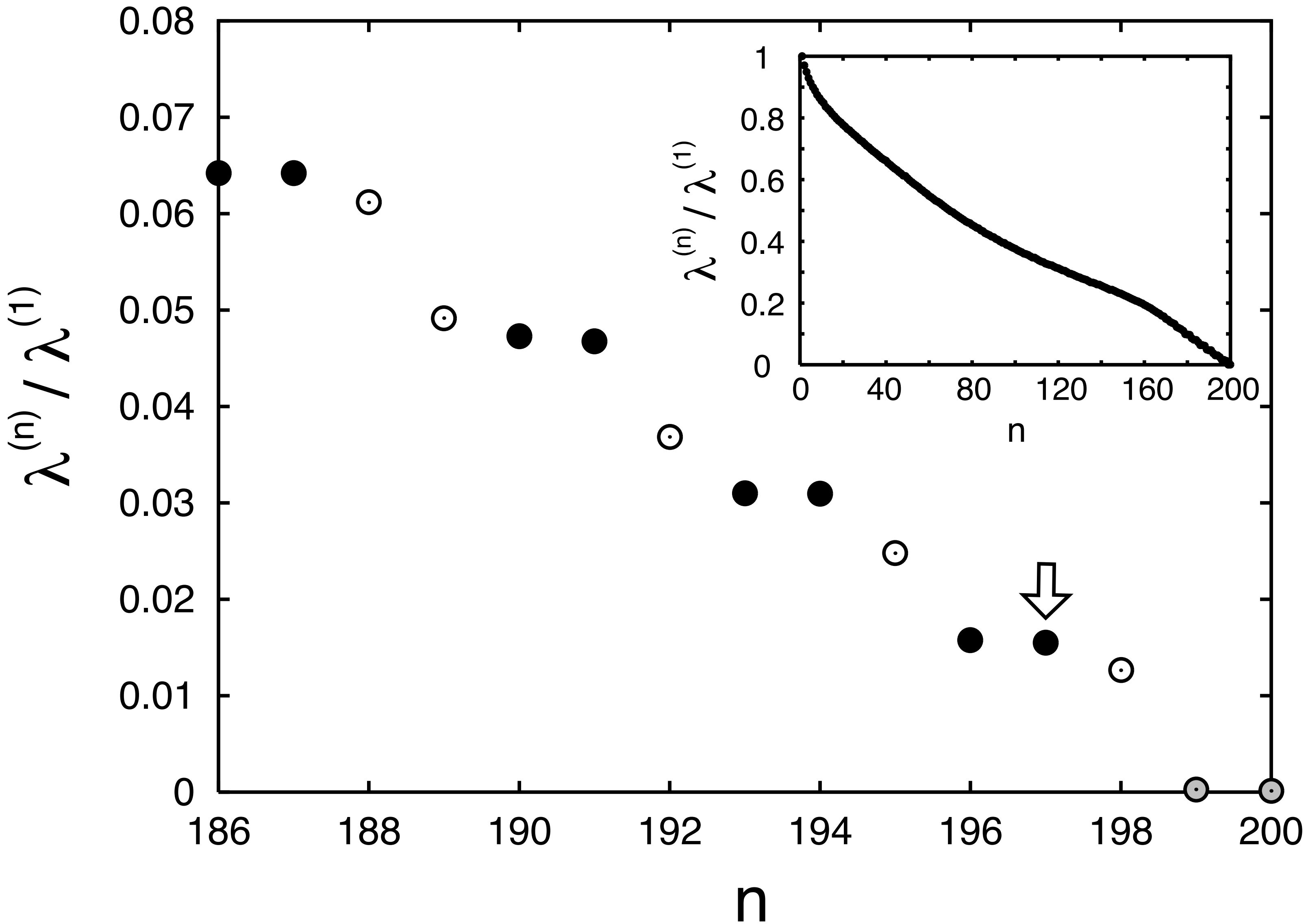
Lyapunov Exponents
Vectors and Modes

by

Gary Morriss, Tooru Taniguchi, Tony Chung &
Dean Robinson

University of New South Wales, Sydney AUSTRALIA

Lyapunov Spectrum



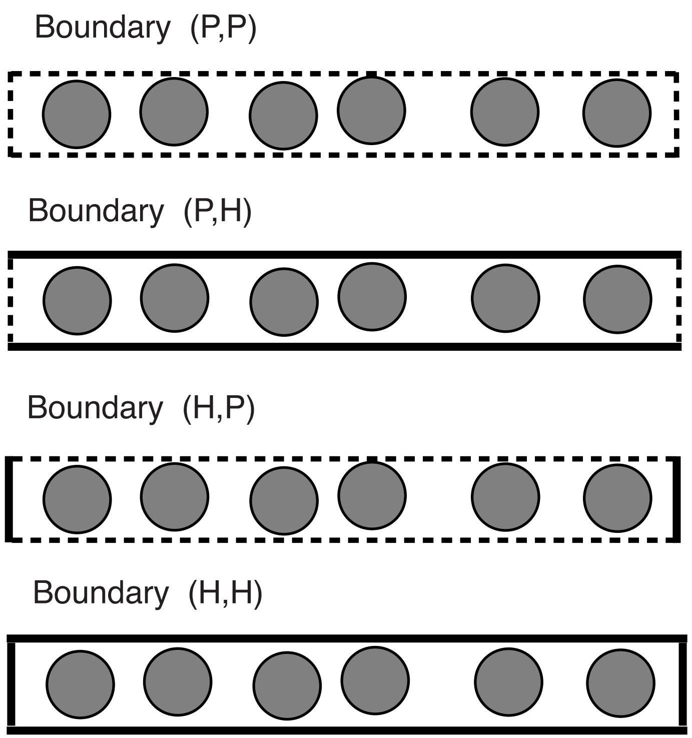
100 hard disks

Contents

- Quasi-one-dimensional system
- Lyapunov modes
- Time dependence
- Two-dimensional systems
- Lyapunov Localization
- Dynamics of the most localized Lyapunov vector

Quasi-one-dimensional Systems

Schematic boundary conditions



Particle order is invariant, so particle index corresponds to x-coordinate.

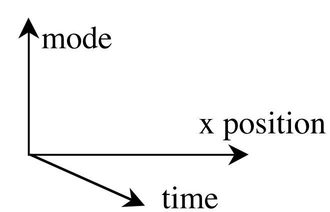
Four types of boundary conditions. We mostly use (H,P) boundary conditions.

The number and pattern of steps changes with boundary conditions.

Modes observed in the long direction only - x-direction

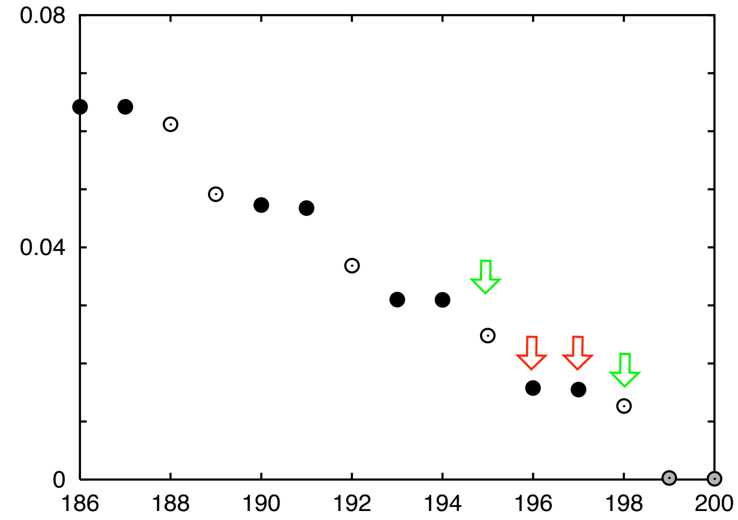
Simplifies the presentation of modes

NOTATION: $\underset{\{P,H\}}{\overset{X}{(\quad}} , \underset{\{P,H\}}{\overset{Y}{\quad)}}$



P = periodic H = hard wall

Numerical Results for Lyapunov exponents



- Quasi-one-dimensional system N=100
- 200 coordinates + 200 momenta -> 400 exponents
- (H,P) -> 4 zero exponents #199, 200, 201, 202
- First 1-point step #198 #203
- First 2-point step #196, 197 #204, 205
- Second 1-point step #195 #206

General Features

- Numerical calculations using Benettin's scheme
- Step structure in the Lyapunov exponents closest to zero (positive and negative)
- Here: 1-point step, then 2-point step (boundary conditions)
- Lyapunov vectors can exhibit stable delocalized structure - called Lyapunov modes

Symplectic structure

Symplectic eigenvalue theorem - pairing of Lyapunov exponents

$$\{\lambda_j, -\lambda_j\}$$

Conjugacy of Lyapunov vectors

$$\lambda_j \quad \Leftrightarrow \quad \delta\Gamma_j = \begin{pmatrix} \delta q_j \\ \delta p_j \end{pmatrix} \qquad\qquad \lambda_{-j} \quad \Leftrightarrow \quad \delta\Gamma_{-j} = \begin{pmatrix} \delta q_{-j} \\ \delta p_{-j} \end{pmatrix}$$

$$\lambda_{-j} = -\lambda_j \quad \Leftrightarrow \quad \delta\Gamma_{-j} = \begin{pmatrix} \delta q_{-j} \\ \delta p_{-j} \end{pmatrix} = \begin{pmatrix} \delta p_j \\ -\delta q_j \end{pmatrix}$$

Benettin's scheme preserves this structure

Conserved Quantities

For each conserved quantity of the dynamics there is a zero Lyapunov exponent.
For (P,P):

Centre of mass

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \qquad \bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$$

Total momentum

$$\bar{p}_x = \frac{1}{N}\sum_{i=1}^{N} p_{xi} \qquad \bar{p}_y = \frac{1}{N}\sum_{i=1}^{N} p_{yi}$$

Energy

$$\tfrac{1}{2}\sum_{i=1}^{N} p_{xi}^2 + p_{yi}^2 = N\bar{e} = NT$$

There can be no exponential separation in the direction of the trajectory.
Time translational invariance $\bar{t}$
Conjugacy $\{\bar{x}, \bar{p}_x\}$ $\{\bar{y}, \bar{p}_y\}$ $\{\bar{e}, \bar{t}\}$

Lyapunov Modes for Zero exponents

Lyapunov Vector notation

$$\delta\Gamma = \begin{pmatrix} \delta\mathbf{q} \\ \delta\mathbf{p} \end{pmatrix} = \begin{pmatrix} \delta x \\ \delta y \\ \delta p_x \\ \delta p_y \end{pmatrix}$$

Noether's theorem transformations corresponding to conserved quantities

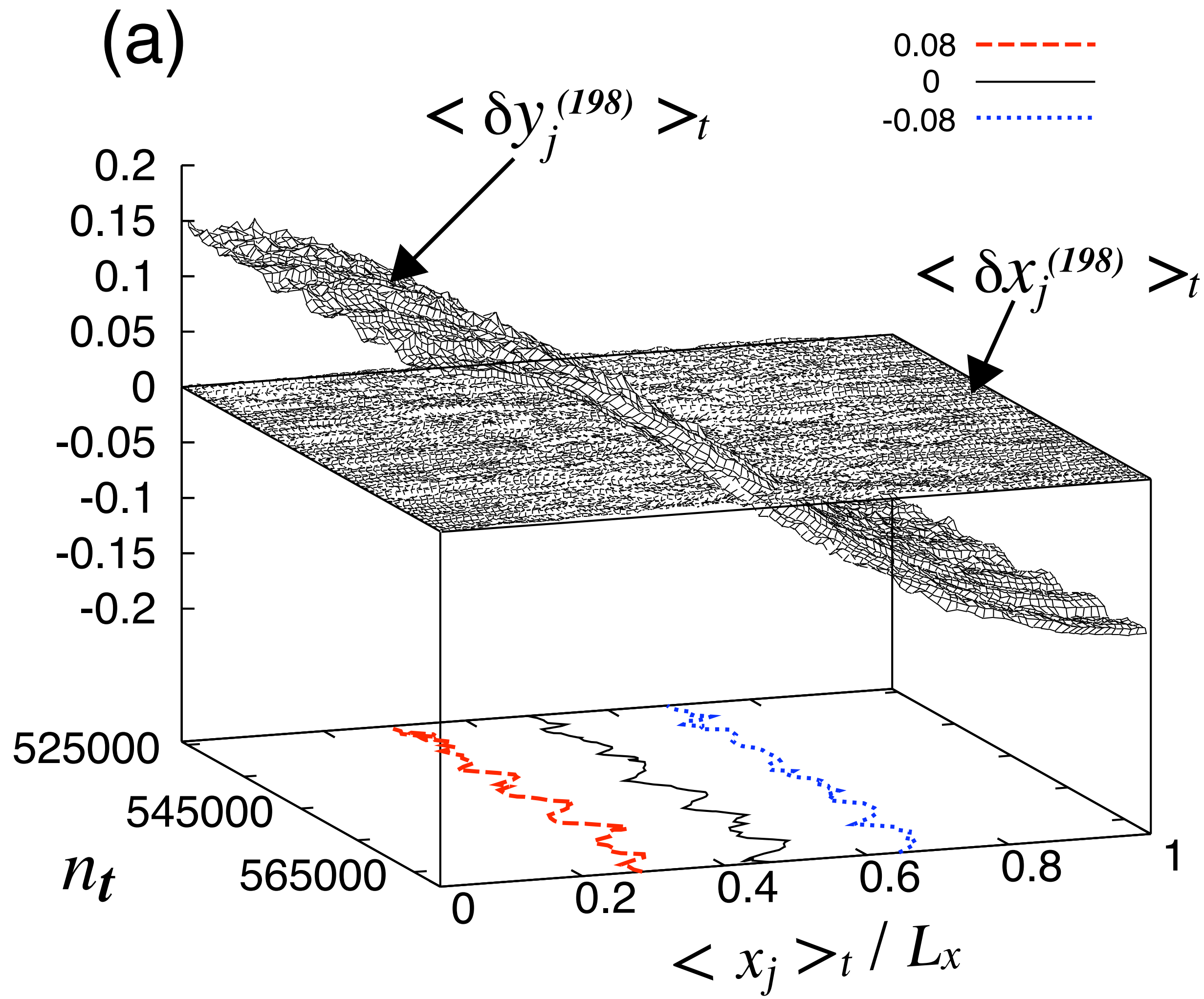
$$\delta\Gamma_x = \frac{1}{\sqrt{N}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \delta\Gamma_y = \frac{1}{\sqrt{N}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad \delta\Gamma_t = \frac{1}{\sqrt{2Ne}}\begin{pmatrix} p_x \\ p_y \\ 0 \\ 0 \end{pmatrix}$$

$$\delta\Gamma_{px} = \frac{1}{\sqrt{N}}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad \delta\Gamma_{py} = \frac{1}{\sqrt{N}}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \qquad \delta\Gamma_e = \frac{1}{\sqrt{2Ne}}\begin{pmatrix} 0 \\ 0 \\ p_x \\ p_y \end{pmatrix}$$

Evidence that these form two independent sub-spaces $\{\delta\Gamma_x, \delta\Gamma_y, \delta\Gamma_t\}$ $\{\delta\Gamma_{px}, \delta\Gamma_{py}, \delta\Gamma_e\}$

Lyapunov Modes

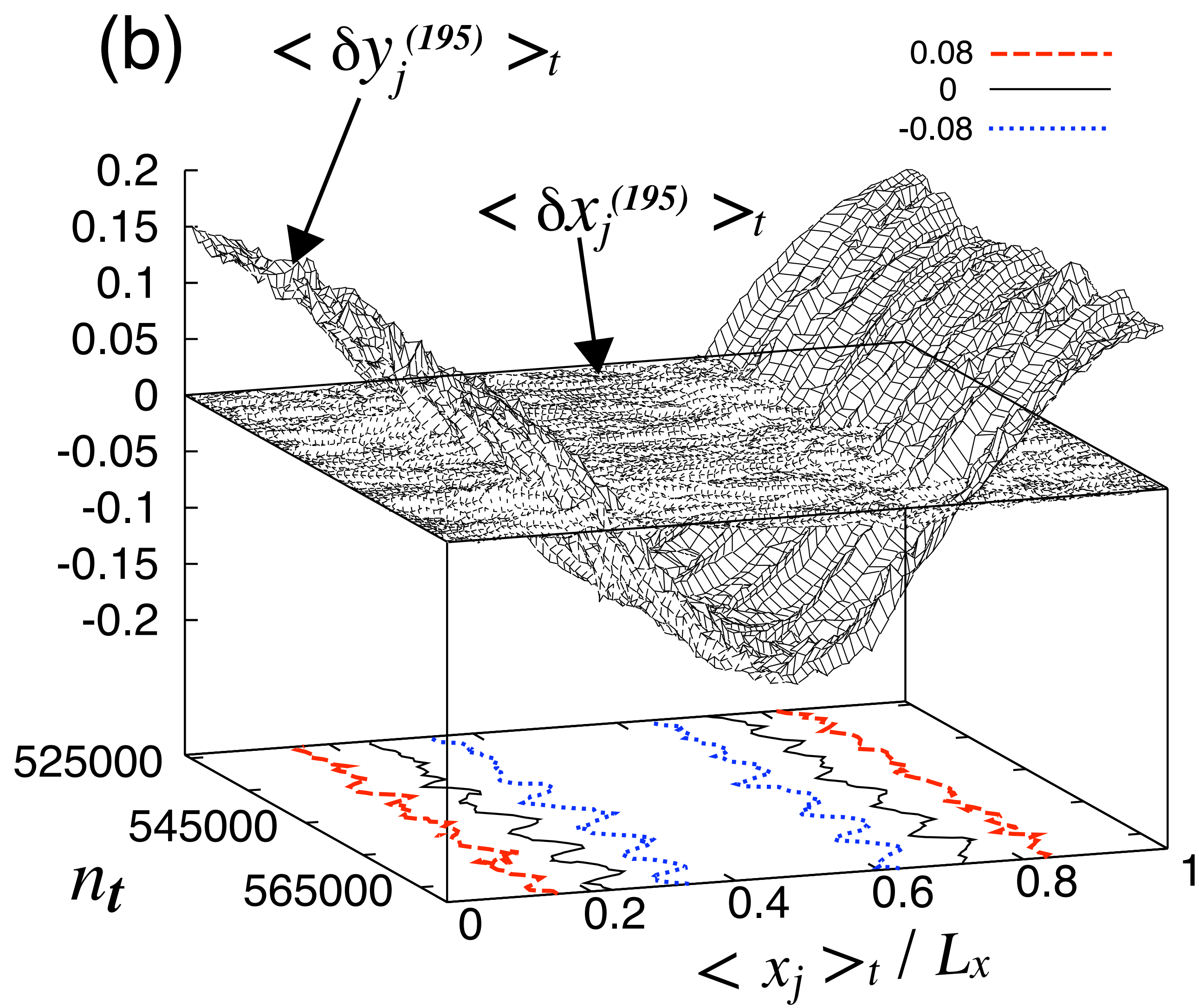
Lyapunov modes First 1-point step



T mode

$$\delta x_j \sim 0 \quad \text{and} \quad \delta y_j \sim \cos\left(\frac{\pi \langle x_j \rangle}{L_x}\right)$$

Lyapunov modes — Second 1-point step

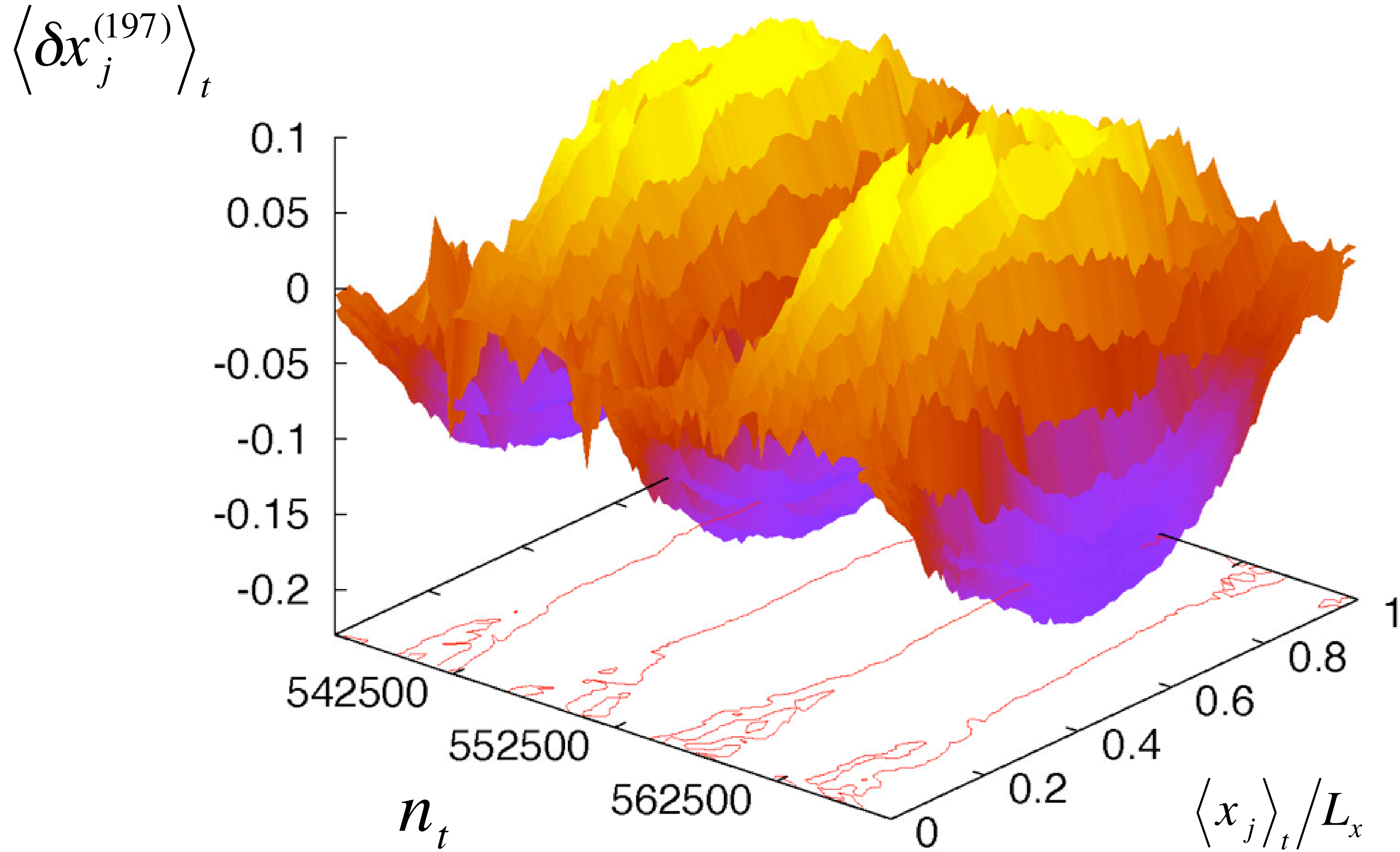


T mode

$$\delta x_j \sim 0 \quad \text{and} \quad \delta y_j \sim \cos\left(\frac{2\pi\langle x_j\rangle}{L_x}\right)$$

Lyapunov modes

First 2-point step

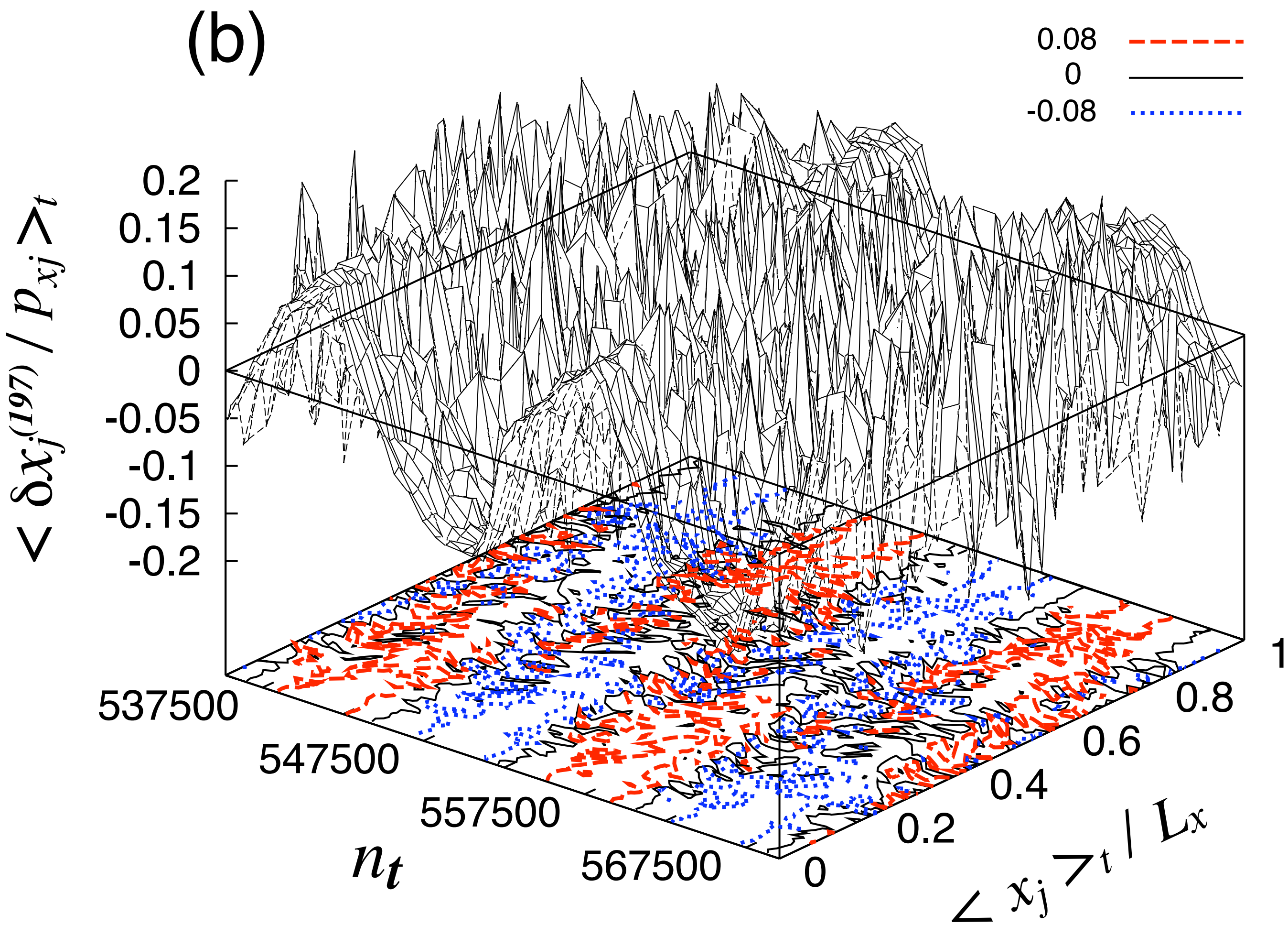


L mode

$$\delta x_j \sim \sin(k_1 x_j)\cos(\omega t)$$

Lyapunov modes

First 2-point step

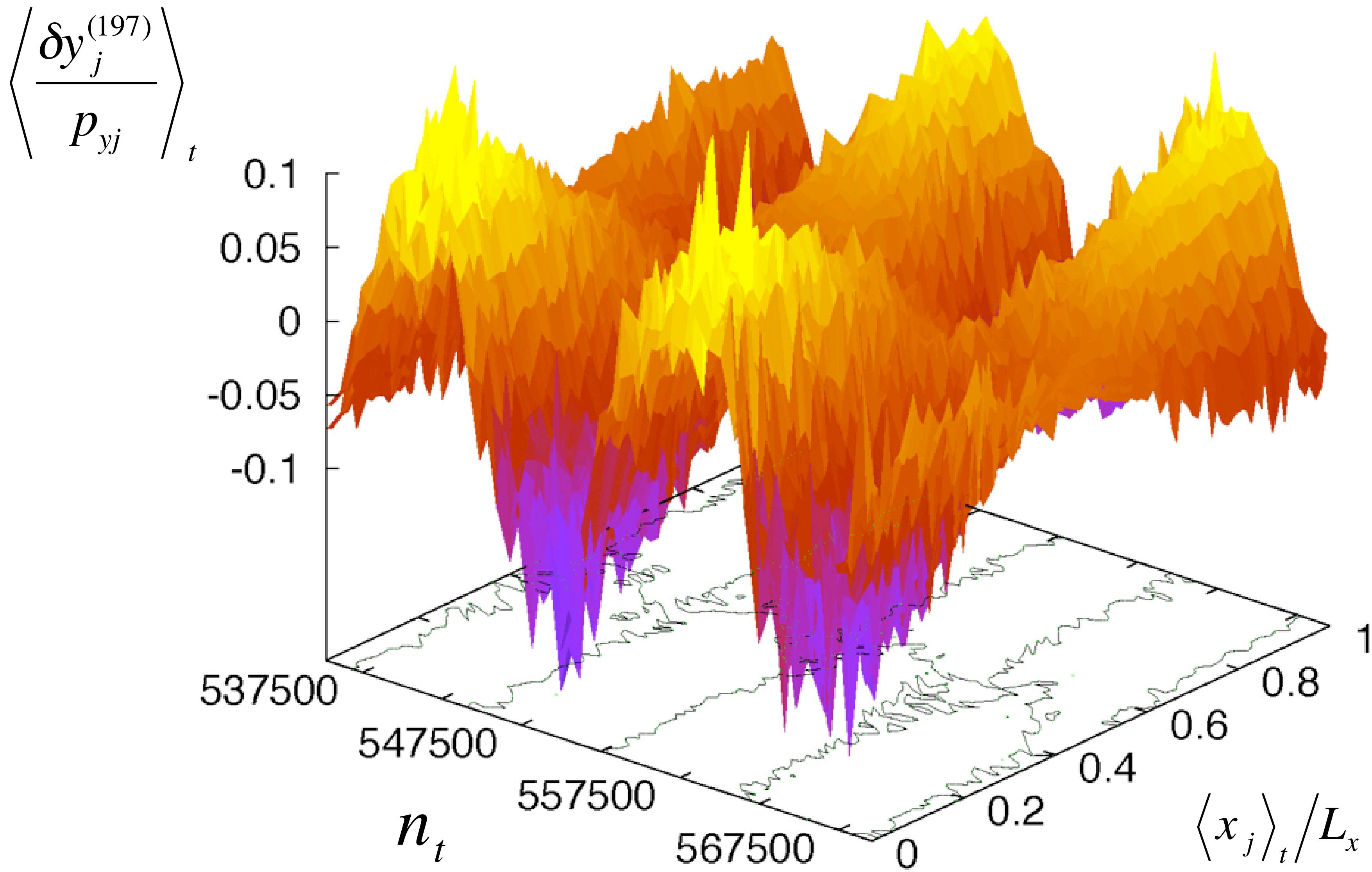


P mode

$$\delta x_j \sim p_{xj} \cos(k_1 x_j) \sin(\omega t)$$

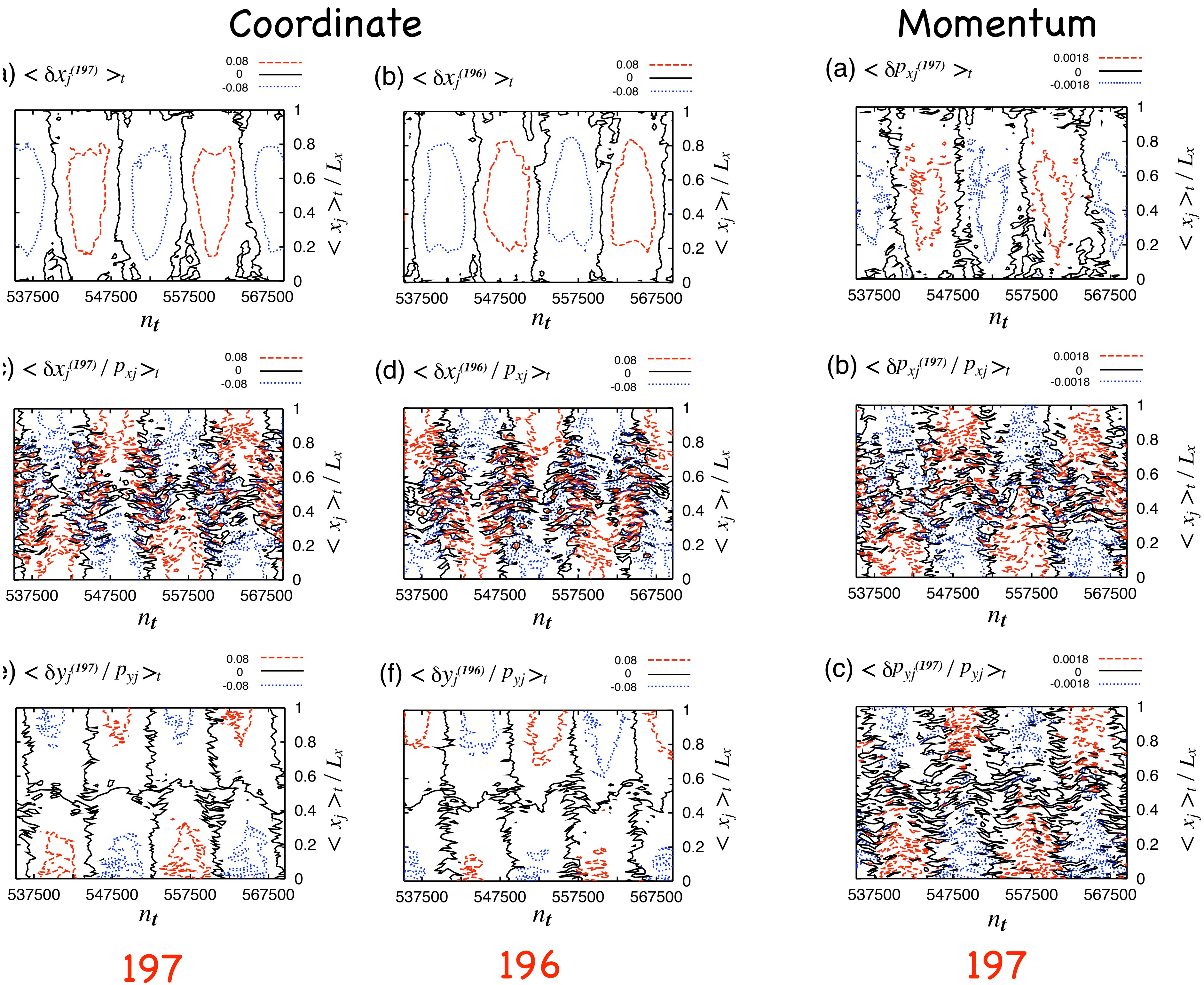
Lyapunov modes

First 2-point step



P mode

$$\delta y_j \sim p_{yj} \cos(k_1 x_j) \sin(\omega t)$$



Coordinate
Momentum
(a) < δx_j^(197) >_t
(b) < δx_j^(196) >_t
(c) < δx_j^(197) / p_xj >_t
(d) < δx_j^(196) / p_xj >_t
(e) < δy_j^(197) / p_yj >_t
(f) < δy_j^(196) / p_yj >_t
(a) < δp_xj^(197) >_t
(b) < δp_xj^(197) / p_xj >_t
(c) < δp_yj^(197) / p_yj >_t
0.08
0
-0.08
0.0018
0
-0.0018
< x_j >_t / L_x
n_t
537500
547500
557500
567500
0
0.2
0.4
0.6
0.8
1
197
196
197

Summary of Modes

For Quasi-one-dimensional system with (H,P)
the principle contribution to the mode

1-point steps - transverse modes

n=0

$$\delta\Gamma_y = \frac{1}{\sqrt{N}}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

n≠0

$$\delta\Gamma_{198} = \begin{pmatrix}0\\ \beta\cos kx_j\\ 0\\ \beta'\cos kx_j\end{pmatrix}$$

k_n - boundary condition dependent

coordinate and momentum components same functional form

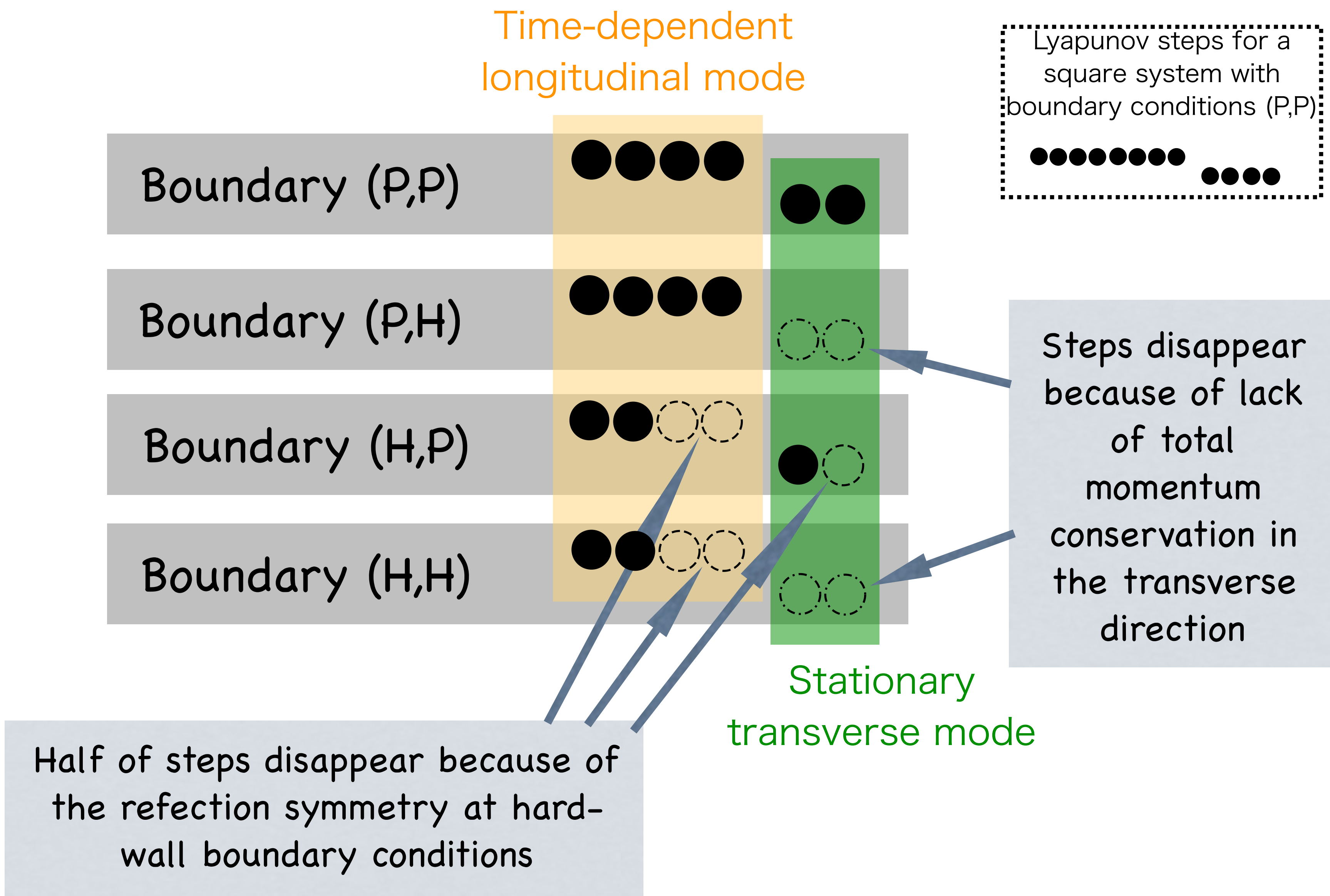
β and β' depend upon density

2-point steps - longitudinal modes

$$\delta\Gamma_{197} = -\cos\omega t \begin{pmatrix} \alpha \sin kx_j \\ 0 \\ \alpha' \sin kx_j \\ 0 \end{pmatrix} + \sin\omega t \begin{pmatrix} \beta p_{xj} \cos kx_j \\ \beta p_{yj} \cos kx_j \\ \beta' p_{xj} \cos kx_j \\ \beta' p_{yj} \cos kx_j \end{pmatrix}$$

$$\delta\Gamma_{196} = -\sin\omega t \begin{pmatrix} \alpha \sin kx_j \\ 0 \\ \alpha' \sin kx_j \\ 0 \end{pmatrix} + \cos\omega t \begin{pmatrix} \beta p_{xj} \cos kx_j \\ \beta p_{yj} \cos kx_j \\ \beta' p_{xj} \cos kx_j \\ \beta' p_{yj} \cos kx_j \end{pmatrix}$$

Comparison of Boundary Conditions



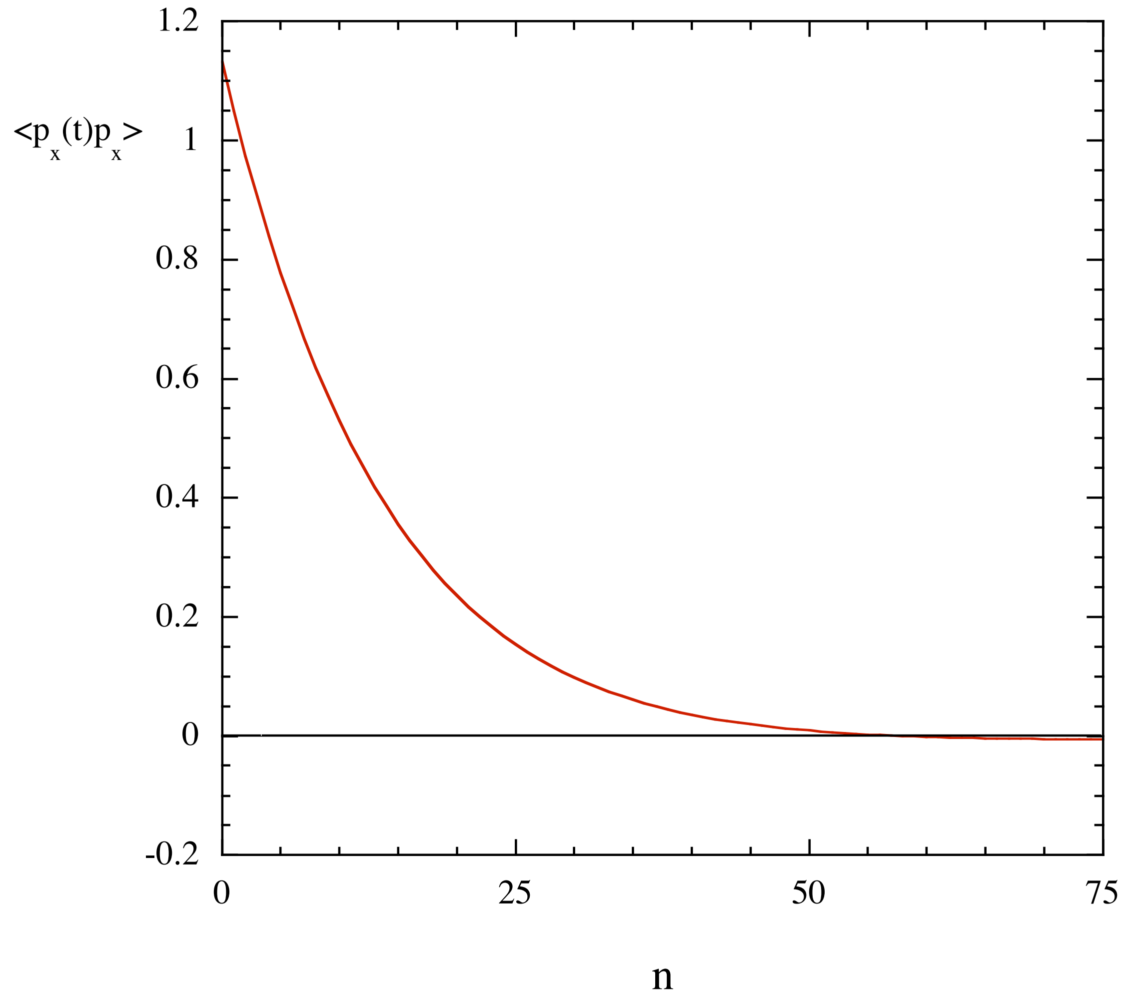
Time Dependence

Time Correlation Functions

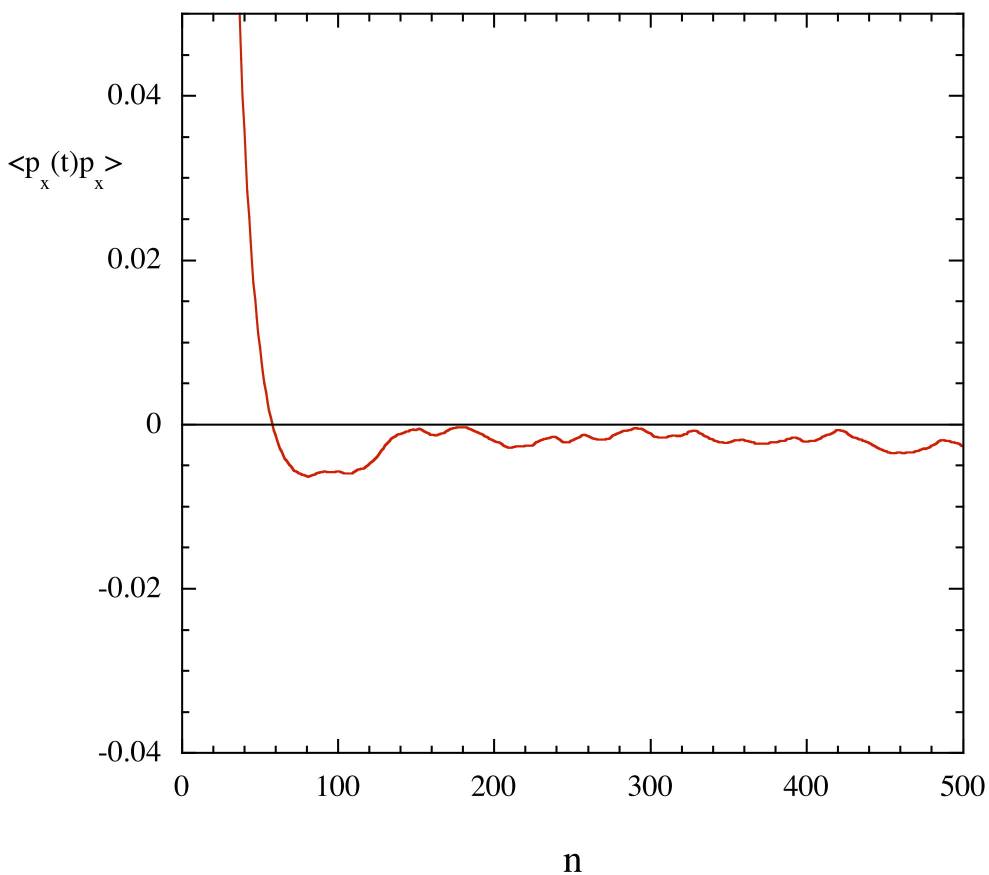
- Experimentally measurable quantities
- Time dependent properties
- Integrals give transport coefficients
- Connections with linear response theory

Velocity autocorrelation function $\langle p_x(t) p_x(0) \rangle$

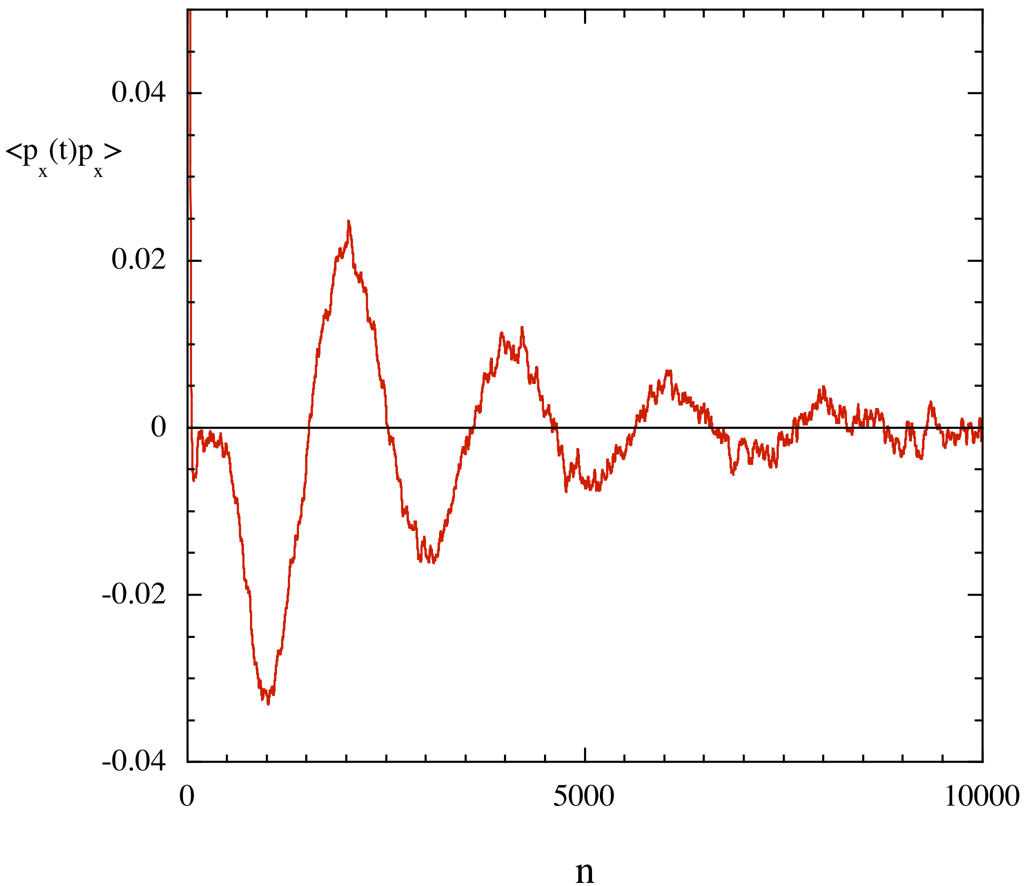
Initial exponential-like decay



At longer time
random behaviour



At very long time



Periods for different Boundary Conditions

	τ	$T_{lyap}\ \tau$	$T_{acf}\ \tau$
(P,P)	0.0369	77.0	37.4
(P,H)	0.0371	91.5	45.9
(H,P)	0.0380	154.5	77.4
(H,H)	0.0383	194.5	96.8

Numerical Results

- Momentum autocorrelation function has oscillatory behaviour at long time

$$\left\langle p_{xj}(t)\, p_{xj}(0) \right\rangle \sim \sin \omega t \qquad (1)$$

- Lyapunov mode for the 2-points steps is oscillatory

$$\delta x_j \sim p_{xj} \cos\left(k_n x_j\right) \sin \omega_L t$$

- which implies

$$\left\langle \delta x_j(t)\, \delta x_j \right\rangle \sim \sin \omega_L t \qquad (2)$$

But:

$$
\begin{aligned}
\langle \delta x_j(t)\delta x_j \rangle &\sim \langle p_{xj}(t) p_{xj} \cos(k_n x_j)\cos(k_n x_j)\rangle \cos\omega_L t \\
&\sim \langle p_{xj}(t) p_{xj} \rangle \cos\omega_L t \\
&\sim \sin\omega t \cos\omega_L t \\
&\sim \sin(\omega - \omega_L)t \qquad (3)
\end{aligned}
$$

comparing (2) & (3)

$$\sin\omega_L t \sim \sin(\omega_L - \omega)t$$

Equating arguments

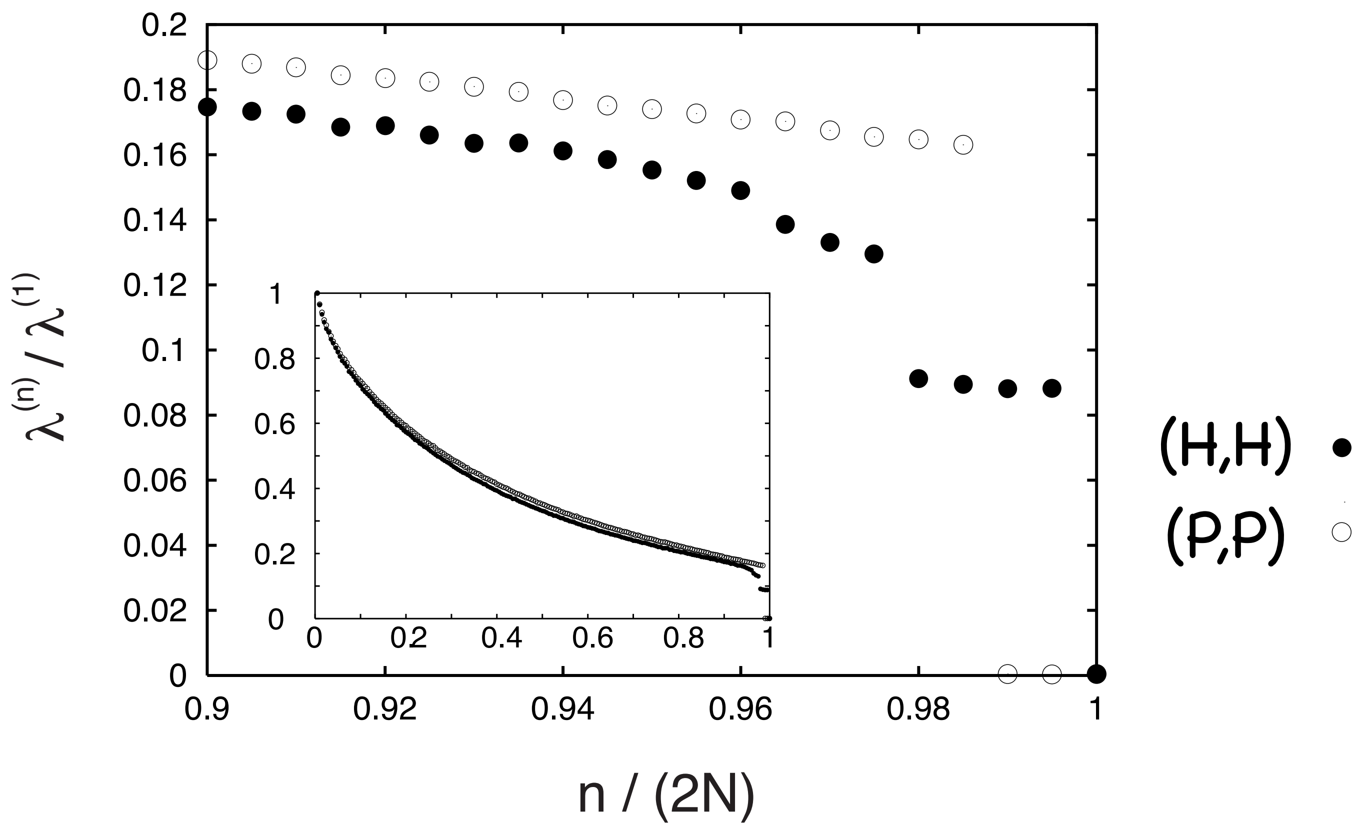
$$\omega_L = \omega - \omega_L$$

$$\Downarrow$$

$$\boxed{\omega_L = \tfrac{1}{2}\omega}$$

Two-dimensional Systems

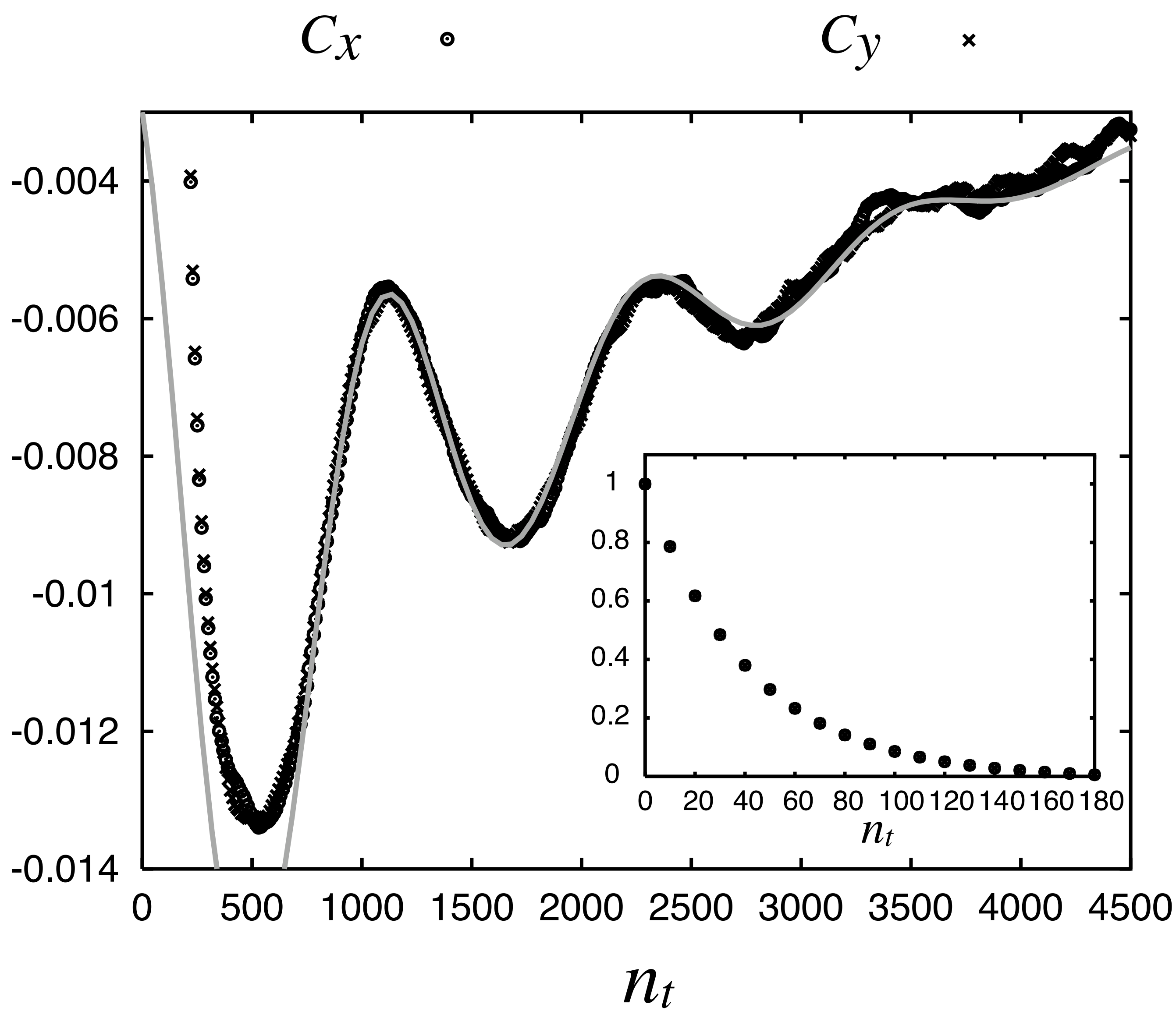
Lyapunov Spectrum in Two-dimensions



Two-dimensional square N=100

(H,H) has 4-point step, (P,P) has no steps

Momentum Autocorrelation Function

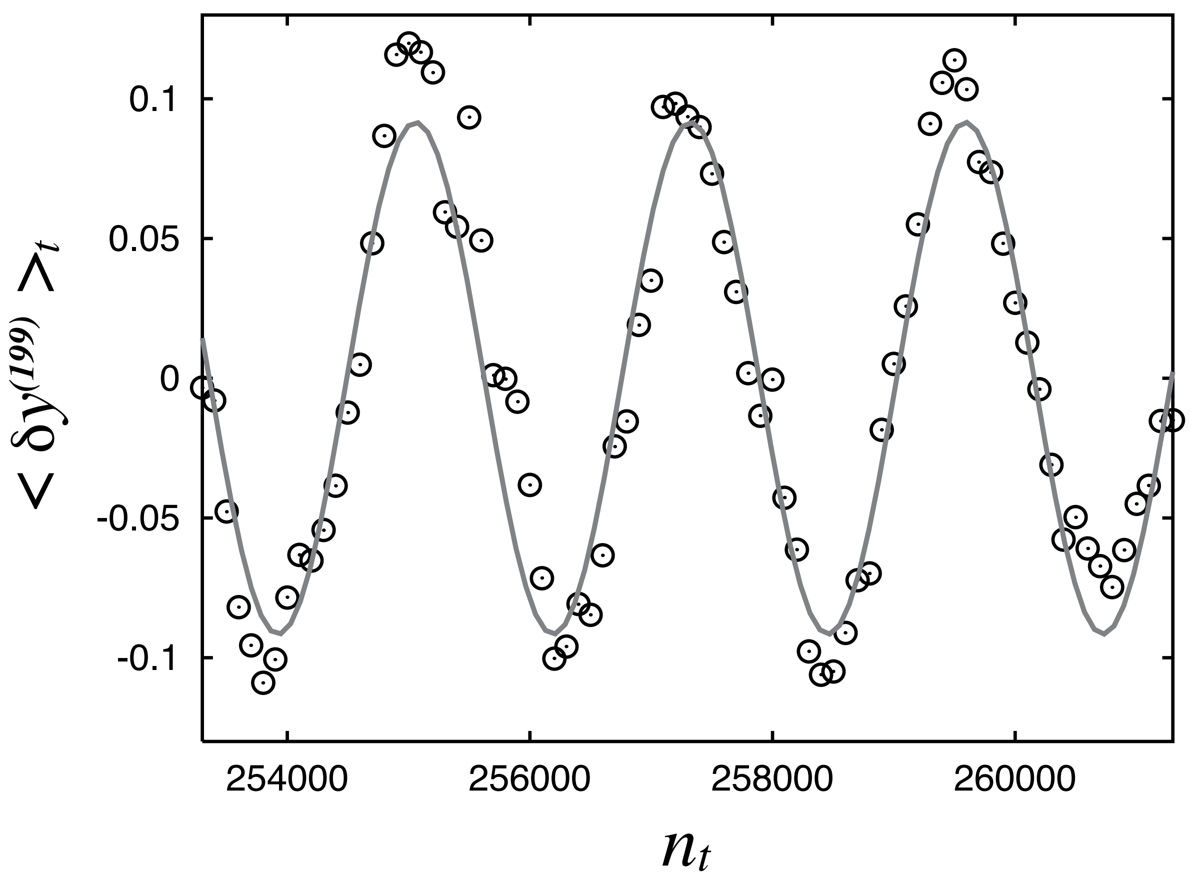


T_{tcf}=1189

Two-dimensional square N=100

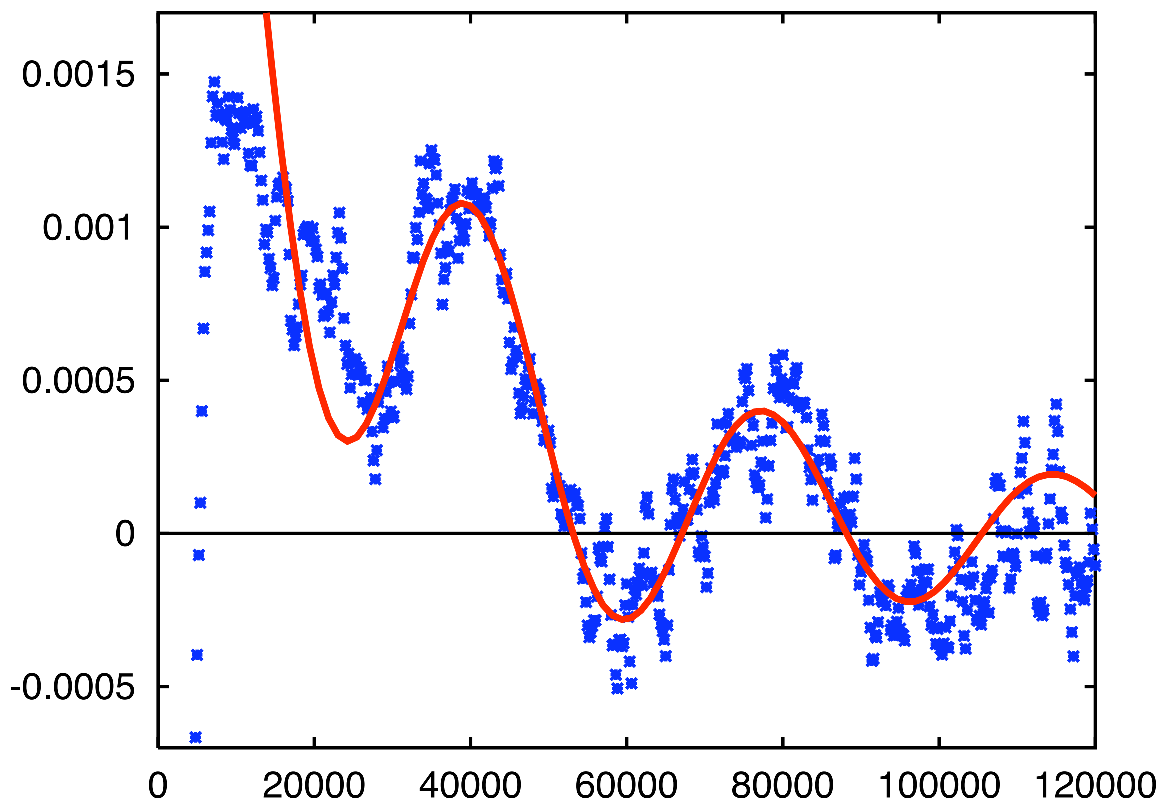
Time Dependence of Lyapunov Mode

Two-dimensional square N=100



T_{lyap}=2267 T_{tcf}=1189

Fully Two-Dimensional System



N=780

(H,H)

$L_y/L_x=0.867$

$N/(L_x\ L_y)=0.8$

$T_{acf}=37120=T_{lyap}/2$ $T_{lyap}=74031$ (Eckmann et. al.)

Lyapunov Localization

Localization

Contribution to n th Lyapunov vector from j th particle

$$\left|\delta\Gamma_j^{(n)}(t)\right|^2 = \left(\delta x_j^{(n)}\right)^2 + \left(\delta y_j^{(n)}\right)^2 + \left(\delta p_{xj}^{(n)}\right)^2 + \left(\delta p_{yj}^{(n)}\right)^2$$

Normalized contribution

$$\gamma_j^{(n)}(t) = \frac{\left|\delta\Gamma_j^{(n)}(t)\right|^2}{\sum_{k=1}^{N}\left|\delta\Gamma_k^{(n)}(t)\right|^2}$$

$$0 \le \gamma_n^{(j)}(t) \le 1$$

Localization 'width'

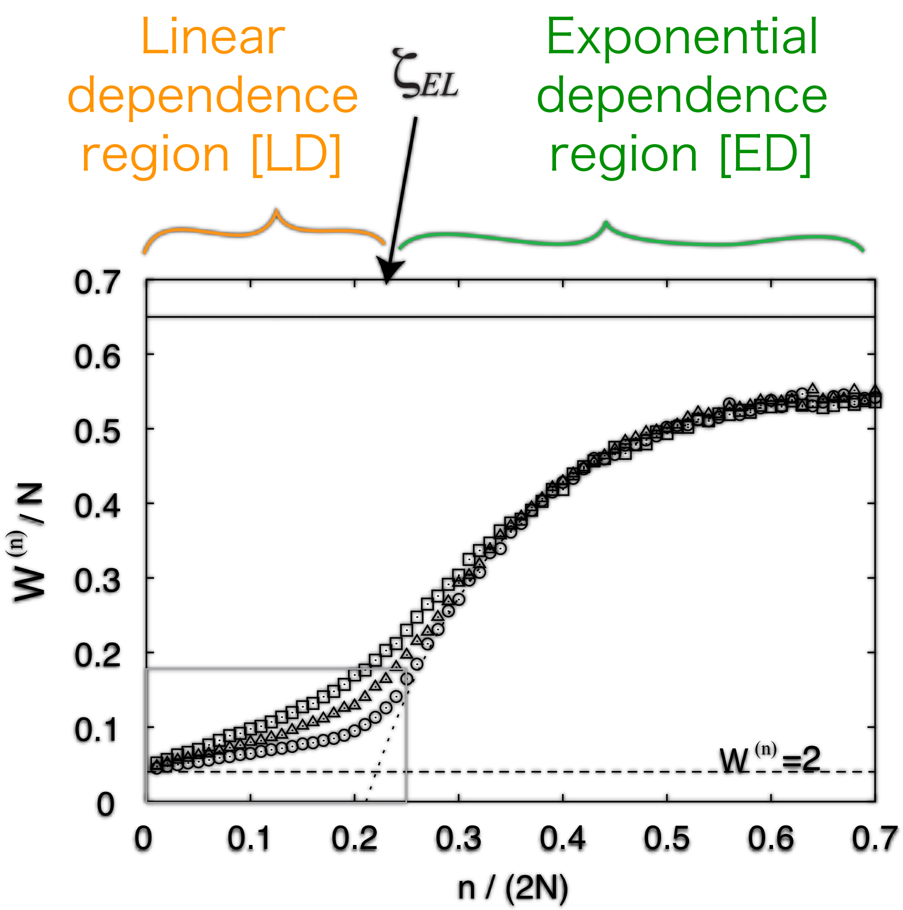
$$\frac{\mathcal{W}^{(n)}}{N} = \frac{1}{N}\exp\left(-\sum_{j=1}^{N}\left\langle \gamma_j^{(n)}(t)\ln\gamma_j^{(n)}(t)\right\rangle\right)$$

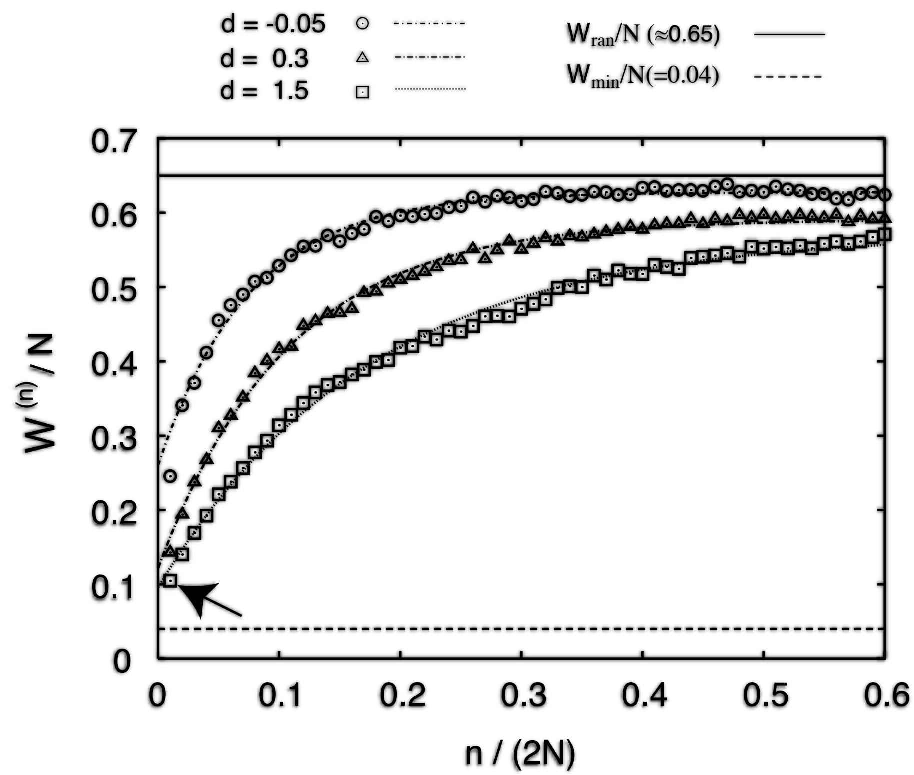
$$\frac{1}{N} \le \frac{\mathcal{W}^{(n)}}{N} \le 1$$

Localization spectra

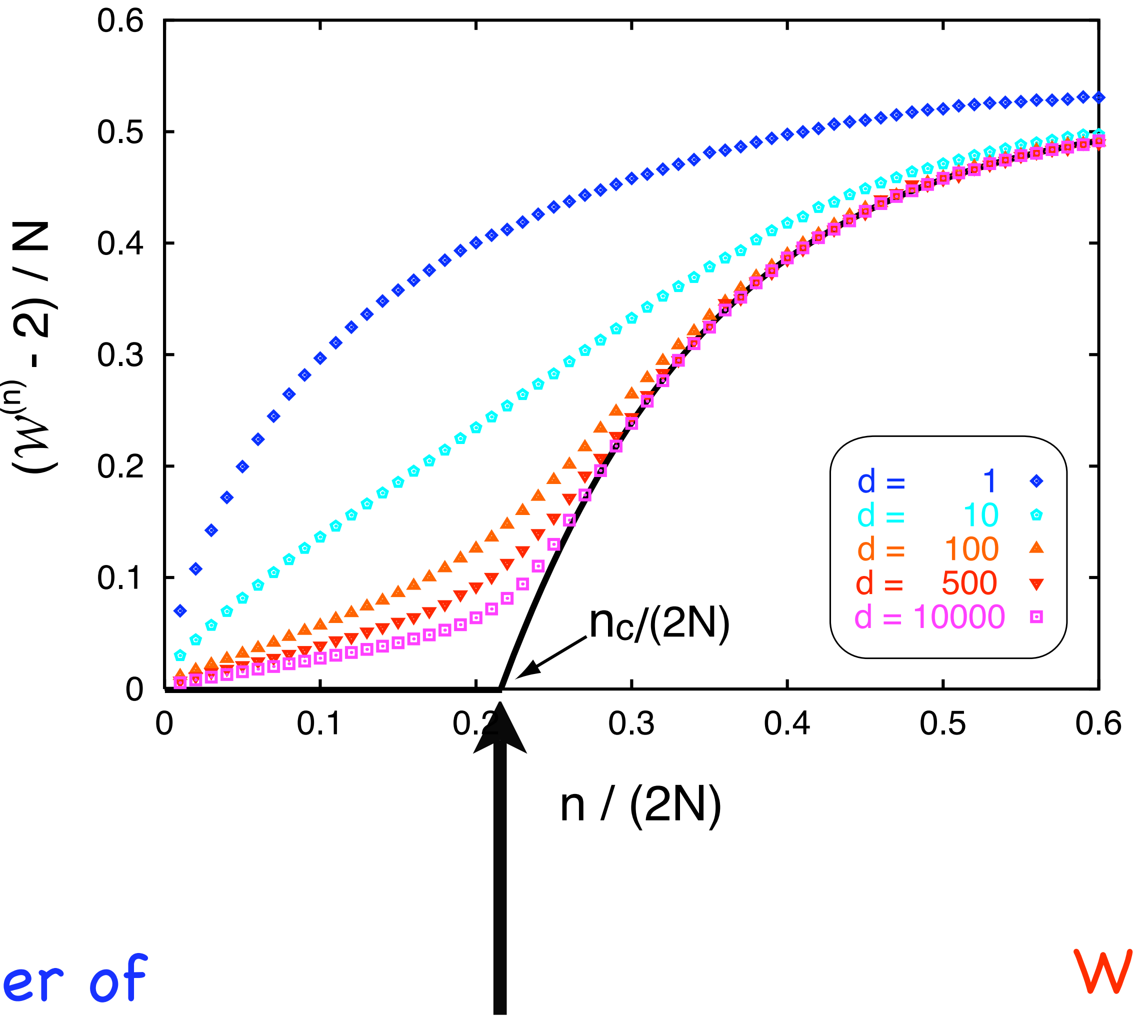
Low Density

High Density





Localization in Low density Limit



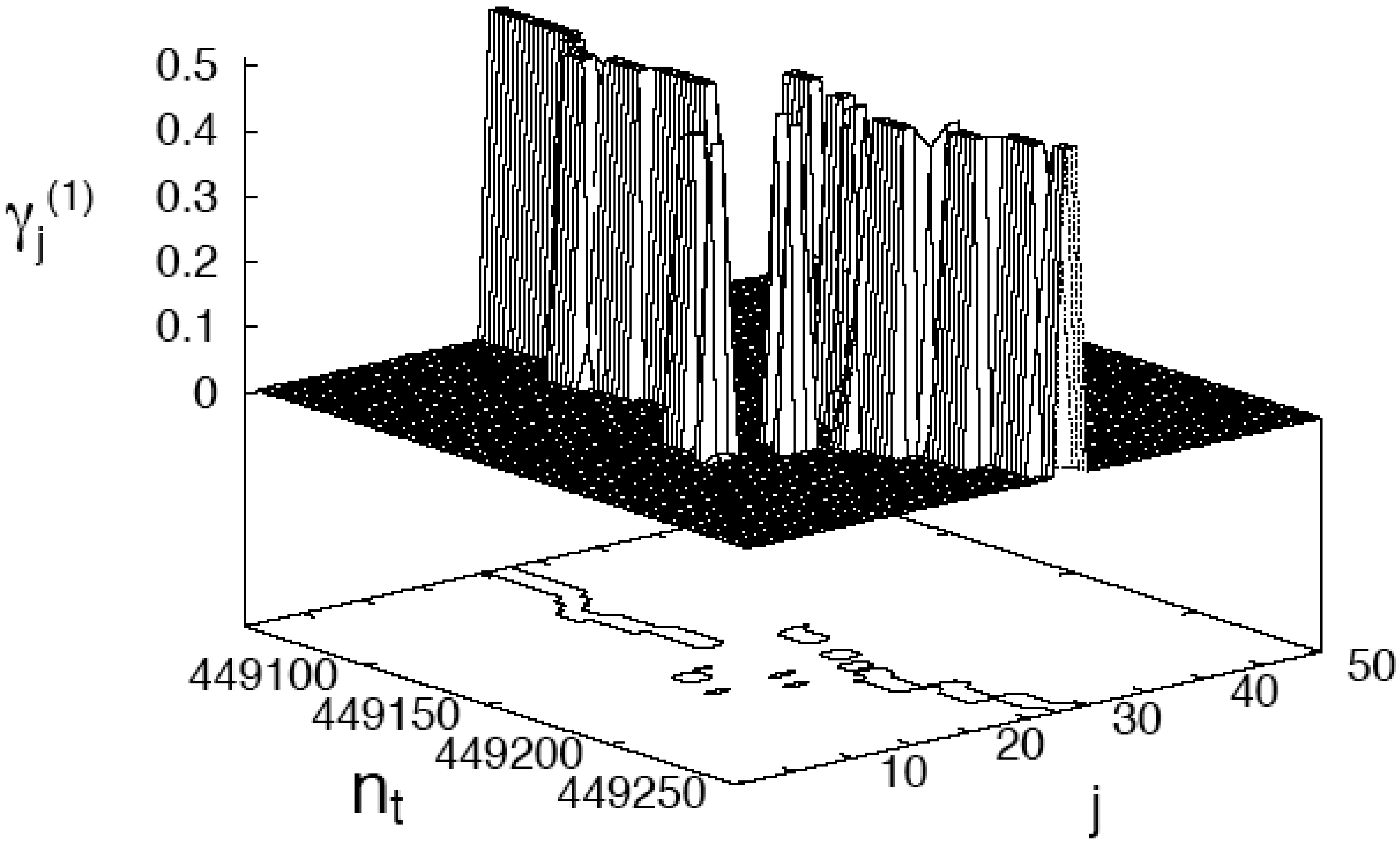
0.219±0.005

A fixed number of strongly localized vectors

Why does this happen?

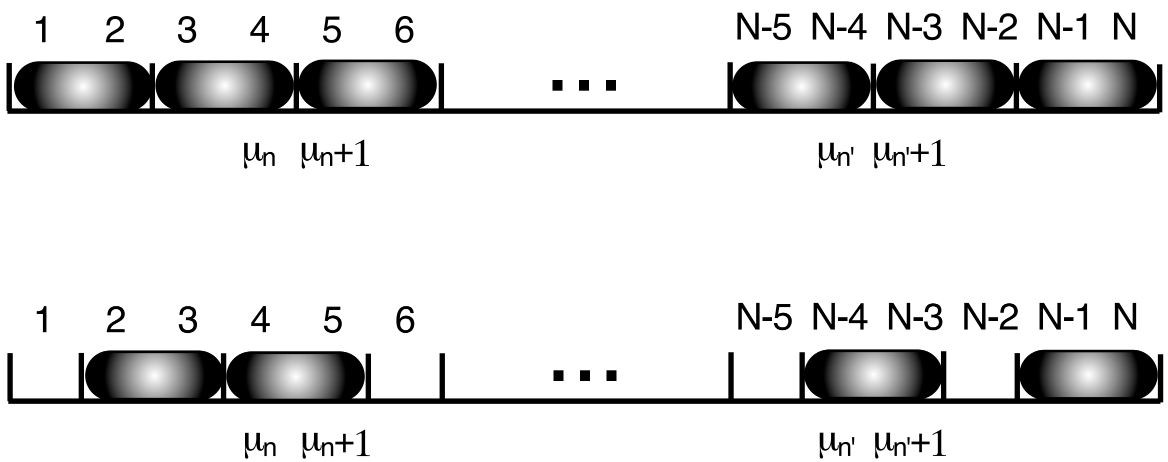
Localization for the Lyapunov vector of the largest exponent

Quasi-one-dimensional System



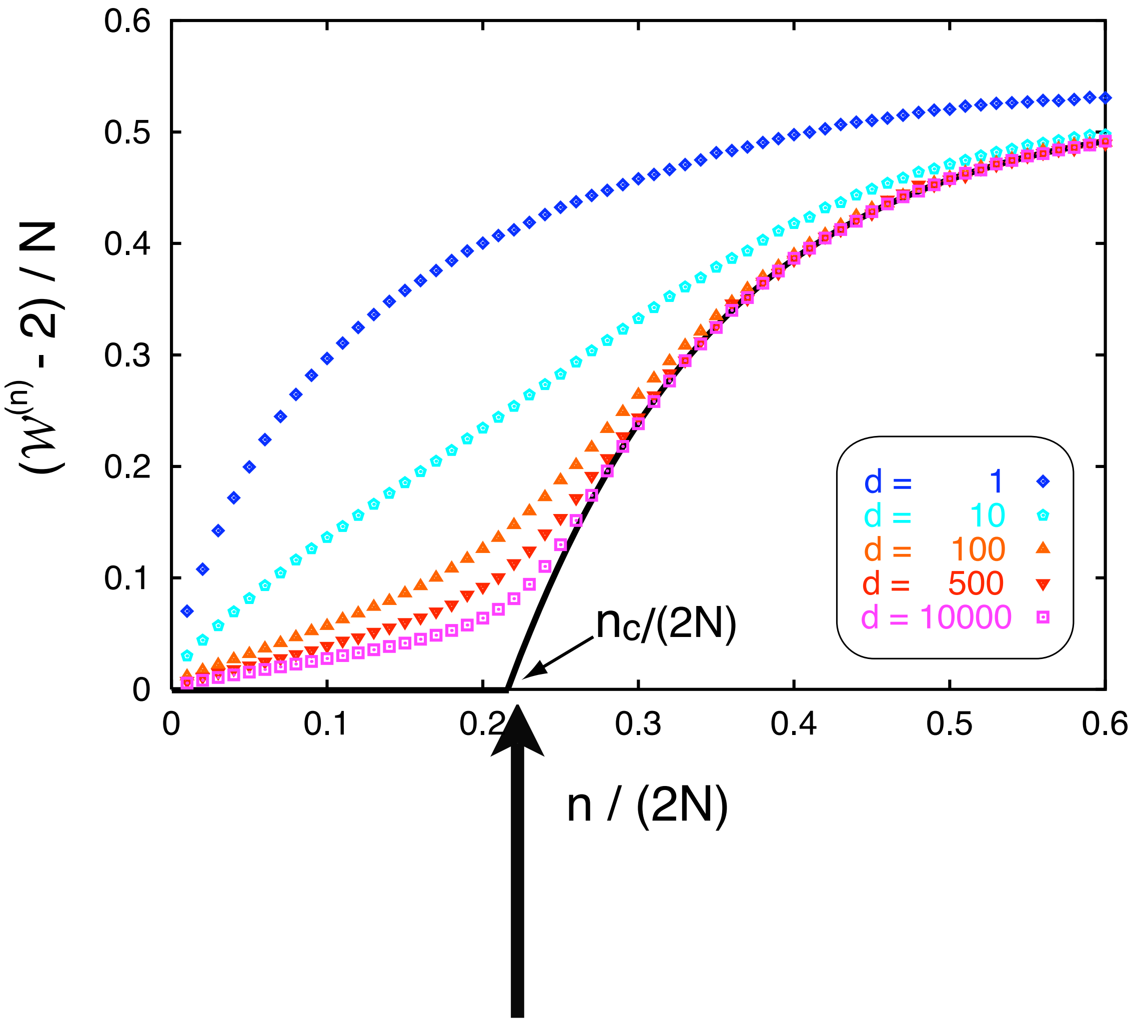
Randomly Distributed Brick Model

Conjecture: The number of most localized Lyapunov vectors is equal to the number of exponents in the linear region



The number of exponents in the linear region is the average number of randomly dropped bricks

Localization in Low density Limit



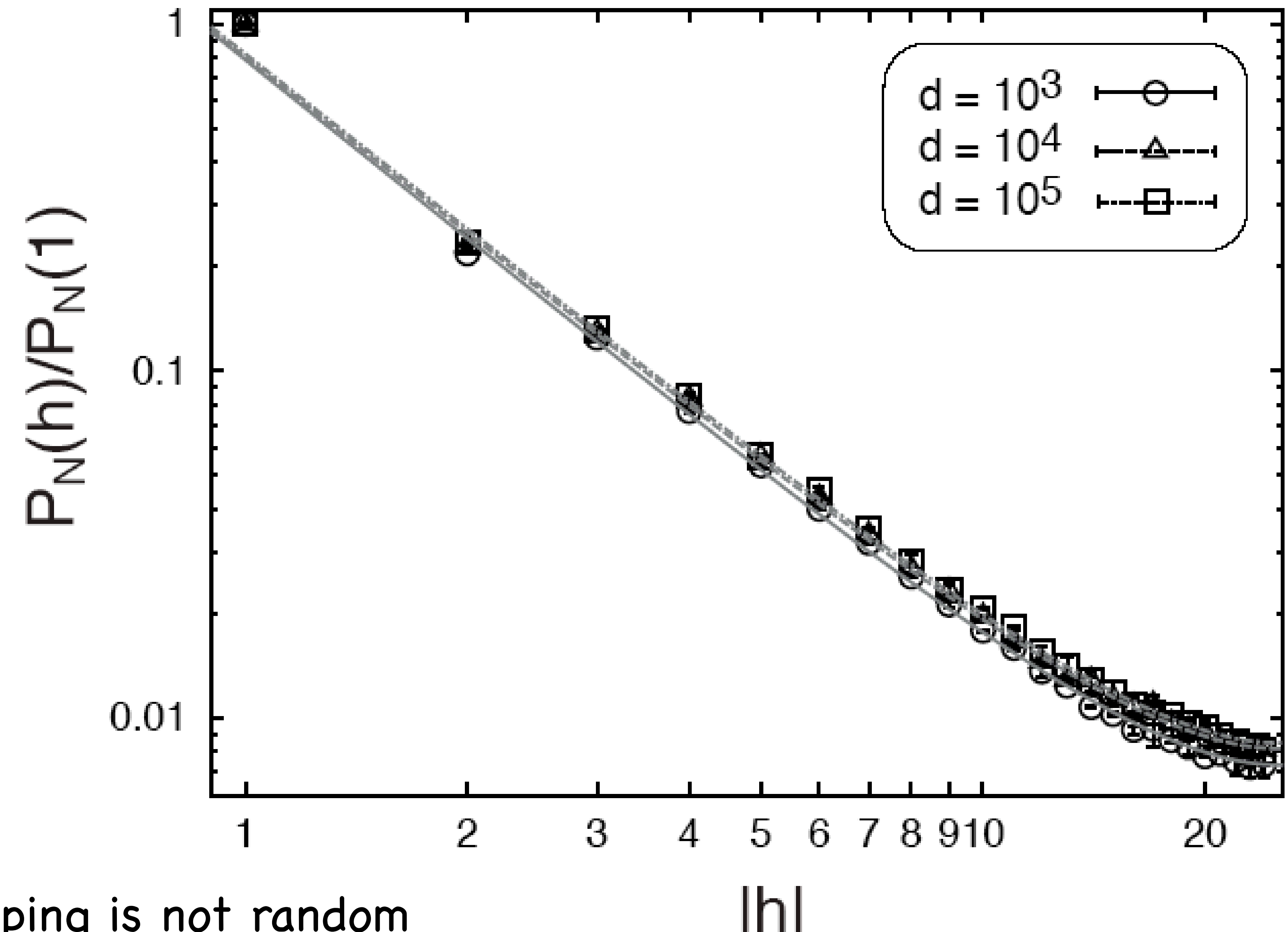
Randomly distributed brick model gives 0.216

(0.219±0.005)

Dynamics of the most Localized Lyapunov vector

Normalized Hopping Rate

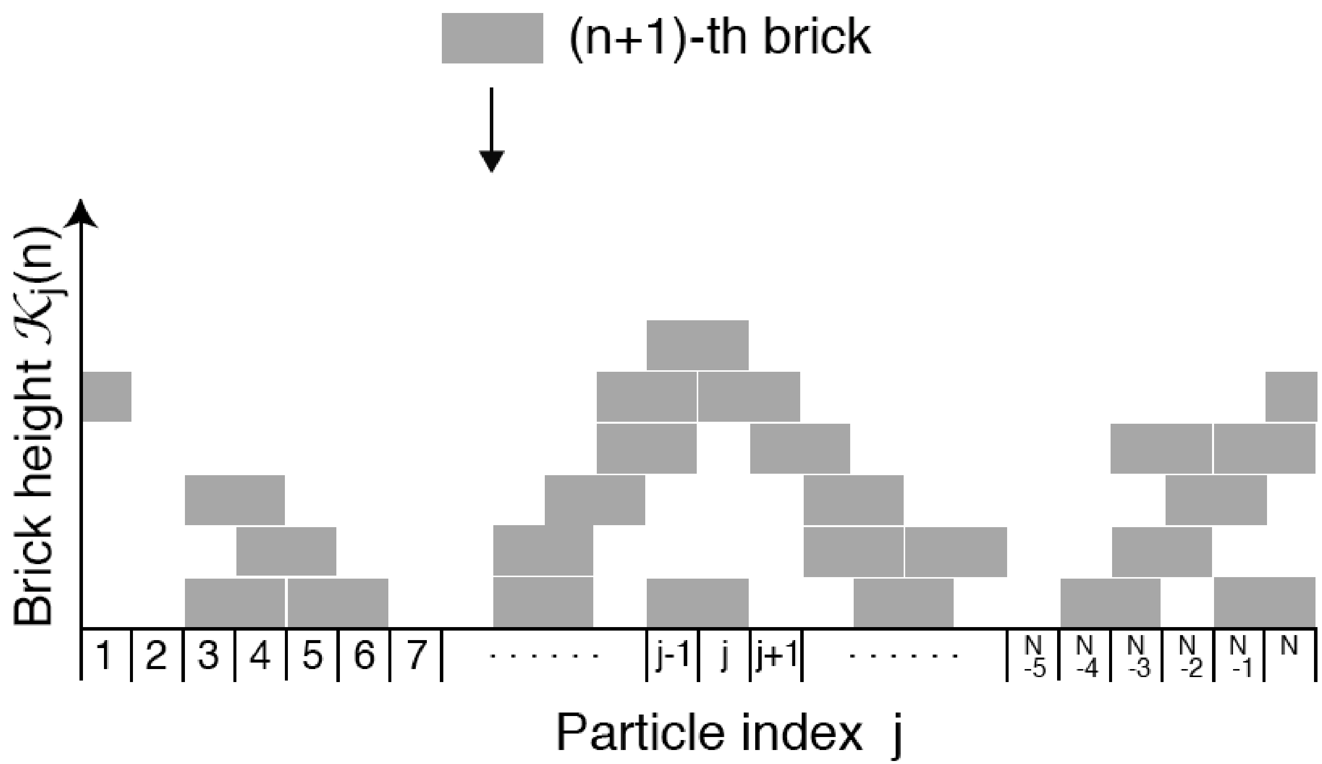
Density dependence



Hopping is not random

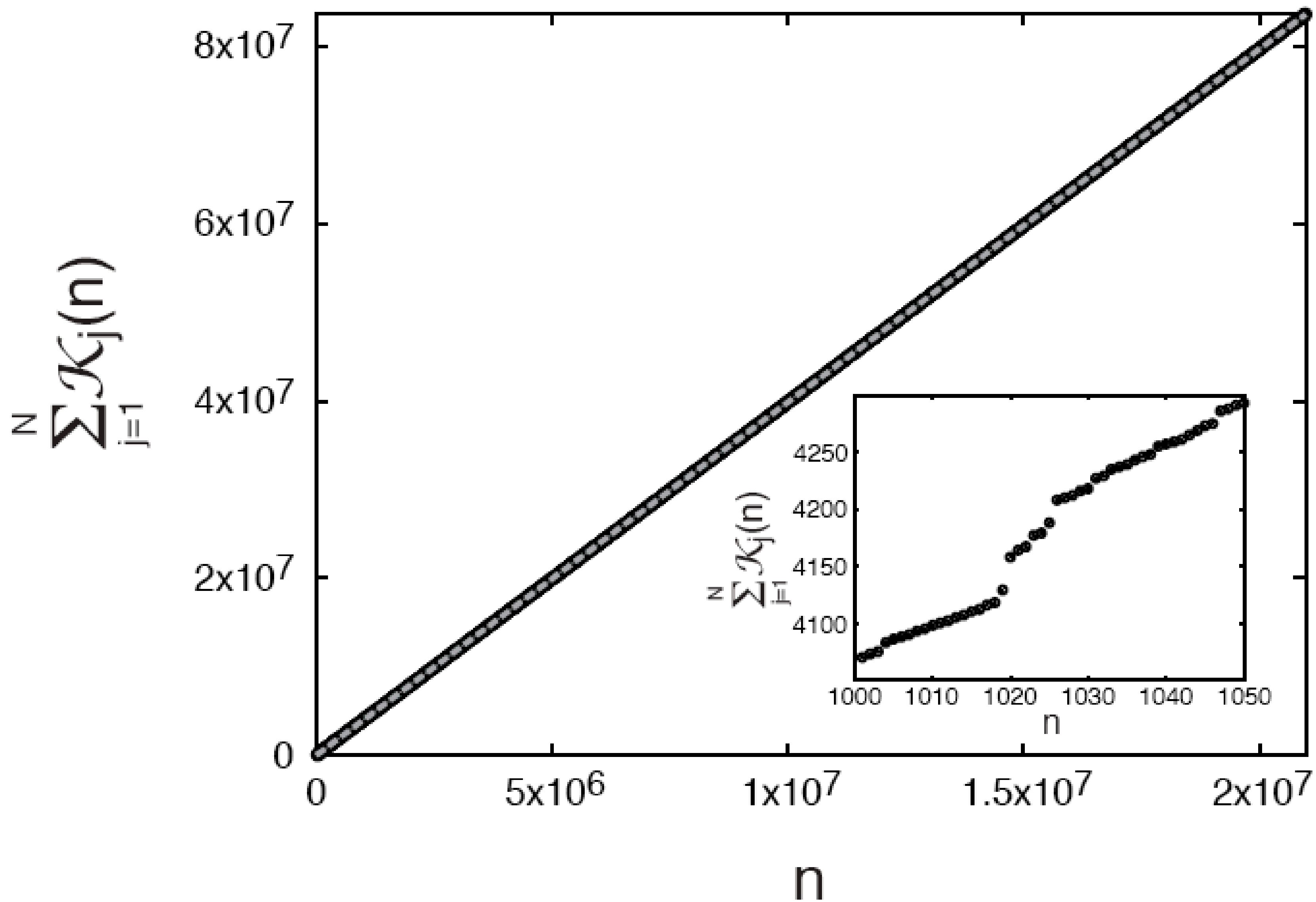
Brick Accumulation Model

$$\mathcal{K}_l(n) = \begin{cases} \max\{\mathcal{K}_j(n-1), \mathcal{K}_k(n-1)\} + 1 & \text{for} \quad j,k \\ \mathcal{K}_l(n-1) & \text{for} \quad l \notin \{j,k\} \end{cases}$$

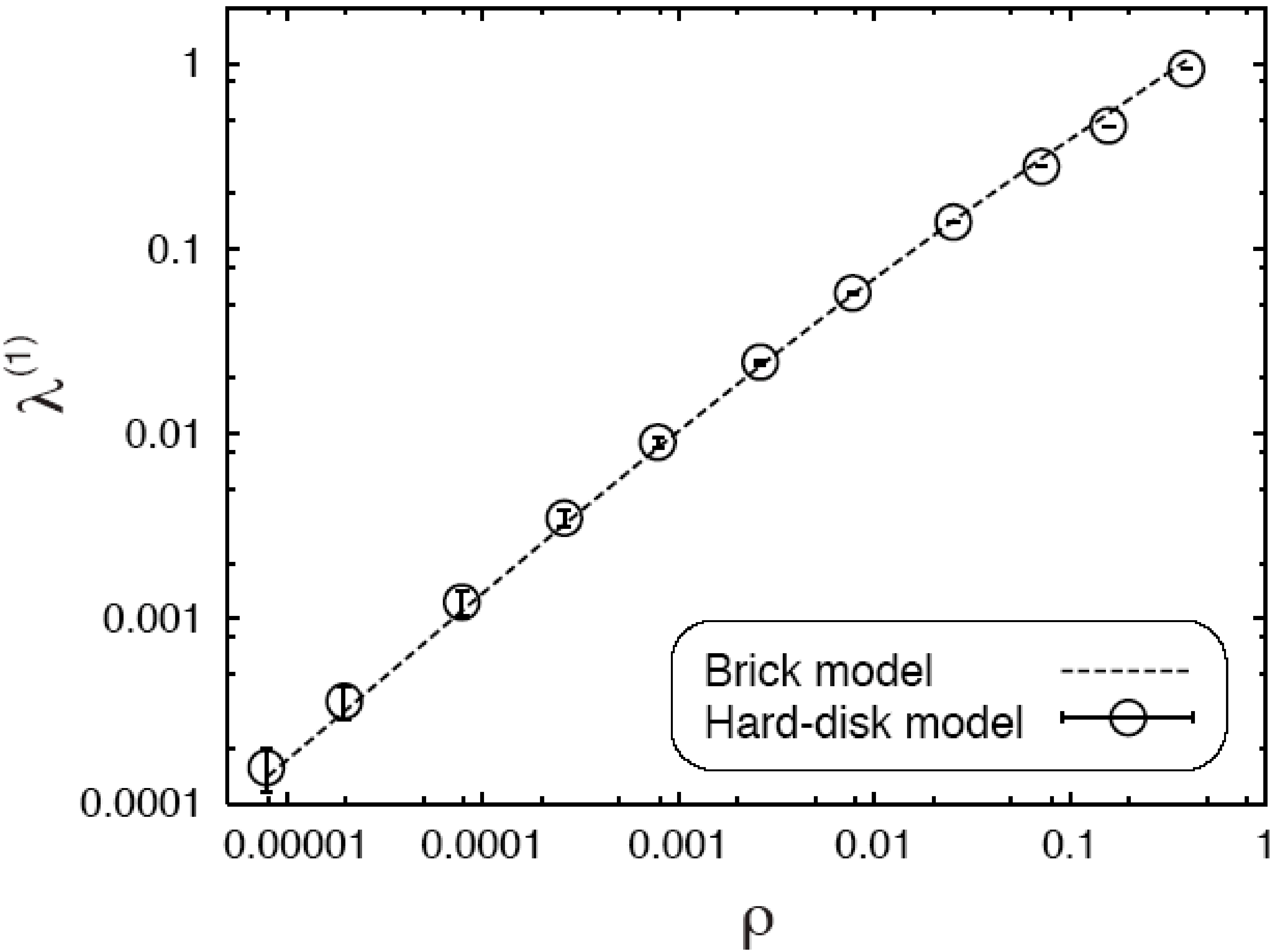


Clock Model

Total Accumulation Rate



Largest Lyapunov Exponent



Conclusions

- Space and time dependent Longitudinal modes

- The period of the oscillating Lyapunov mode and the period of oscillations in the momentum auto-correlation function are related.

- This connection is independent of the boundary conditions:
ω and ω_L change but $\omega_L = \frac{1}{2}\omega$ remains!

- The relation is correct for fully two-dimensional systems.

- Linear region in Localization spectrum is explained

- Dynamics explained by brick accumulation model

NEXT

Nonequilibrium Heat flow

Left-side boundary condition

$$p_x' = \varepsilon p_{T_L} - (1-\varepsilon)\, p_x$$

Right-side boundary condition

$$p_x' = -\varepsilon p_{T_R} - (1-\varepsilon)\, p_x$$

HOT | Quasi-one-dimensional system | COLD

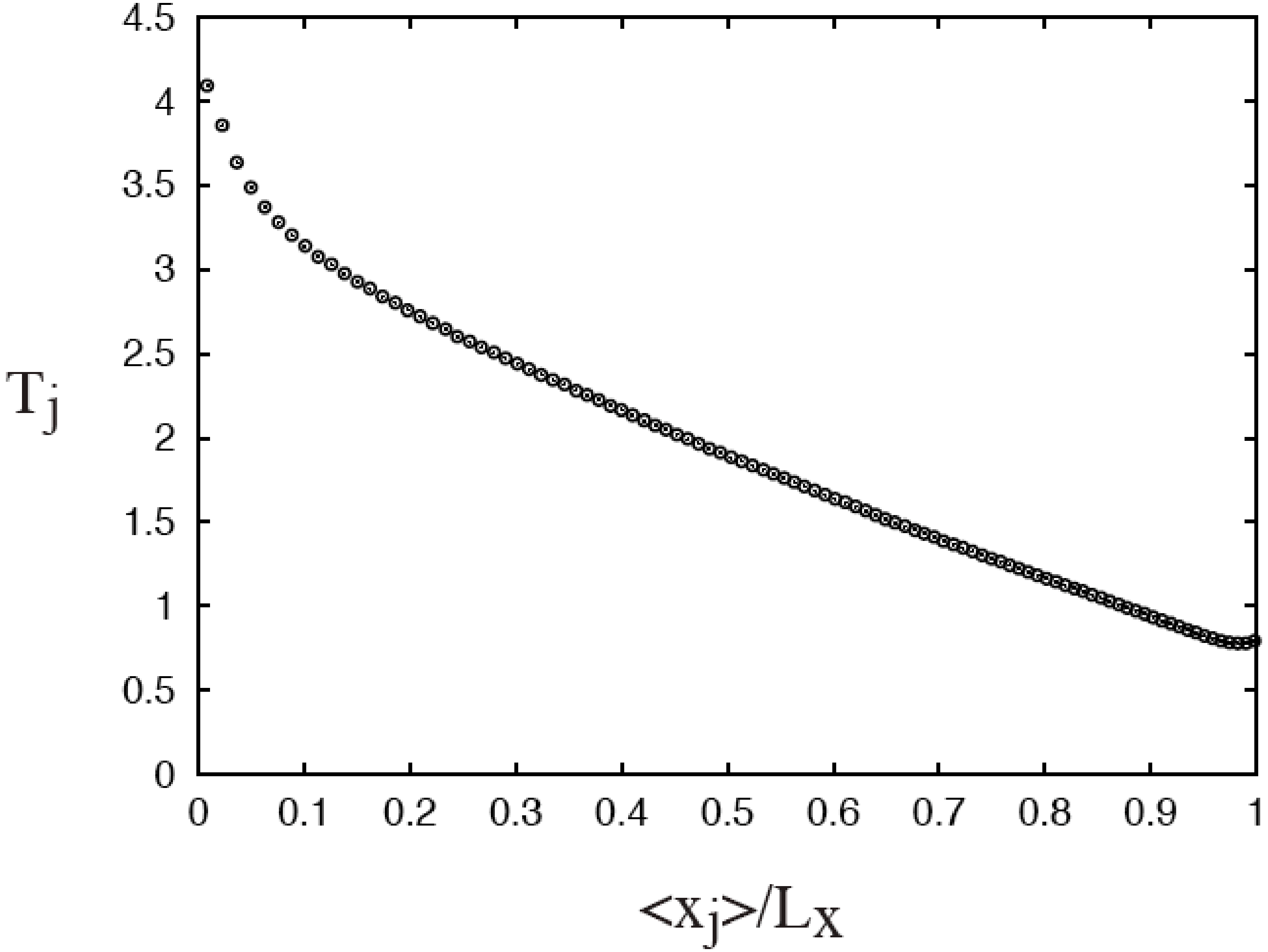
T=10 | T=1

N=100

$$\varepsilon = 0.5$$

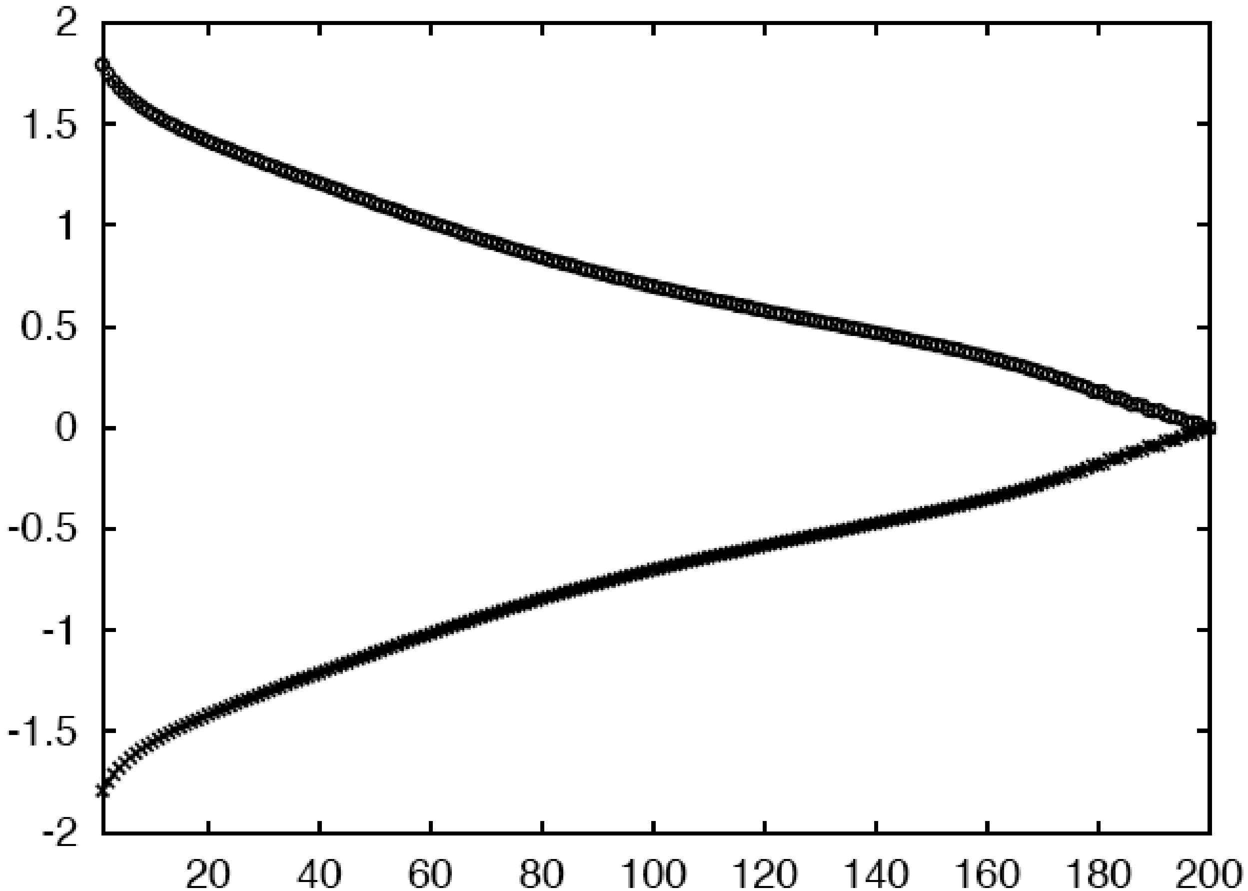
Temperature Profile

T=10

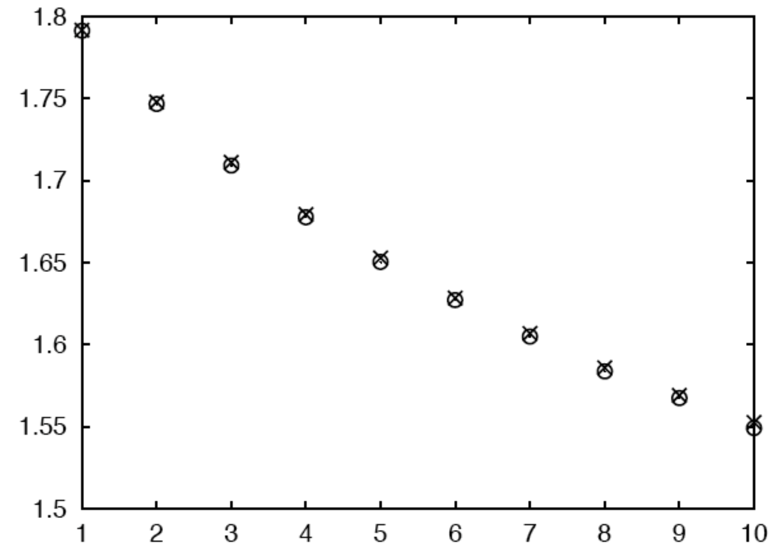


T=1

Full Spectrum of Lyapunov Exponents



Largest positive and negative exponents



Smallest positive and negative exponents