Lyapunov instability of hard-particle systems

Harald A. Posch
Hadrien Bosetti, Jacobus van Meel

University of Vienna

Exploring Complex Dynamics in High-Dimensional Chaotic Systems:
From Weather Forecasting to Oceanic Flows
MPI für Physik komplexer Systeme, Dresden, 25 – 29 January 2010

Outline

“Smooth“ hard elastic particles:

- Gram-Schmidt and covariant Lyapunov vectors
- Localized and delocalized Lyapunov modes
- L and P-mode reconstruction
- Transversality

Physical consequences

“Rough“ hard particles

Lyapunov instability in phase space

$$\mathbf{\Gamma} = \{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N, \mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N\}$$

$$\dot{\mathbf{\Gamma}} = \mathbf{F}(\mathbf{\Gamma})$$

$$\delta\mathbf{\Gamma} = \{\delta\mathbf{q}_1, \delta\mathbf{q}_2, \ldots, \delta\mathbf{q}_N, \delta\mathbf{p}_1, \delta\mathbf{p}_2, \ldots, \delta\mathbf{p}_N\}$$

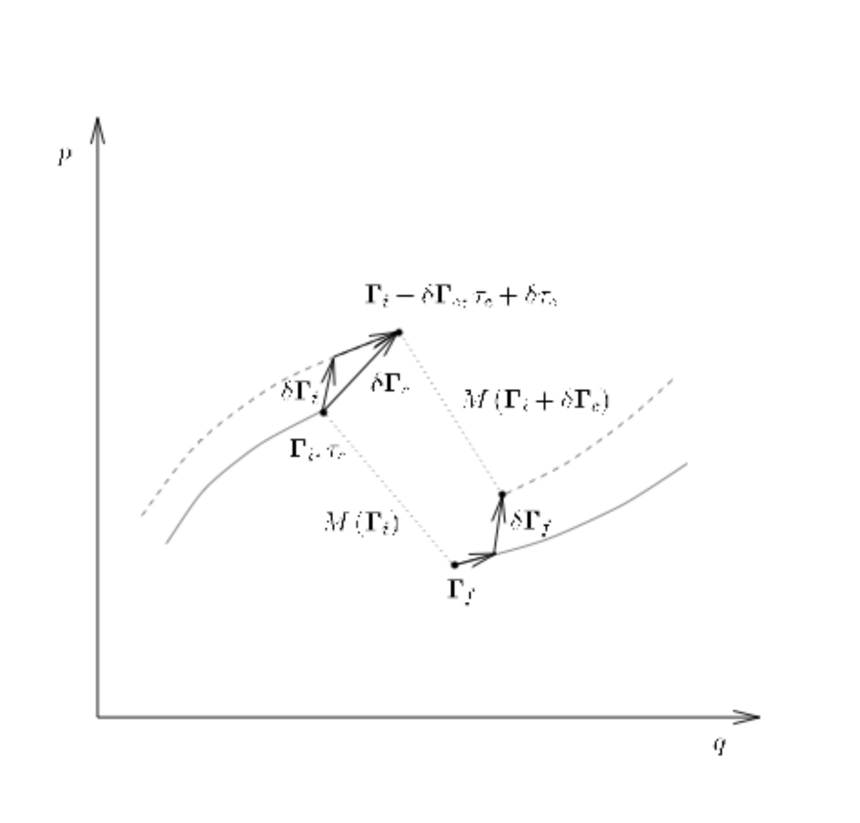
$$\delta\dot{\mathbf{\Gamma}} = \frac{\partial \mathbf{F}(\mathbf{\Gamma})}{\partial \mathbf{\Gamma}} \cdot \delta\mathbf{\Gamma}$$

$$\lambda_l = \lim_{t\to\infty} \frac{1}{t} \log \frac{|\delta\mathbf{\Gamma}_l\,(t)|}{|\delta\mathbf{\Gamma}_l\,(0)|}.$$

$$\delta\mathbf{\Gamma}_l\,(0)\,, \quad l = 1, \ldots, 2dN$$

$$\{\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_L\}$$

Perturbations in tangent space



$$\Gamma(t) = \{\mathbf{q}_i(t), \mathbf{p}_i(t); i = 1, \ldots, N\}$$

$$\dot{\Gamma} = \mathbf{F}(\Gamma),$$

$$\Gamma(t) = \Phi^t(\Gamma(0))$$

$$\Gamma_f = \mathbf{M}(\Gamma_i)$$

$$\delta\Gamma_f = \frac{\partial \mathbf{M}}{\partial \Gamma_i} \cdot \delta\Gamma_i + \left[\frac{\partial \mathbf{M}}{\partial \Gamma_i} \cdot \mathbf{F}(\Gamma_i) - \mathbf{F}(\mathbf{M}(\Gamma_i))\right] \delta\tau_c(\Gamma_i, \delta\Gamma_i)$$

$$\lambda = \lim_{t \to \infty} \frac{1}{t} \log \frac{|\delta\Gamma(t)|}{|\delta\Gamma(0)|}.$$

Streaming between collisions:

$$\mathbf{q}_j(t) = \mathbf{q}_j(0) + \mathbf{p}_j(0)/m \cdot t$$
$$\mathbf{p}_j(t) = \mathbf{p}_j(0)$$

$$\mathbf{J}_s : \begin{cases} \delta\mathbf{q}_j(t) = \delta\mathbf{q}_j(0) + \delta\mathbf{p}_j(0)/m \cdot t \\ \delta\mathbf{p}_j(t) = \delta\mathbf{p}_j(0) \end{cases}$$

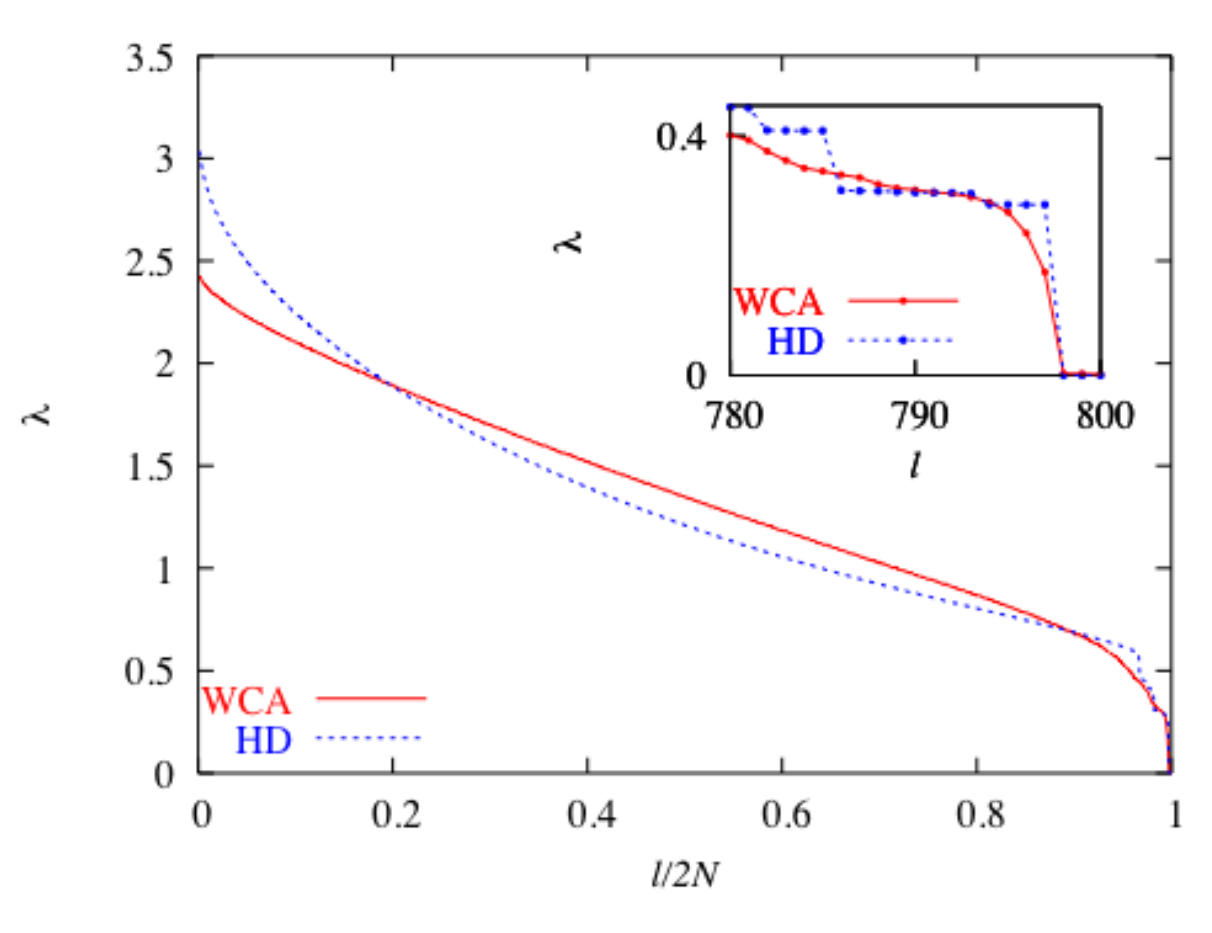
Collision between k and l:

$$\mathbf{p}_k^f = \mathbf{p}_k^i + (\mathbf{p}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 \qquad \mathbf{q} \equiv \mathbf{q}_l - \mathbf{q}_k$$
$$\mathbf{p}_l^f = \mathbf{p}_l^i - (\mathbf{p}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 \qquad \mathbf{p} \equiv \mathbf{p}_l - \mathbf{p}_k$$

$$\mathbf{J}_c : \begin{cases} \delta\mathbf{q}_k^f = \delta\mathbf{q}_k^i + (\delta\mathbf{q}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 & \delta\mathbf{q} \equiv \delta\mathbf{q}_l - \delta\mathbf{q}_k \\ \delta\mathbf{q}_l^f = \delta\mathbf{q}_l^i - (\delta\mathbf{q}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 & \delta\mathbf{p} \equiv \delta\mathbf{p}_l - \delta\mathbf{p}_k \\ \delta\mathbf{p}_k^f = \delta\mathbf{p}_k^i + (\delta\mathbf{p}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 + \frac{1}{\sigma^2}\left[(\mathbf{p}\cdot\delta\mathbf{q}_c)\,\mathbf{q} + (\mathbf{p}\cdot\mathbf{q})\,\delta\mathbf{q}_c\right] & \\ \delta\mathbf{p}_l^f = \delta\mathbf{p}_l^i - (\delta\mathbf{p}\cdot\mathbf{q})\,\mathbf{q}/\sigma^2 - \frac{1}{\sigma^2}\left[(\mathbf{p}\cdot\delta\mathbf{q}_c)\,\mathbf{q} + (\mathbf{p}\cdot\mathbf{q})\,\delta\mathbf{q}_c\right] & \end{cases}$$

$$\delta\mathbf{q}_c = \delta\mathbf{q} - \frac{(\delta\mathbf{q}\cdot\mathbf{q})}{(\mathbf{p}\cdot\mathbf{q})}\mathbf{p}$$

Lyapunov spectra for soft and hard disks

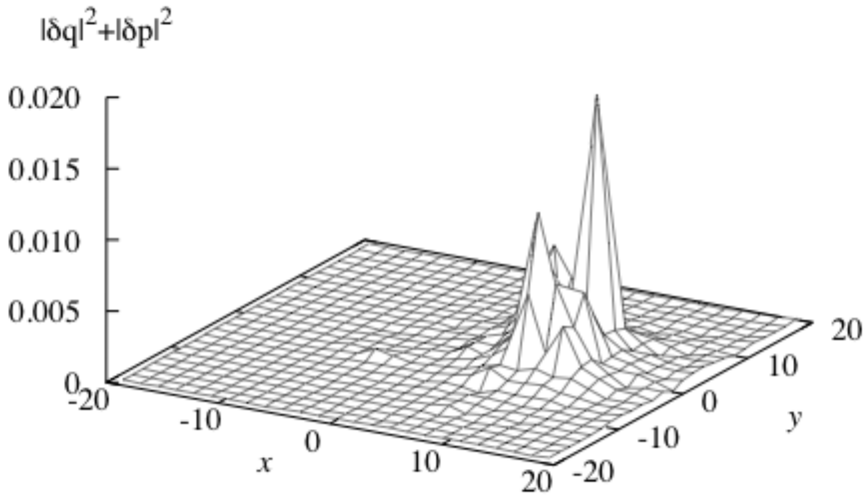


400 disks, rho = 0.4, T = 1

Properties of Lyapunov instability

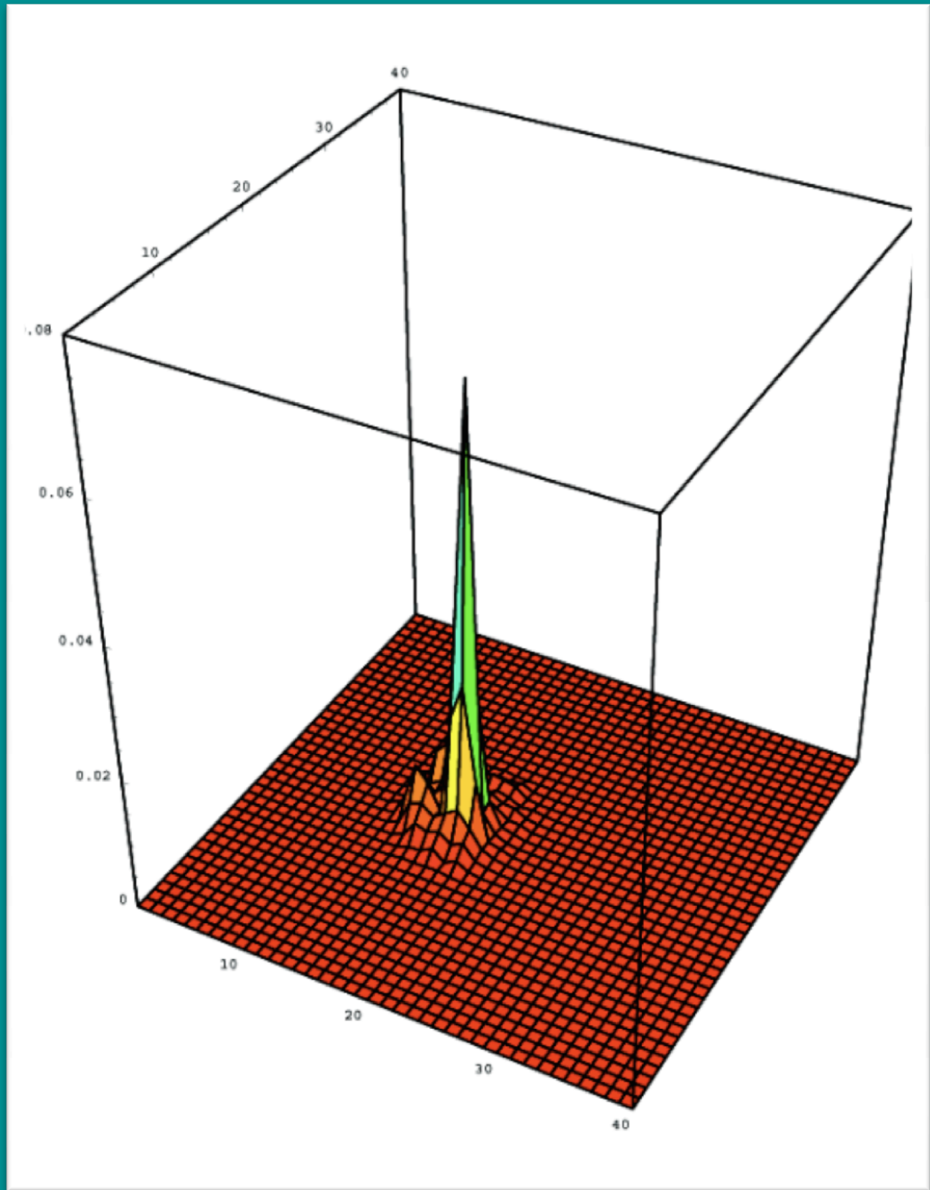
- Conjugate pairing
- Localized Lyapunov modes
- Delocalized Lyapunov modes
- Gram-Schmidt versus Covariant Lyapunov vectors

Localization of Gram-Schmidt vectors for hard disks



$N = 1024; \quad L_x/L_y = 1; \quad \rho = 0.7$

102400 soft disks, density = 1



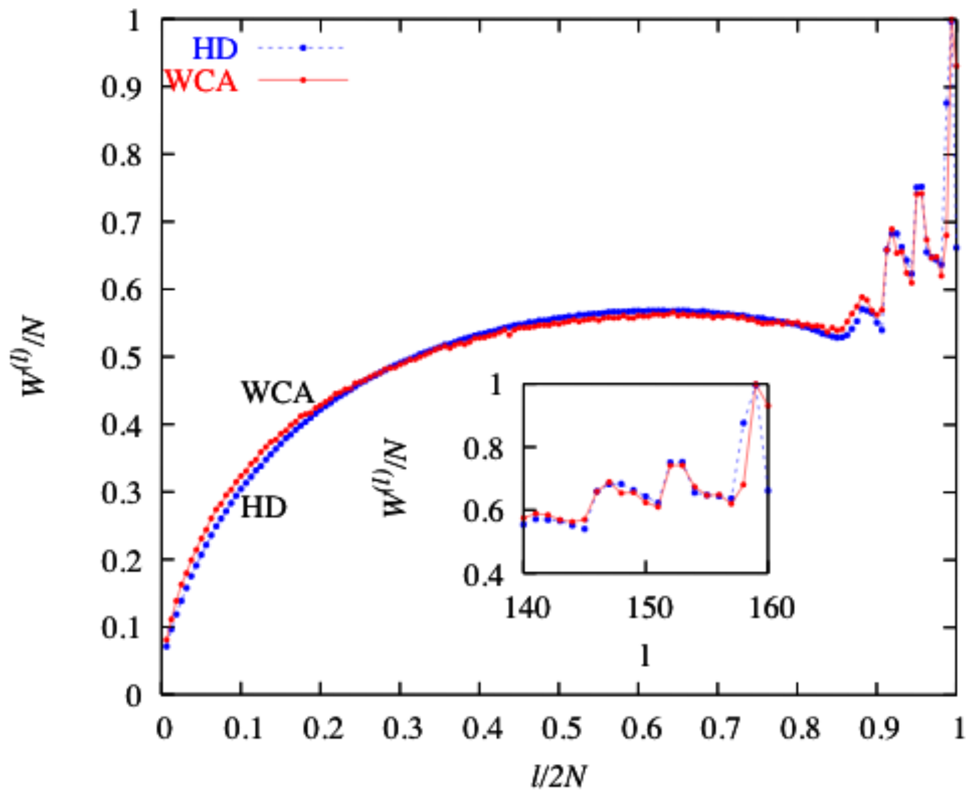
Wm.G. Hoover, K. Boercker, and HAP, Phys. Rev. E 57, 3911 (1998)

Localization measure at low density 0.2

$$\gamma_i^{(l)} \equiv \left(\delta q_i^{(l)}\right)^2 + \left(\delta p_i^{(l)}\right)^2$$

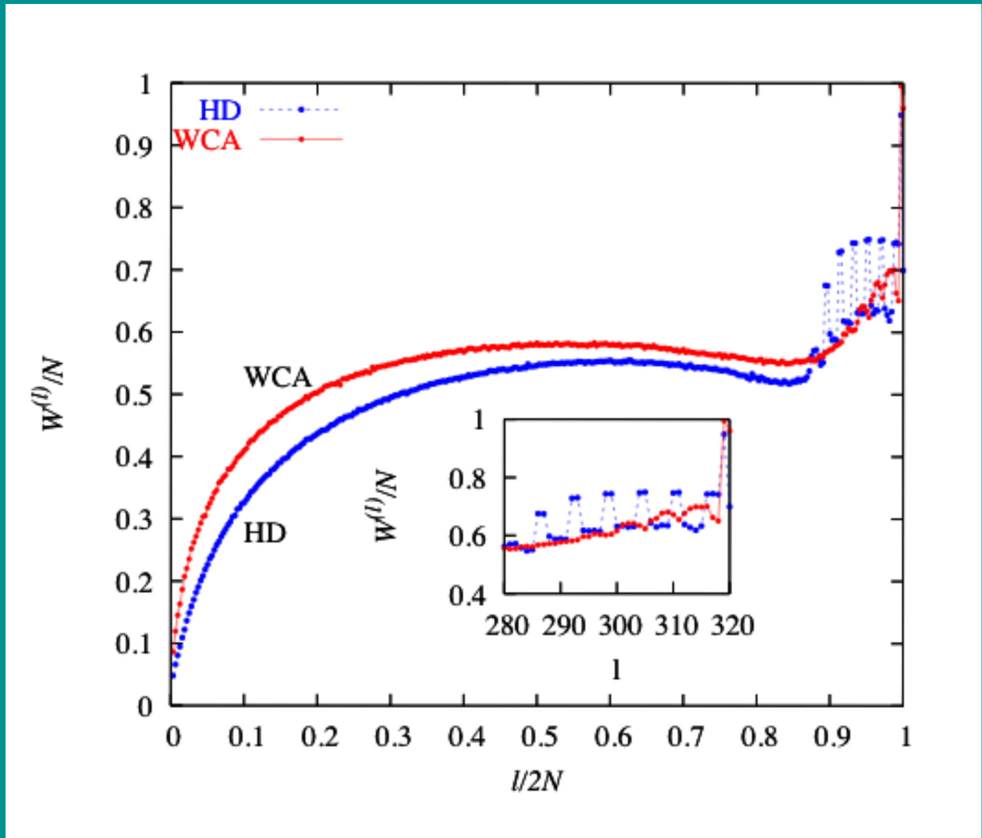
$$S^{(l)} = -\sum_{i=1}^{N} \langle \gamma_i^{(l)}(t) \ln \gamma_i^{(l)}(t) \rangle$$

$$W^{(l)} \equiv \exp\left(S^{(l)}\right)$$

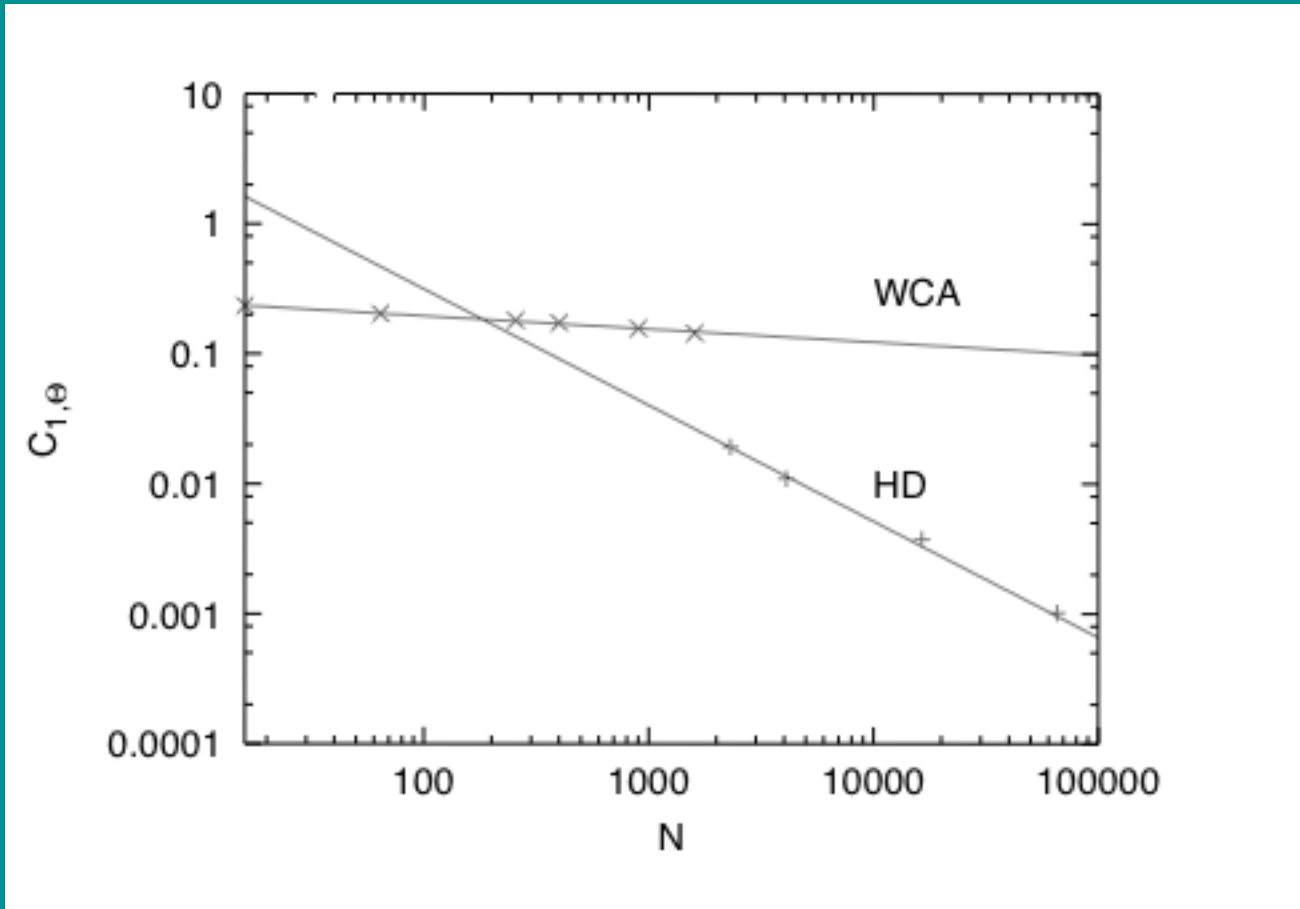


T. Taniguchi, G. Morriss, PRE 68, 046204 (2003)

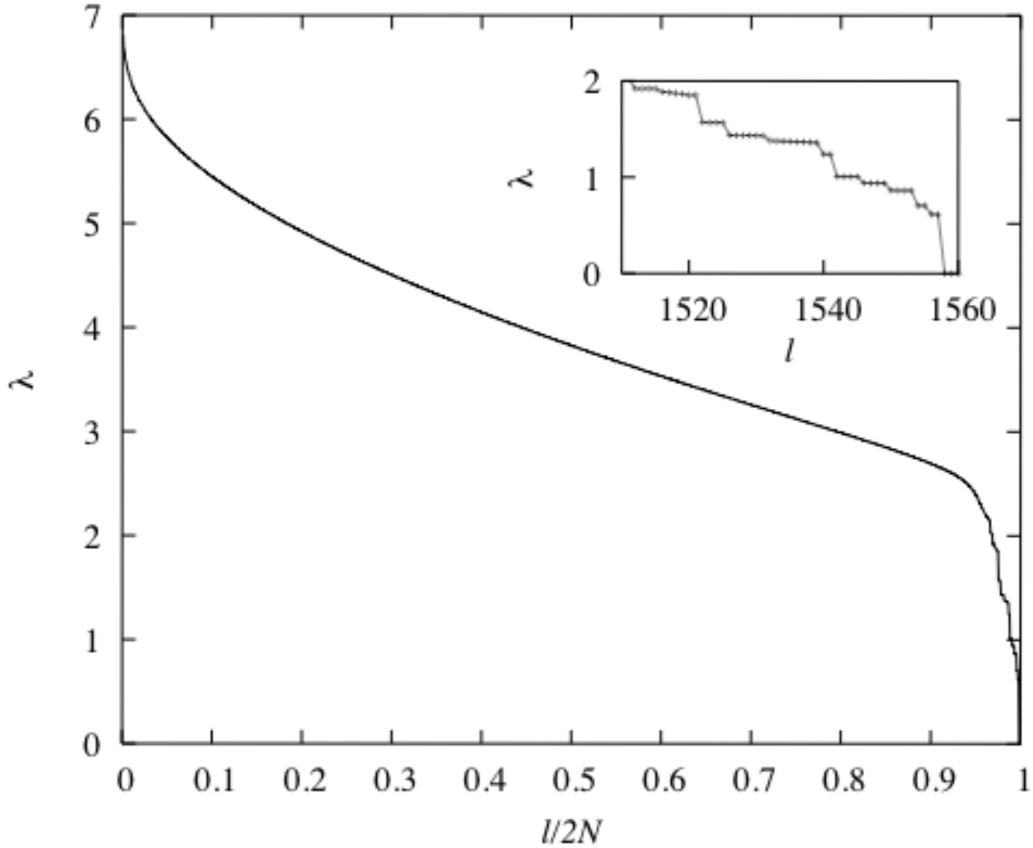
Localization measure for density 0.5



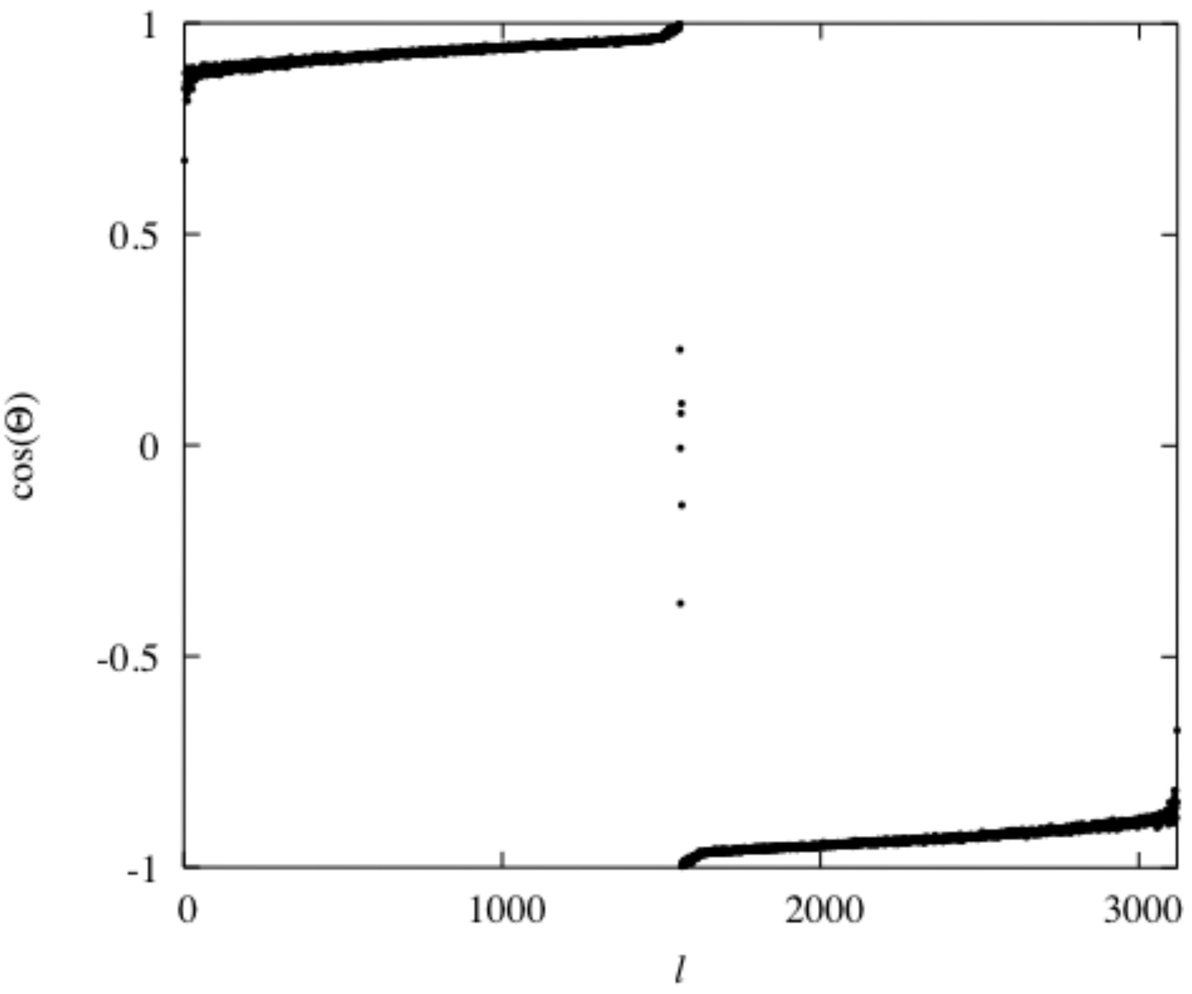
N-dependence of localization measure

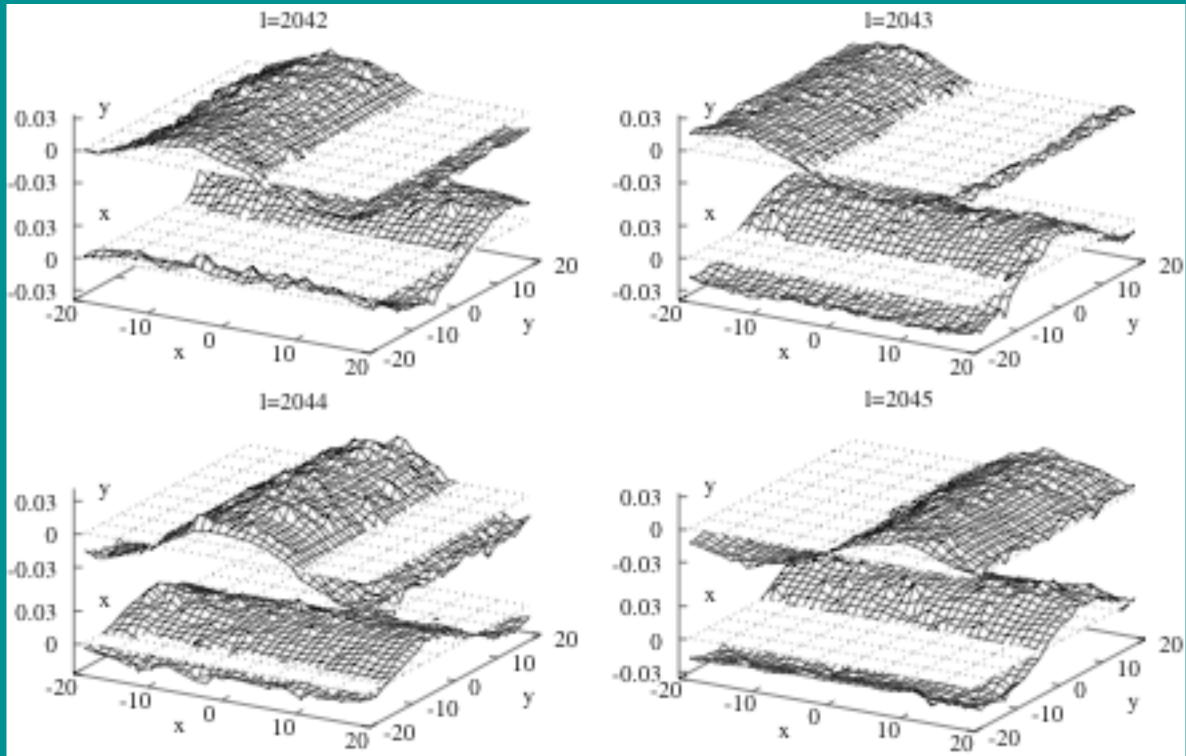


N = 780 hard disks, rho = 0.8, A = 0.8, periodic boundaries



$$\langle \cos(\Theta_l) \rangle \equiv \left\langle \frac{\sum_{i=1}^{N} (\delta q_i^{(l)} \cdot \delta p_i^{(l)})}{\sum_{i=1}^{N} (\delta q_i^{(l)})^2 \sum_{i=1}^{N} (\delta p_i^{(l)})^2} \right\rangle$$





H. A. Posch, R. Hirschl, and Wm.G. Hoover (2000)

Hard disks: Generators of symmetry transformations

Transformation	Generator
$(p,q) \mapsto (p_x + \varepsilon 1, p_y, q_x, q_y)$	$\delta\xi_1 = (1,0,0,0)$
$(p,q) \mapsto (p_x, p_y + \varepsilon 1, q_x, q_y)$	$\delta\xi_2 = (0,1,0,0)$
$(p,q) \mapsto (p_x, p_y, q_x + \varepsilon 1, q_y)$	$\delta\xi_3 = (0,0,1,0)$
$(p,q) \mapsto (p_x, p_y, q_x, q_y + \varepsilon 1)$	$\delta\xi_4 = (0,0,0,1)$
$(p,q) \mapsto (p_x + \varepsilon p_x, p_y + \varepsilon p_y, q_x, q_y)$	$\delta\xi_5 = (p_x, p_y, 0, 0)$
$(p,q) \mapsto (p_x, p_y, q_x + \varepsilon p_x, q_y + \varepsilon p_y)$	$\delta\xi_6 = (0,0,p_x,p_y)$

$$\delta\xi_3 : (q_{x,j}, q_{y,j}) \mapsto (q_{x,j} + \varepsilon, q_{y,j})$$
$$\delta\xi_4 : (q_{x,j}, q_{y,j}) \mapsto (q_{x,j}, q_{y,j} + \varepsilon)$$
$$\delta\xi_6 : (q_{x,j}, q_{y,j}) \mapsto (q_{x,j} + \varepsilon p_{x,j}, q_{y,j} + \varepsilon p_{y,j}) ,$$

$$A(x,y) = \sum_{|\ell|=n_x, |m|=n_y} c_{\ell,m} \exp\left(i(\ell\, k_x x + m\, k_y y)\right)$$

Classification of modes for 2d hard-disk systems

1) **Transverse branch:**

Transverse modes: modulations of $\delta\xi_3$ and $\delta\xi_4$
divergence-free vector field $\in \mathrm{T}(\mathbf{n})$.

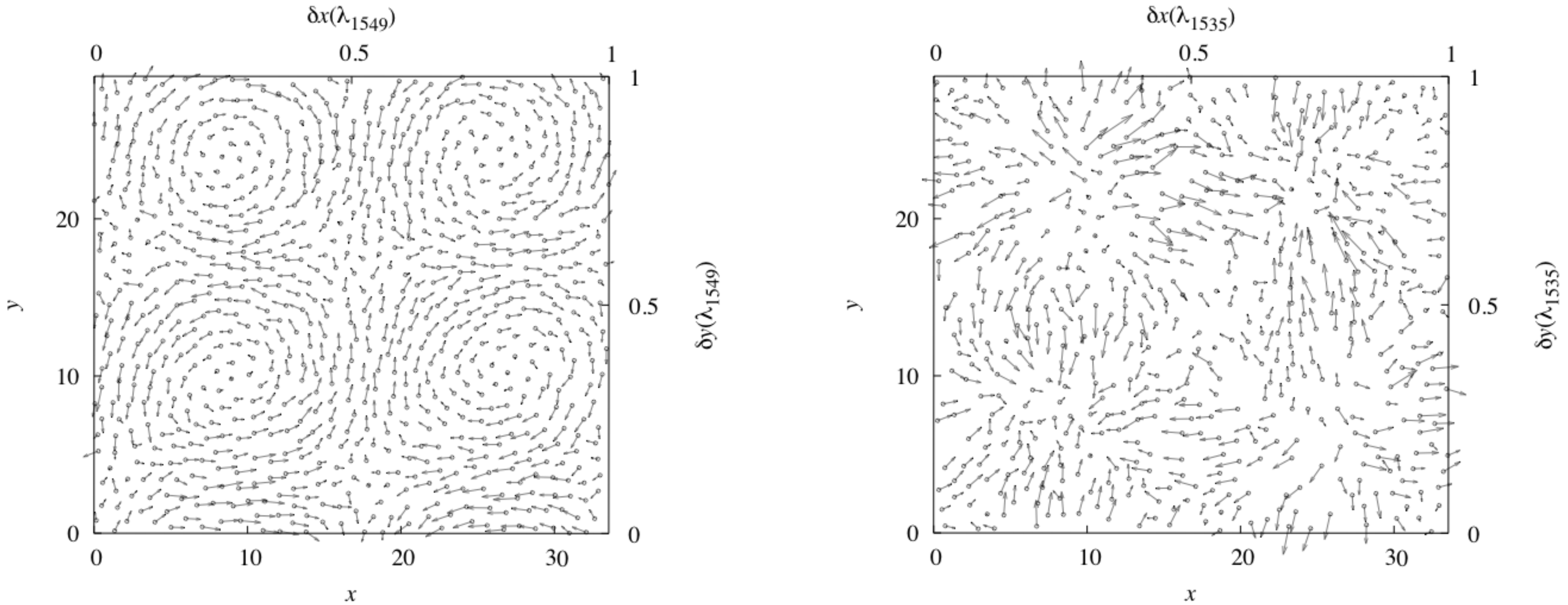
2) **Longitudinal branch:**

(i) **Longitudinal modes:** modulations of $\delta\xi_3$ and $\delta\xi_4$.
irrotational vector fields $\in \mathrm{L}(\mathbf{n})$.

(ii) P-**modes:** modulations of $\delta\xi_6$, $\in \mathrm{P}(\mathbf{n})$.

$\mathrm{T}(\mathbf{n})$, $\mathrm{L}(\mathbf{n})$, $\mathrm{P}(\mathbf{n})$ have dimension 4 (or 2 if $n_x = 0$ or $n_y = 0$).
$\mathrm{LP}(\mathbf{n}) \equiv \mathrm{L}(\mathbf{n}) \oplus \mathrm{P}(\mathbf{n})$ has dimension 8 (or 4 if $n_x = 0$ or $n_y = 0$).

Lyapunov modes as vector fields

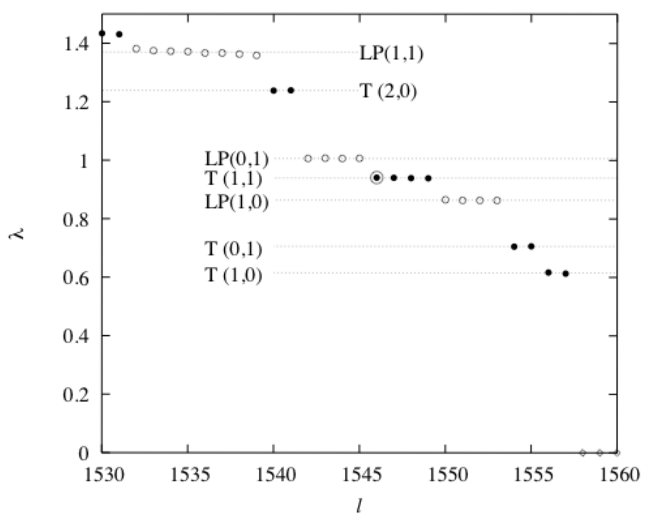


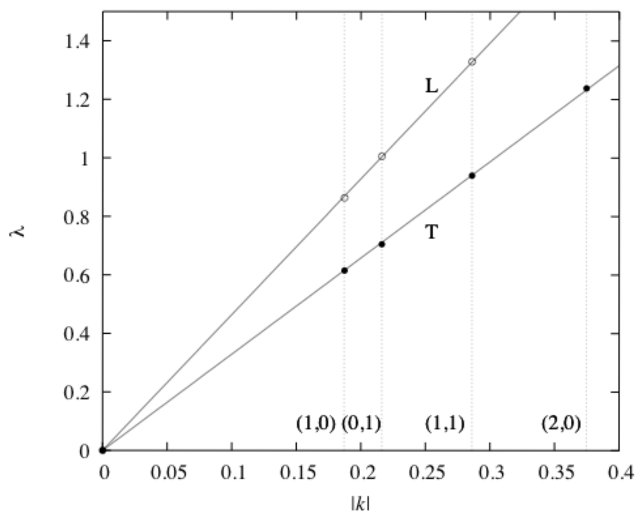
T(1,1)

LP(1,1)

$N = 780; \quad \rho = 0.8$

Dispersion relation





N = 780 hard disks, [illegible] = 0.8, A = 0.867

H.A. Posch, R. Hirschl, and Wm.G. Hoover (2000)

Oseledec Theorem

$$\Lambda_{\pm} = \lim_{t \to \pm\infty} \left(\left[D\phi^t|_{\mathbf{\Gamma}} \right]^T D\phi^t|_{\mathbf{\Gamma}} \right)^{1/2|t|}$$

$$\exp(\lambda^{(1)}) > \cdots > \exp(\lambda^{(\ell)})$$

$$\mathbf{TX}(\mathbf{\Gamma}) = \boldsymbol{U}_{\pm}^{(1)}(\mathbf{\Gamma}) \oplus \cdots \oplus \boldsymbol{U}_{\pm}^{(\ell)}(\mathbf{\Gamma})$$

$$\mathbf{TX}(\mathbf{\Gamma}) = \boldsymbol{E}^{(1)}(\mathbf{\Gamma}) \oplus \cdots \oplus \boldsymbol{E}^{(\ell)}(\mathbf{\Gamma})$$

$$\lim_{t \to \pm\infty} \frac{1}{|t|} \log \| D\phi^t|_{\mathbf{\Gamma}} \cdot \delta\mathbf{\Gamma} \| = \pm\lambda^{(j)} \qquad \forall j \in \{1, \ldots, \ell\}$$

$$D\phi^t|_{\mathbf{\Gamma}_0} \boldsymbol{E}^{(i)}(\mathbf{\Gamma}_0) = \boldsymbol{E}^{(i)}(\phi^t(\mathbf{\Gamma}_0)).$$

$$\boldsymbol{E}^{(j)} = \left(\boldsymbol{U}_{-}^{(1)} \oplus \cdots \oplus \boldsymbol{U}_{-}^{(j)} \right) \cap \left(\boldsymbol{U}_{+}^{(j)} \oplus \cdots \oplus \boldsymbol{U}_{+}^{(\ell)} \right)$$

Gram-Schmidt vectors

$$\tilde{g}^{(1)} = g^{(1)} R_{11}$$

$$\tilde{g}^{(2)} = g^{(1)} R_{12} + g^{(2)} R_{22}$$

$$\vdots$$

$$\tilde{g}^{(L)} = g^{(1)} R_{1L} + \cdots + g^{(L)} R_{LL}$$

$$\begin{pmatrix} \vdots & \vdots & & \vdots \\ \tilde{g}^{(1)} & \tilde{g}^{(2)} & \ldots & \tilde{g}^{(L)} \\ \vdots & \vdots & & \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & & \vdots \\ g^{(1)} & g^{(2)} & \ldots & g^{(L)} \\ \vdots & \vdots & & \vdots \end{pmatrix} \cdot \begin{pmatrix} R_{11} & \ldots & R_{1L} \\ 0 & \ddots & \vdots \\ 0 & \ldots & R_{LL} \end{pmatrix}$$

$$\tilde{\mathbf{G}}_m = \mathbf{G}_m \cdot \mathbf{R}_m \quad , \quad \tilde{\mathbf{G}}_{m-1} = \mathbf{G}_{m-1} \cdot \mathbf{R}_{m-1}$$

$$\tilde{\mathbf{G}}_m = \mathbf{J}_{m-1} \cdot \mathbf{G}_{m-1}$$

F. Ginelli, P.Poggi, A. Turchi, H. Chate, R. Livi, A. Politi, PRL 99, 130601 (2007)

Covariant Lyapunov vectors

$$v_m^{(1)} \in \text{span}\{g_m^{(1)}\}$$

$$v_m^{(2)} \in \text{span}\{g_m^{(1)}, g_m^{(2)}\}$$

$$\vdots$$

$$v_m^{(L)} \in \text{span}\{g_m^{(1)}, g_m^{(2)}, \ldots, g_m^{(L)}\}$$

$$\begin{pmatrix} \vdots & \vdots & & \vdots \\ v_m^{(1)} & v_m^{(2)} & \ldots & v_m^{(L)} \\ \vdots & \vdots & & \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & & \vdots \\ g_m^{(1)} & g_m^{(2)} & \ldots & g_m^{(L)} \\ \vdots & \vdots & & \vdots \end{pmatrix} \cdot \begin{pmatrix} c_{11} & \ldots & c_{1L} \\ 0 & \ddots & \vdots \\ 0 & \ldots & c_{LL} \end{pmatrix}$$

$$\mathbf{V}_m = \mathbf{G}_m \cdot \mathbf{C}_m$$

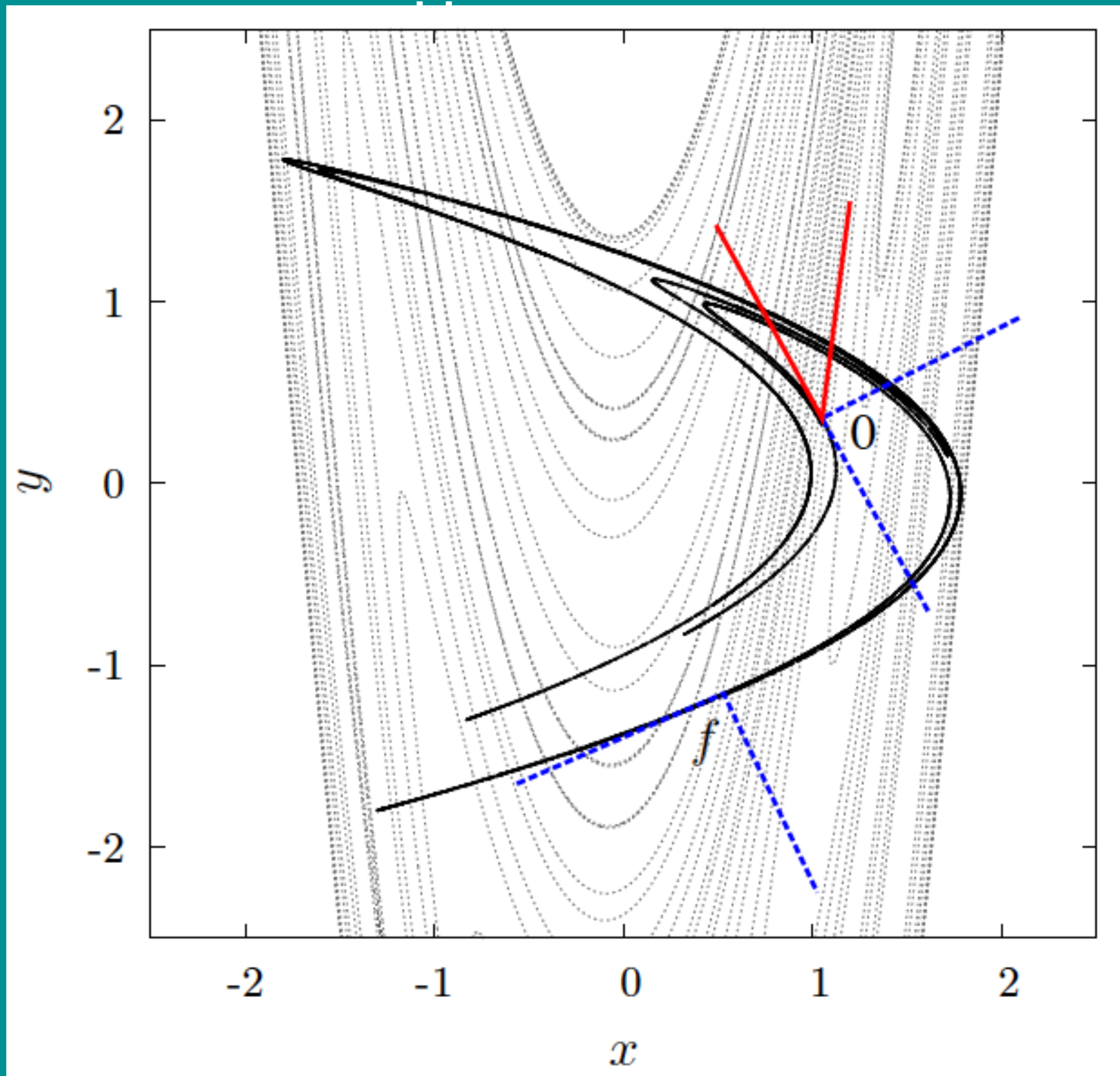
Proposition: $\mathbf{C}_{m-1} = \mathbf{R}_m^{-1} \cdot \mathbf{C}_m \quad \Rightarrow \quad \mathbf{V}_m = \mathbf{J}_{m-1} \cdot \mathbf{V}_{m-1}$

F. Ginelli, P.Poggi, A. Turchi, H. Chate, R. Livi, A. Politi, PRL 99, 130601 (2007)

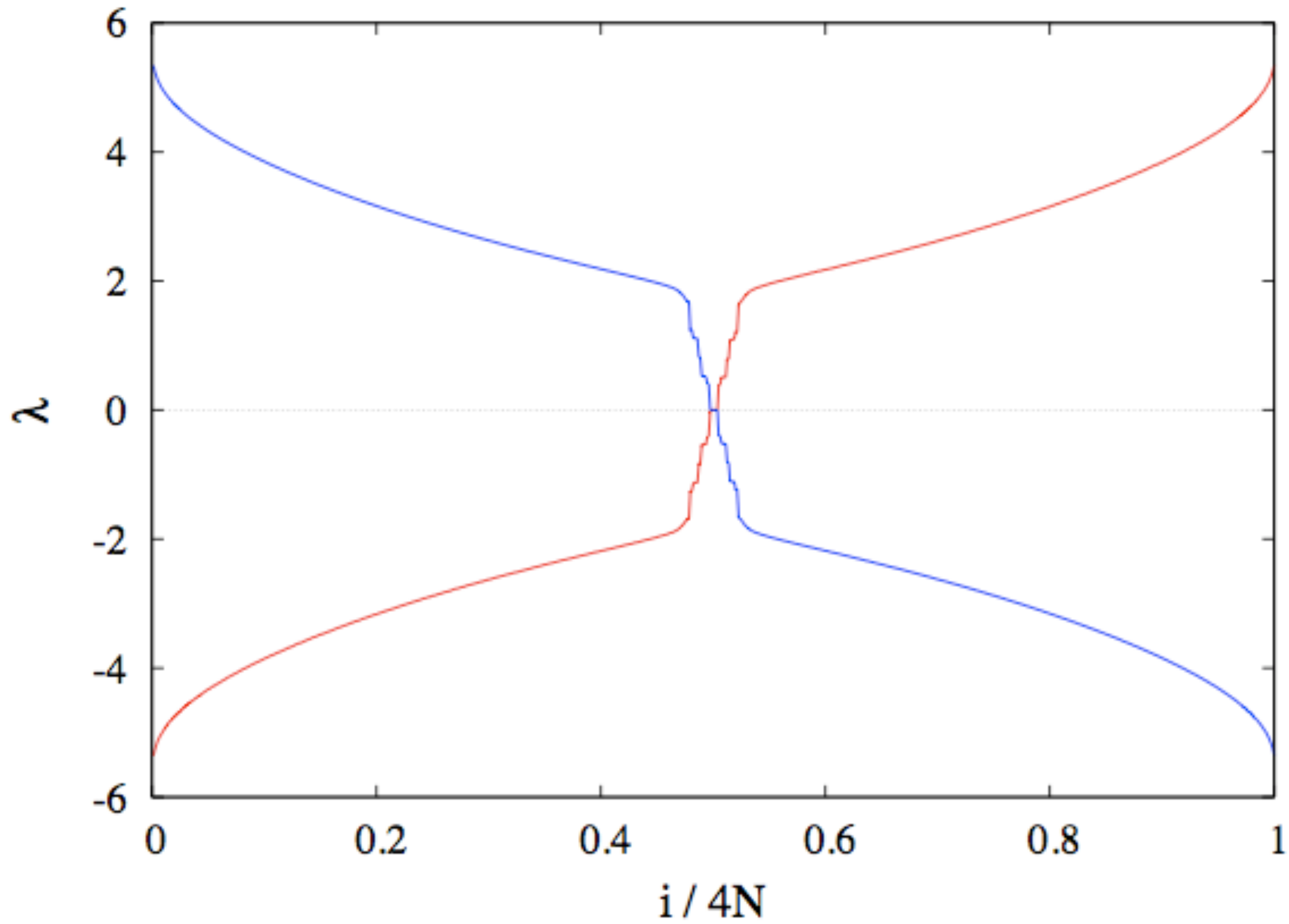
Covariant Lyapunov vectors

(F. Ginelli, P. Poggi, A. Turchi, H. Chate, R. Livi, and A. Politi, PRL 99, 130601 (2007))

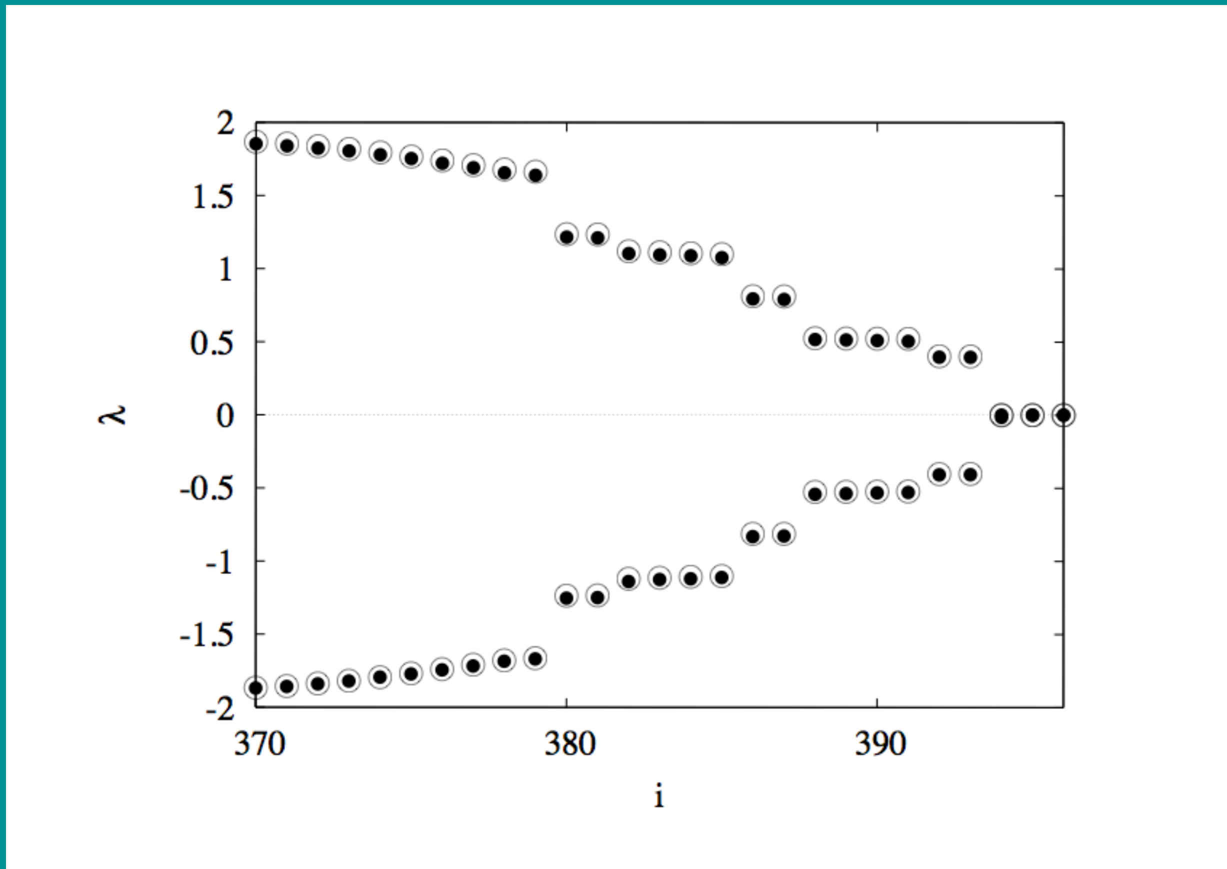
Application to the Henon map



Hard disks, N = 198, N/V = 0.7, A = 2/11, K/N = 1

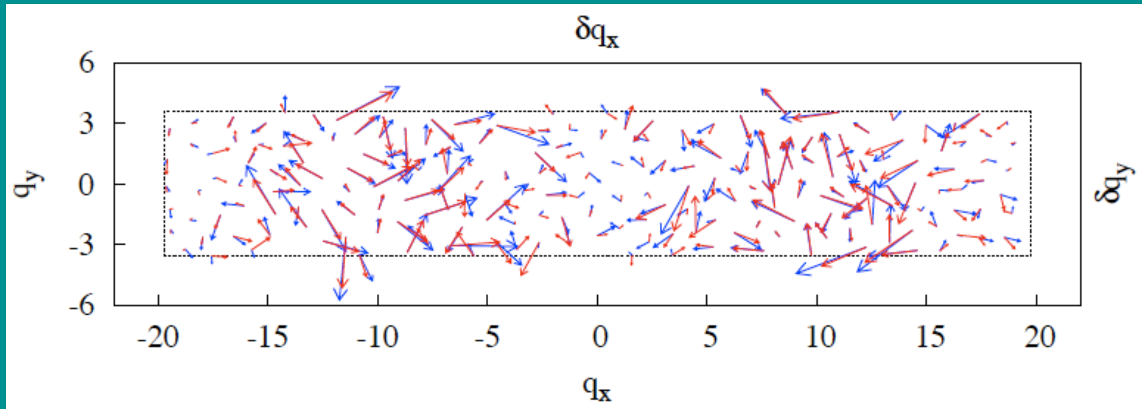


Lyapunov modes



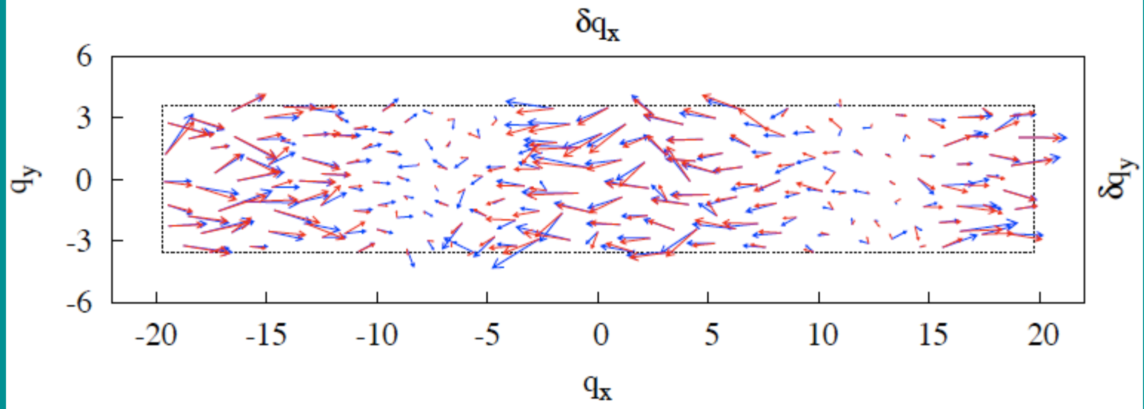
Hard disks, N = 198, N/V = 0.7, A = 2/11, K/N = 1

LP



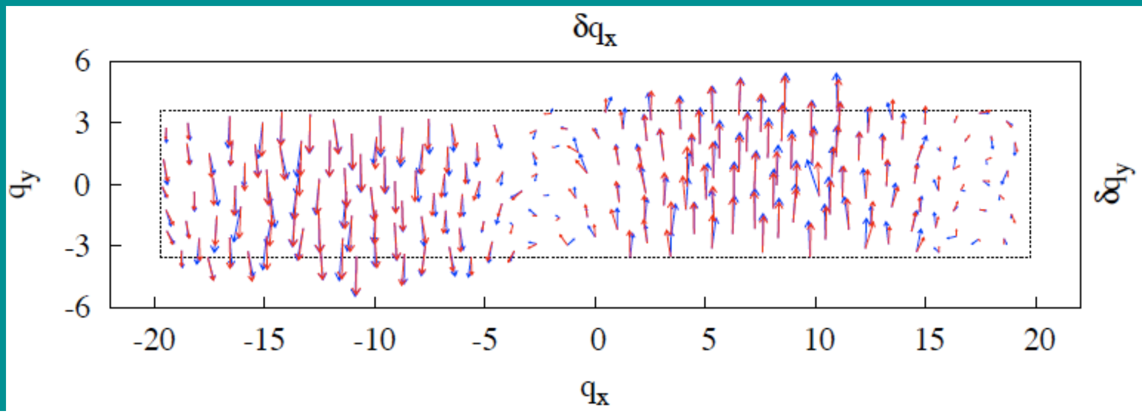
I = 388

L



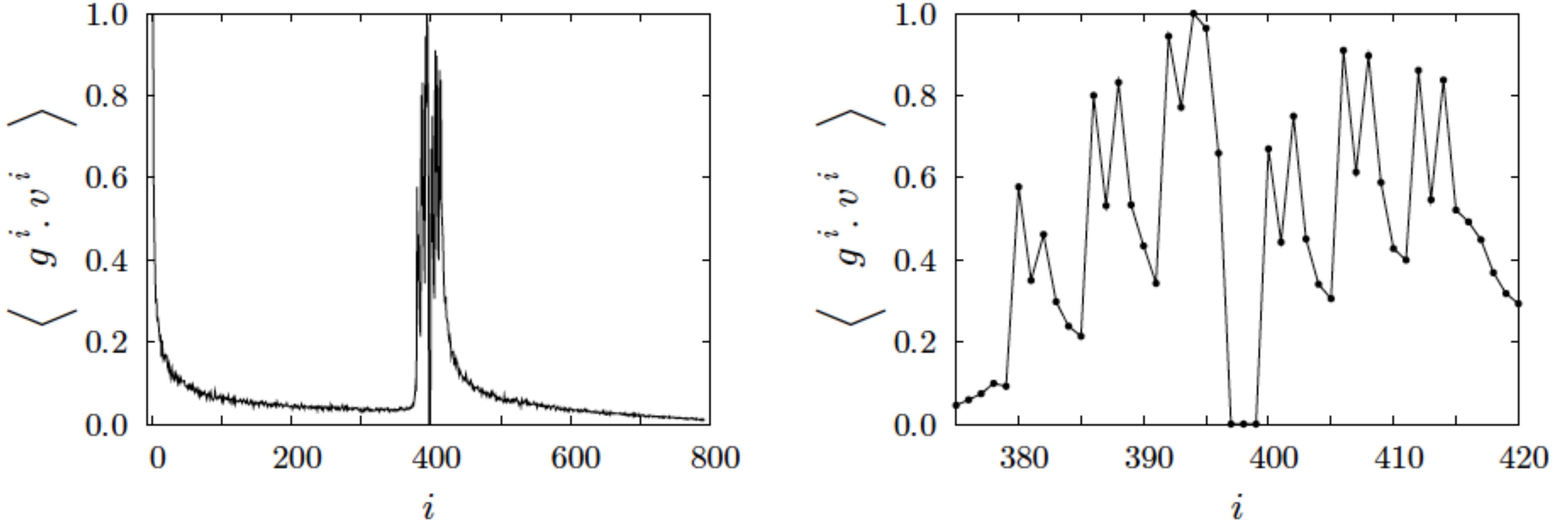
I = 389

T

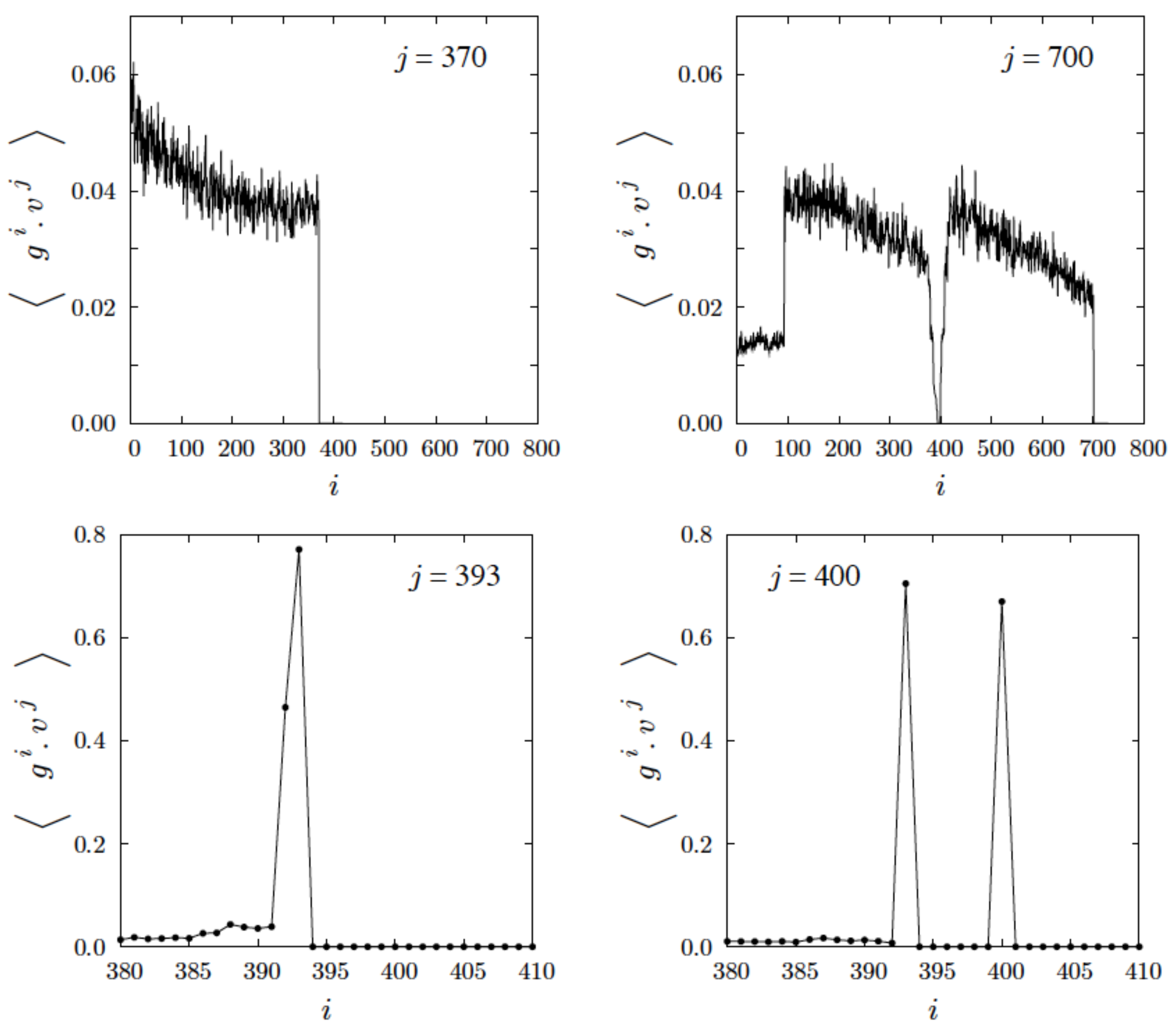


I = 392

Covariant versus Gram-Schmidt



Covariant versus Gram-Schmidt II



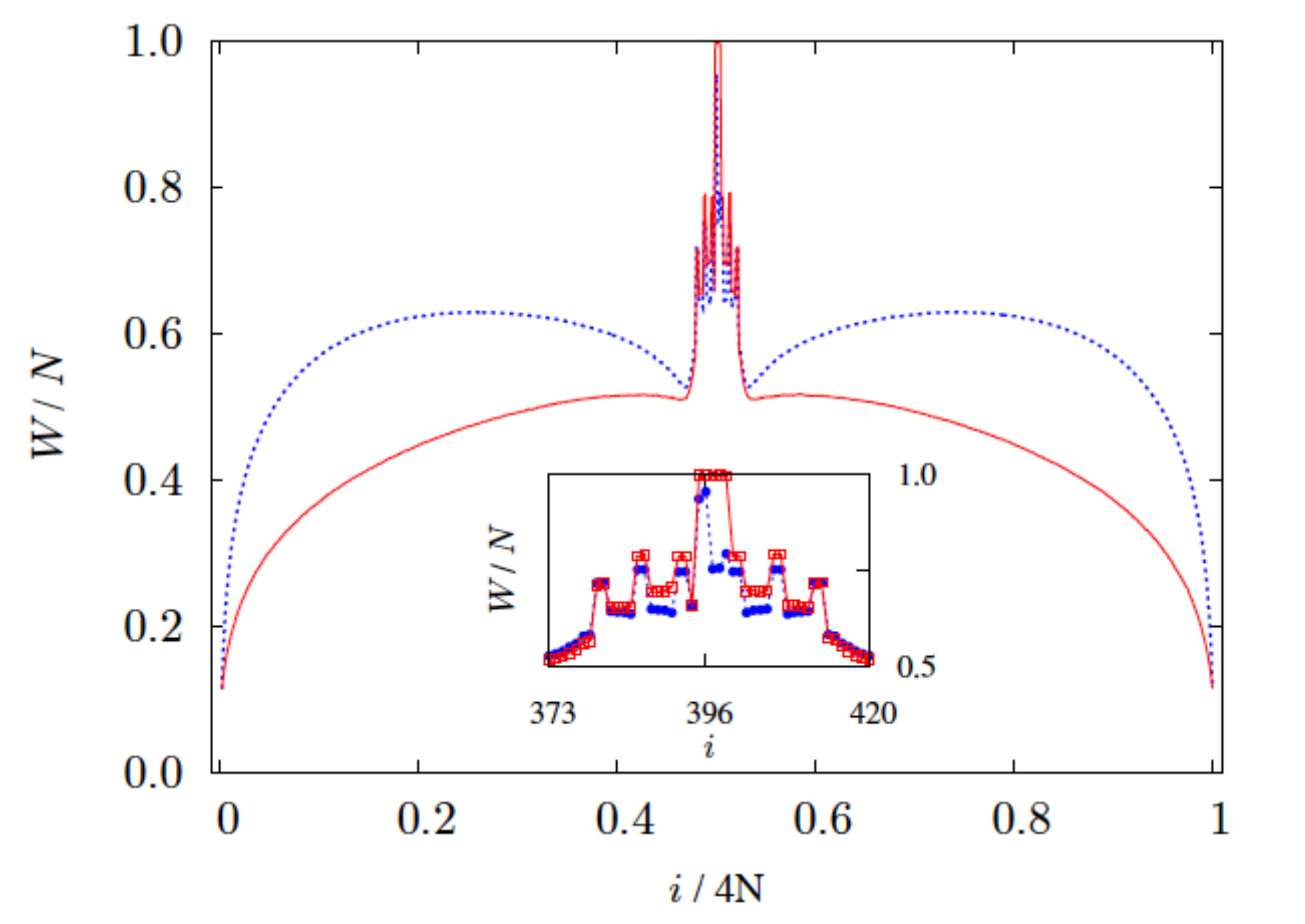
The null subspace is covariant

	$\boldsymbol{v}^{394}$	$\boldsymbol{v}^{395}$	$\boldsymbol{v}^{396}$	$\boldsymbol{v}^{397}$	$\boldsymbol{v}^{398}$	$\boldsymbol{v}^{399}$
$\boldsymbol{g}^{394}$	-1.00000	-0.00317	0.12143	0.34122	0.31370	0.63834
$\boldsymbol{g}^{395}$	0	0.99999	0.71271	-0.37819	-0.34895	0.30478
$\boldsymbol{g}^{396}$	0	0	0.69087	-0.86052	-0.88305	-0.70681
$\boldsymbol{g}^{397}$	0	0	0	0.00671	0.00670	0.00475
$\boldsymbol{g}^{398}$	0	0	0	0	0.00031	0.00124
$\boldsymbol{g}^{399}$	0	0	0	0	0	0.00453

TABLE I: Snapshot values for the scalar products $\boldsymbol{v}^i \cdot \boldsymbol{g}^j$ for $(i,j) \in \{2N-2, \cdots, 2N+3\}$ for $N = 198$.

Localization for density 0.7, N = 198

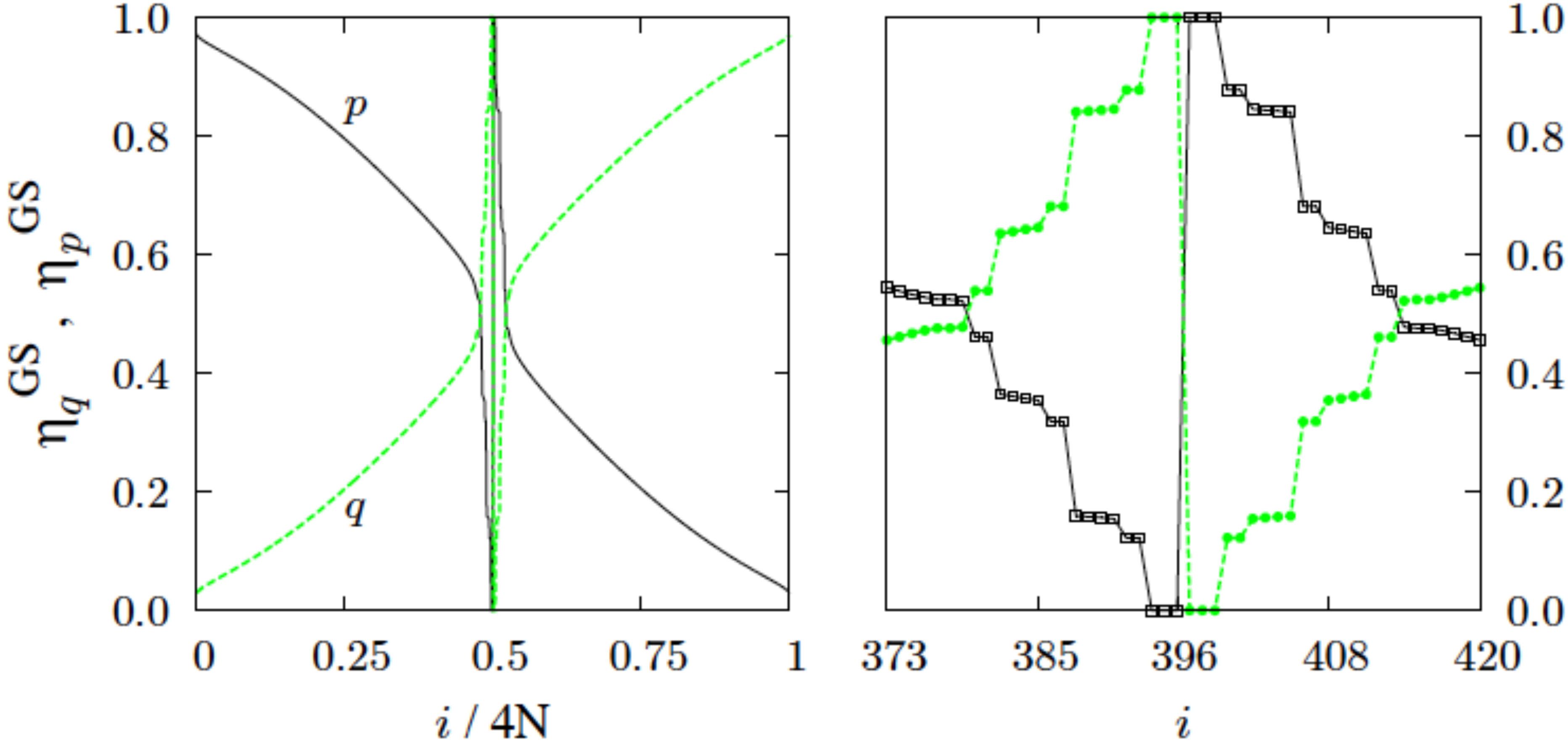
G-S vectors: blue; covariant vectors: red



$$\mu_n = (\delta \boldsymbol{q}_n)^2 + (\delta \boldsymbol{p}_n)^2.$$

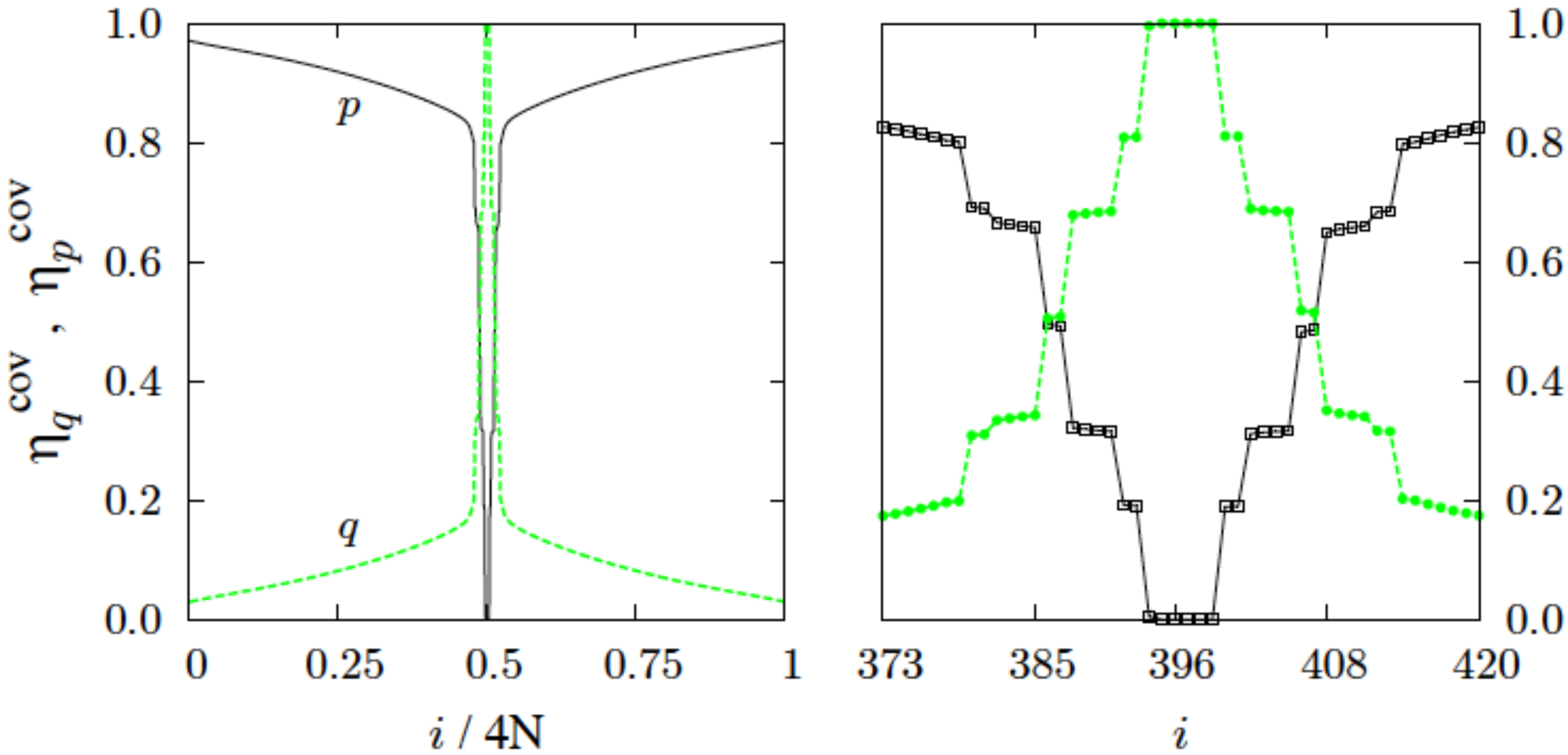
$$W = \exp[S]/N, \quad S = \left\langle -\sum_{n=1}^{N} \mu_n \ln \mu_n \right\rangle.$$

Projection of GS vectors onto Q and P-subspaces



$$\eta_q = \left\langle \sum_{n=1}^{N} \delta \boldsymbol{q}_n^2 \right\rangle \quad , \quad \eta_p = \left\langle \sum_{n=1}^{N} \delta \boldsymbol{p}_n^2 \right\rangle$$

Projection of covariant vectors onto Q and P subspaces



$$\eta_q = \left\langle \sum_{n=1}^{N} \delta \boldsymbol{q}_n^2 \right\rangle \quad , \quad \eta_p = \left\langle \sum_{n=1}^{N} \delta \boldsymbol{p}_n^2 \right\rangle$$

Continuous symmetries and vanishing Lyapunov exponents

$$\mathbf{e}_\alpha(\mathbf{\Gamma}) = \left(\frac{\partial \mathbf{G}_\alpha(\mathbf{\Gamma})}{\partial \alpha}\right)_{\alpha=\mathbf{0}}$$

$$C_\alpha(\mathbf{\Gamma}) = const.$$

$$\mathbf{e}_\alpha(\mathbf{\Gamma}) = \mathbf{\Sigma} \cdot \frac{\partial C_\alpha(\mathbf{\Gamma})}{\partial \mathbf{\Gamma}},$$

$$\mathbf{f}_\alpha(\mathbf{\Gamma}) = \frac{\partial C_\alpha(\mathbf{\Gamma})}{\partial \mathbf{\Gamma}}.$$

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}.$$

$$\mathbf{r}_i \rightarrow \mathbf{r}_i' = \mathbf{r}_i + \alpha \mathbf{b},$$

$$t \rightarrow t' + \alpha,$$

$$\mathbf{r}_i \rightarrow \mathbf{r}_i' = \mathbf{r}_i + \alpha \mathbf{v} t,$$

Central manifold

$$\mathbf{\Gamma} = (q_x^1, q_y^1, \ldots, q_x^N, q_y^N \,;\, p_x^1, p_y^1, \ldots, p_x^N, p_y^N)$$

$$\boldsymbol{e}_1 = \frac{1}{\sqrt{2K}} (p_x^1, p_y^1, \ldots, p_x^N, p_y^N \,;\, 0, 0, \ldots, 0, 0) \,,$$

$$\boldsymbol{e}_2 = \frac{1}{\sqrt{N}} (1, 0, \ldots, 1, 0 \,;\, 0, 0, \ldots, 0, 0) \,,$$

$$\boldsymbol{e}_3 = \frac{1}{\sqrt{N}} (0, 1, \ldots, 0, 1 \,;\, 0, 0, \ldots, 0, 0) \,,$$

$$\boldsymbol{e}_4 = \frac{1}{\sqrt{2K}} (0, 0, \ldots, 0, 0 \,;\, p_x^1, p_y^1, \ldots, p_x^N, p_y^N) \,,$$

$$\boldsymbol{e}_5 = \frac{1}{\sqrt{N}} (0, 0, \ldots, 0, 0 \,;\, 1, 0, \ldots, 1, 0) \,,$$

$$\boldsymbol{e}_6 = \frac{1}{\sqrt{N}} (0, 0, \ldots, 0, 0 \,;\, 0, 1, \ldots, 0, 1) \,.$$

Projections of GS-vectors

TABLE II: Instantaneous projection matrix α of Gram-Schmidt vectors (for $i \in \{2N-2, \cdots, 2N+3\}$) onto the natural basis $\{\boldsymbol{e}_k, 1 \le k \le 6\}$ of the central manifold. The system contains $N = 4$ disks. The powers of 10 are given in square brackets.

i	$\alpha_{i,1}$	$\alpha_{i,2}$	$\alpha_{i,3}$	$\alpha_{i,4}$	$\alpha_{i,5}$	$\alpha_{i,6}$
$2N-2$	-0.766	0.582	0.273	$-0.766[-6]$	$0.582[-6]$	$0.273[-6]$
$2N-1$	0.256	-0.114	0.960	$0.256[-6]$	$-0.114[-6]$	$0.960[-6]$
$2N$	0.590	0.805	-0.062	$0.590[-6]$	$0.805[-6]$	$-0.062[-6]$
$2N+1$	$-0.611[-6]$	$0.782[-6]$	$-0.121[-6]$	0.611	-0.782	0.121
$2N+2$	$0.575[-6]$	$0.544[-6]$	$0.611[-6]$	-0.575	-0.544	-0.611
$2N+3$	$-0.543[-6]$	$-0.304[-6]$	$0.783[-6]$	0.543	0.304	-0.783

$$\alpha_{i,k} = \boldsymbol{g}^i \cdot \boldsymbol{e}_k; \quad \beta_{i,k} = \boldsymbol{v}^i \cdot \boldsymbol{e}_k, \quad k \in \{1, \dots, 6\} \quad i \in \{2N-2, \cdots, 2N+3\}.$$

Projections of covariant vectors

TABLE III: Instantaneous projection matrix matrix β for the the six central covariant vectors onto the natural basis $\{\boldsymbol{e}_k, 1 \leq k \leq 6\}$ of the central manifold. The system contains of $N = 4$ particles. The powers of 10 are given in square brackets.

i	$\beta_{i,1}$	$\beta_{i,2}$	$\beta_{i,3}$	$\beta_{i,4}$	$\beta_{i,5}$	$\beta_{i,6}$
$2N-2$	-0.766	0.582	0.273	−0.766[−6]	0.582[−6]	0.273[−6]
$2N-1$	0.256	-0.114	0.960	0.256[−6]	−0.114[−6]	0.960[−6]
$2N$	0.590	0.805	-0.062	0.590[−6]	0.805[−6]	−0.062[−6]
$2N+1$	-0.611	0.782	-0.121	0.611 [-5]	-0.782 [-5]	0.121 [-5]
$2N+2$	0.575	0.544	0.611	-0.575 [-5]	-0.544[-5]	-0.611[-5]
$2N+3$	-0.543	-0.304	0.783	0.543 [-5]	0.304 [-5]	-0.783[-5]

$$\alpha_{i,k} = \boldsymbol{g}^i \cdot \boldsymbol{e}_k; \quad \beta_{i,k} = \boldsymbol{v}^i \cdot \boldsymbol{e}_k, \quad k \in \{1, \ldots, 6\} \quad i \in \{2N-2, \cdots, 2N+3\}.$$

Covariant subspaces of the null space

$$D\phi^t_{\mathbf{\Gamma}_0} \cdot \boldsymbol{e}^j\,(\mathbf{\Gamma}_0) \;=\; \boldsymbol{e}^j\,(\mathbf{\Gamma}_t)\,,$$

$$D\phi^t_{\mathbf{\Gamma}_0} \cdot \boldsymbol{e}^{j+3}\,(\mathbf{\Gamma}_0) \;=\; t\,\boldsymbol{e}^j\,(\mathbf{\Gamma}_t) + \boldsymbol{e}^{j+3}\,(\mathbf{\Gamma}_t)\,, \quad \text{for} \;\; j \in \{1,2,3\}$$

$$\mathcal{N}_1 \;=\; span\{\boldsymbol{e}_1\}$$

$$\mathcal{N}_2 \;=\; span\{\boldsymbol{e}_2\}$$

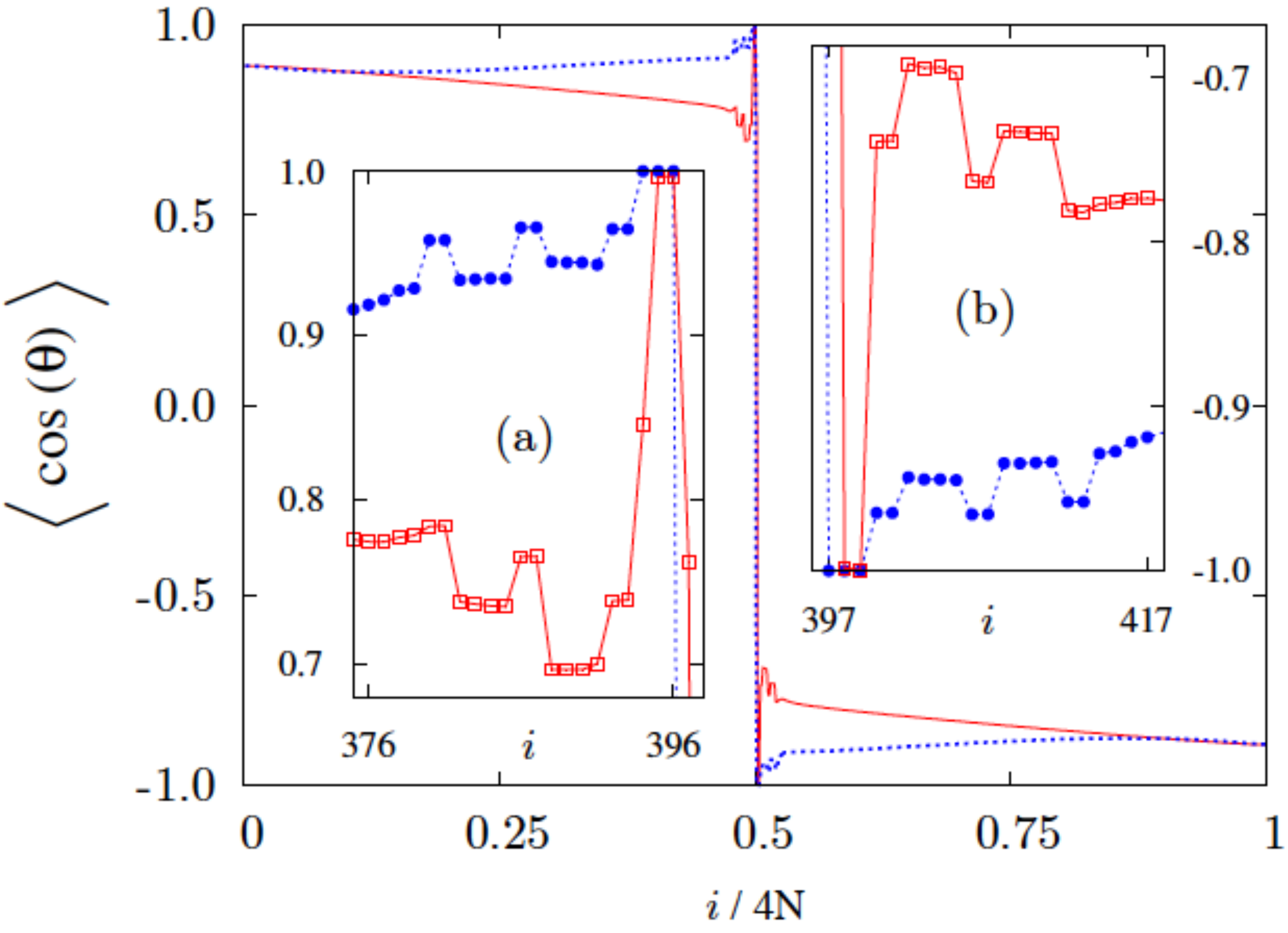
$$\mathcal{N}_3 \;=\; span\{\boldsymbol{e}_3\}$$

$$\mathcal{N}_p = span\{\boldsymbol{e}_1, \boldsymbol{e}_4\}$$

$$\mathcal{N}_x = span\{\boldsymbol{e}_2, \boldsymbol{e}_5\}$$

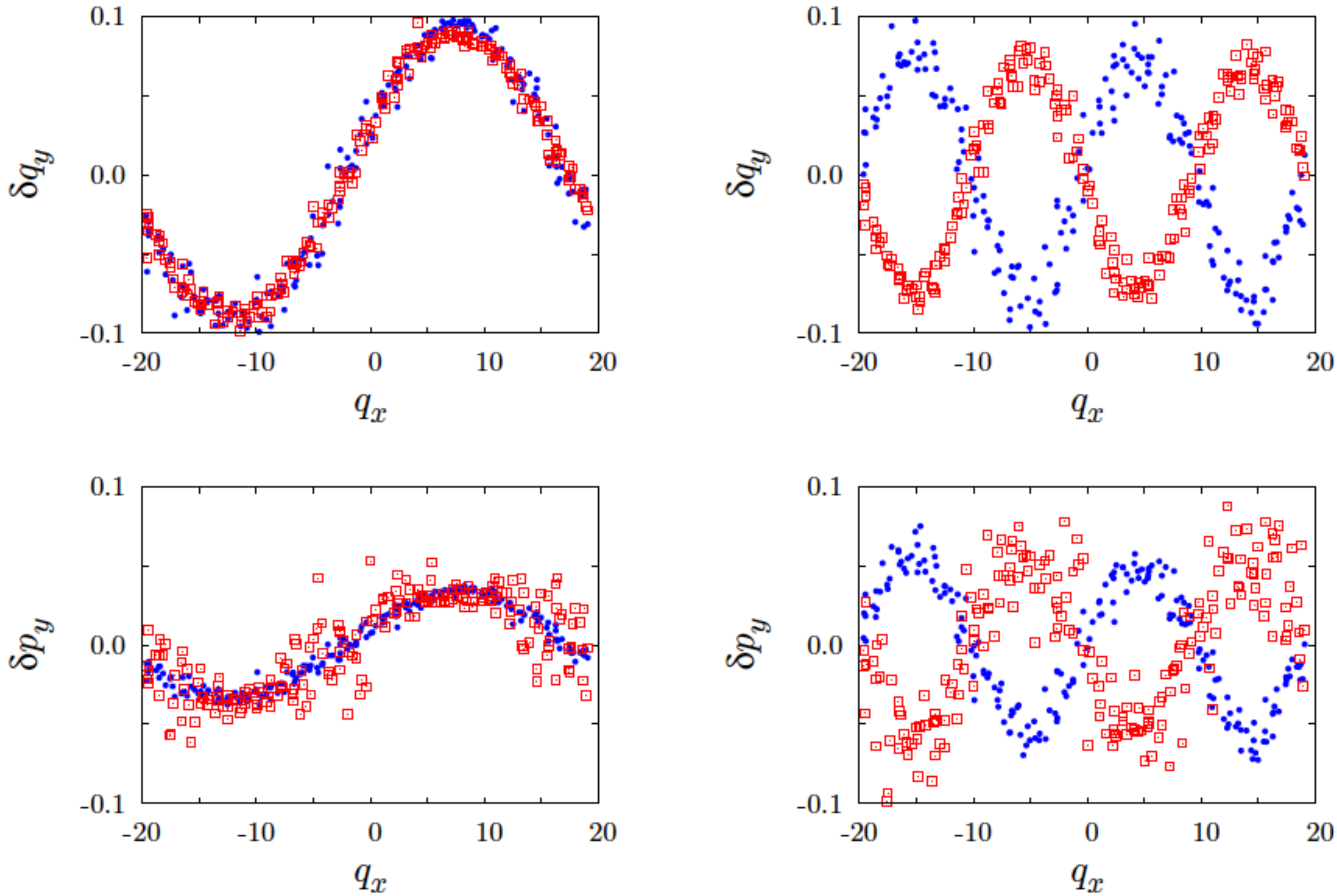
$$\mathcal{N}_y = span\{\boldsymbol{e}_3, \boldsymbol{e}_6\}$$

Angles between 2N-vectors from Q and P



$$\cos(\Theta) = (\delta \boldsymbol{q} \cdot \delta \boldsymbol{p})/(|\delta \boldsymbol{q}|| \cdot \delta \boldsymbol{p}|)$$

Transverse modes T(1,0) and T(2,0)



Mode reconstruction for LP-Modes

TABLE IV: Basis vectors of $(n_x, 0)$ modes for a hard disk system in a rectangular box with periodic boundaries. We use the notation $c_x = \cos(k_x x)$, and $s_x = \sin(k_x x)$, where the wave vector is given by $\boldsymbol{k} = (k_x, k_y) = (2\pi n_x / L_x, 0)$. Here $n_x \in \{1, 2, 3\}$.

$\boldsymbol{n}$	Basis of $\mathbf{T}(\boldsymbol{n})$	Basis of $\mathbf{L}(\boldsymbol{n})$	Basis of $\mathbf{P}(\boldsymbol{n})$
$\begin{pmatrix} n_x \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ c_x \end{pmatrix}, \begin{pmatrix} 0 \\ s_x \end{pmatrix}$	$\begin{pmatrix} c_x \\ 0 \end{pmatrix}, \begin{pmatrix} s_x \\ 0 \end{pmatrix}$	$\begin{pmatrix} p_x \\ p_y \end{pmatrix} s_x, \begin{pmatrix} p_x \\ p_y \end{pmatrix} c_x$

boundaries. We use the notation $c_x = \cos(k_x x)$, and $s_x = \sin(k_x x)$, where the wave vector is given by $\boldsymbol{k} = (k_x, k_y) = (2\pi n_x/L_x, 0)$. Here $n_x \in \{1, 2, 3\}$.

$\boldsymbol{n}$	Basis of $\mathbf{T}(\boldsymbol{n})$	Basis of $\mathbf{L}(\boldsymbol{n})$	Basis of $\mathbf{P}(\boldsymbol{n})$
$\begin{pmatrix} n_x \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ c_x \end{pmatrix}, \begin{pmatrix} 0 \\ s_x \end{pmatrix}$	$\begin{pmatrix} c_x \\ 0 \end{pmatrix}, \begin{pmatrix} s_x \\ 0 \end{pmatrix}$	$\begin{pmatrix} p_x \\ p_y \end{pmatrix} s_x, \begin{pmatrix} p_x \\ p_y \end{pmatrix} c_x$

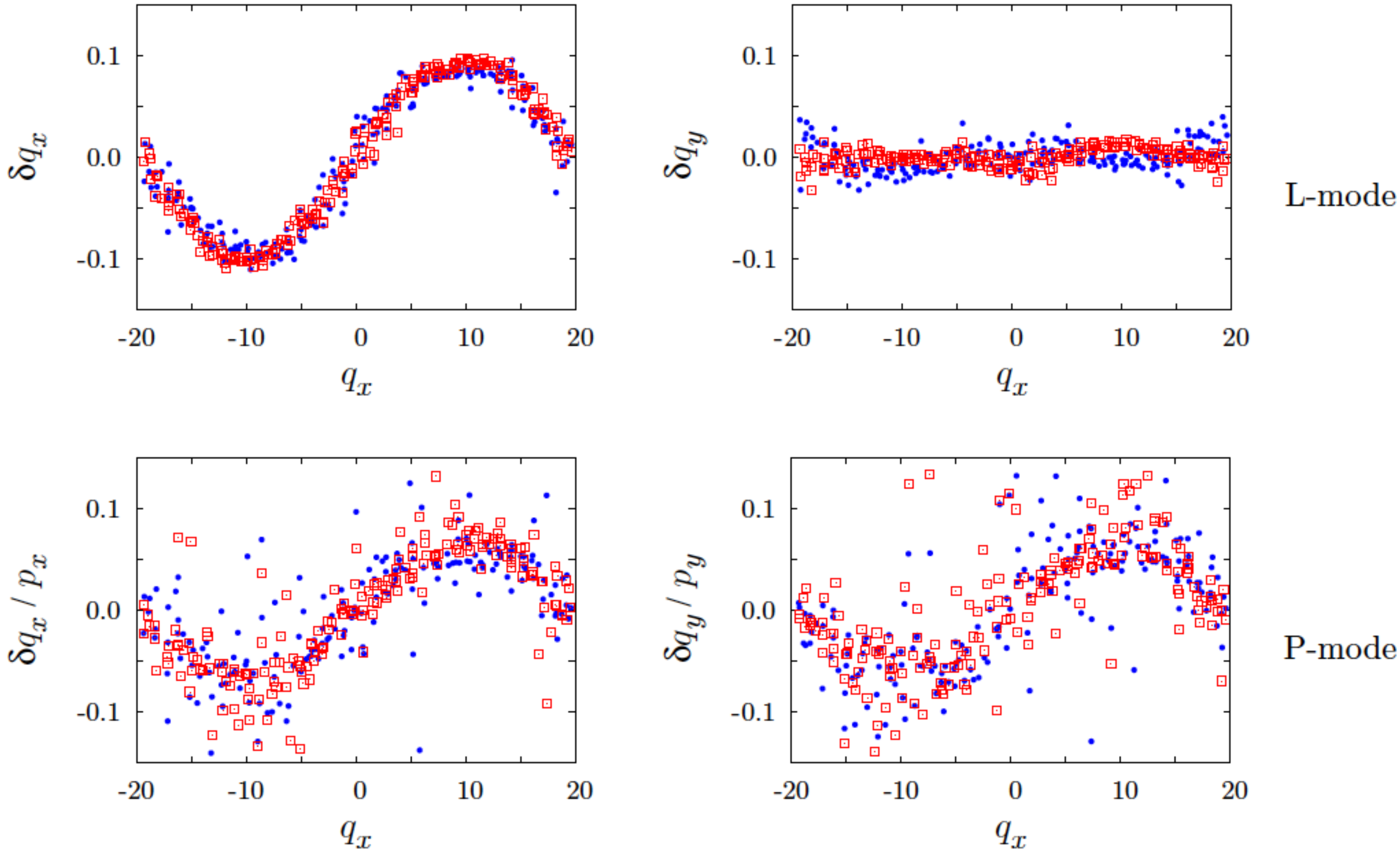
$$\begin{pmatrix} \sin k_x q_{x,i} \\ 0 \end{pmatrix} = a_1 \begin{pmatrix} \delta q_{x,i}^{388} \\ \delta q_{y,i}^{388} \end{pmatrix} + b_1 \begin{pmatrix} \delta q_{x,i}^{389} \\ \delta q_{y,i}^{389} \end{pmatrix} + c_1 \begin{pmatrix} \delta q_{x,i}^{390} \\ \delta q_{y,i}^{390} \end{pmatrix} + d_1 \begin{pmatrix} \delta q_{x,i}^{391} \\ \delta q_{y,i}^{391} \end{pmatrix}$$

$$\begin{pmatrix} \cos k_x q_{x,i} \\ 0 \end{pmatrix} = a_2 \begin{pmatrix} \delta q_{x,i}^{388} \\ \delta q_{y,i}^{388} \end{pmatrix} + b_2 \begin{pmatrix} \delta q_{x,i}^{389} \\ \delta q_{y,i}^{389} \end{pmatrix} + c_2 \begin{pmatrix} \delta q_{x,i}^{390} \\ \delta q_{y,i}^{390} \end{pmatrix} + d_2 \begin{pmatrix} \delta q_{x,i}^{391} \\ \delta q_{y,i}^{391} \end{pmatrix}$$

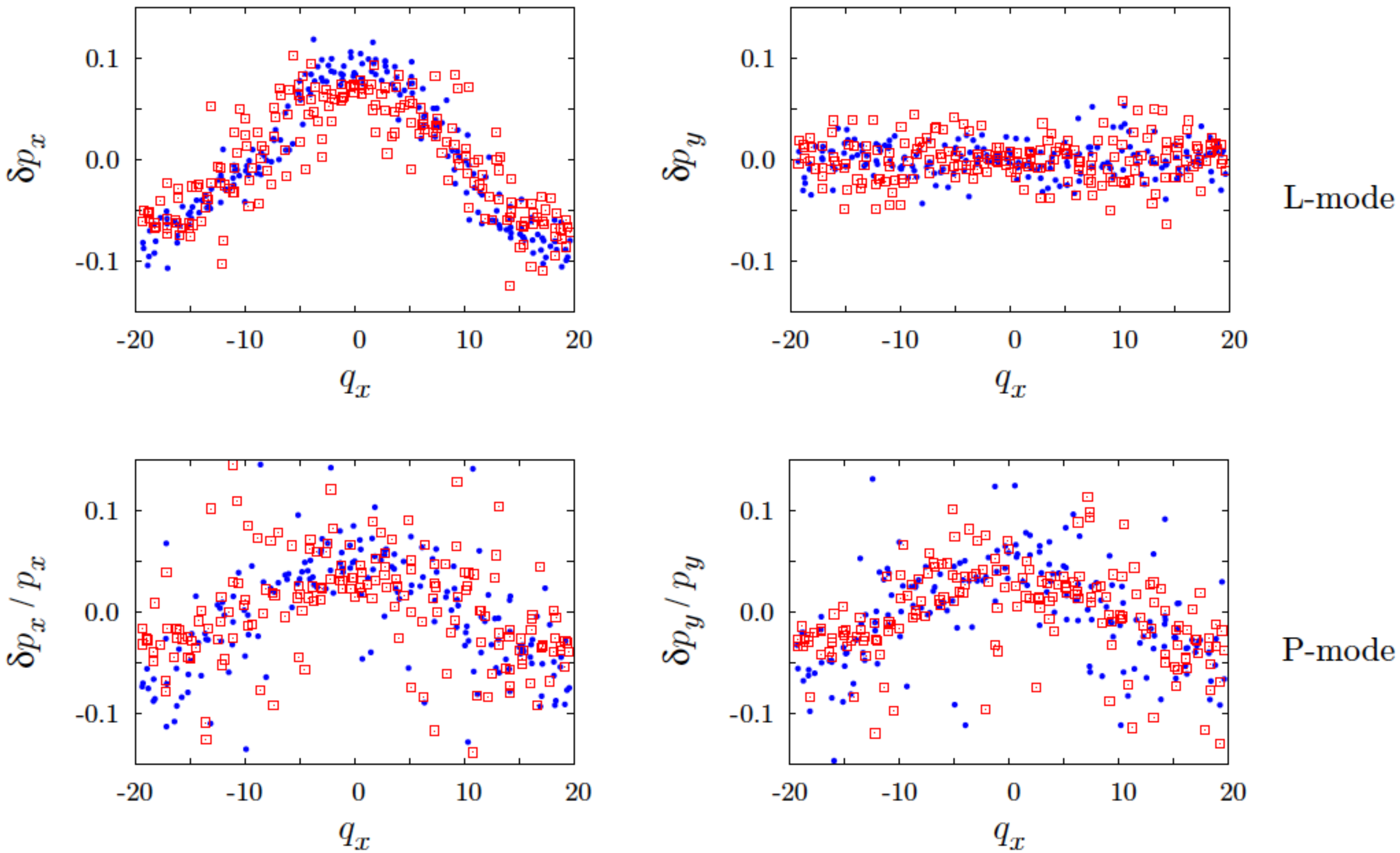
$$\begin{pmatrix} p_{x,i} \sin k_x q_{x,i} \\ p_{y,i} \sin k_x q_{x,i} \end{pmatrix} = a_3 \begin{pmatrix} \delta q_{x,i}^{388} \\ \delta q_{y,i}^{388} \end{pmatrix} + b_3 \begin{pmatrix} \delta q_{x,i}^{389} \\ \delta q_{y,i}^{389} \end{pmatrix} + c_3 \begin{pmatrix} \delta q_{x,i}^{390} \\ \delta q_{y,i}^{390} \end{pmatrix} + d_3 \begin{pmatrix} \delta q_{x,i}^{391} \\ \delta q_{y,i}^{391} \end{pmatrix}$$

$$\begin{pmatrix} p_{x,i} \cos k_x q_{x,i} \\ p_{y,i} \cos k_x q_{x,i} \end{pmatrix} = a_4 \begin{pmatrix} \delta q_{x,i}^{388} \\ \delta q_{y,i}^{388} \end{pmatrix} + b_4 \begin{pmatrix} \delta q_{x,i}^{389} \\ \delta q_{y,i}^{389} \end{pmatrix} + c_4 \begin{pmatrix} \delta q_{x,i}^{390} \\ \delta q_{y,i}^{390} \end{pmatrix} + d_4 \begin{pmatrix} \delta q_{x,i}^{391} \\ \delta q_{y,i}^{391} \end{pmatrix}$$

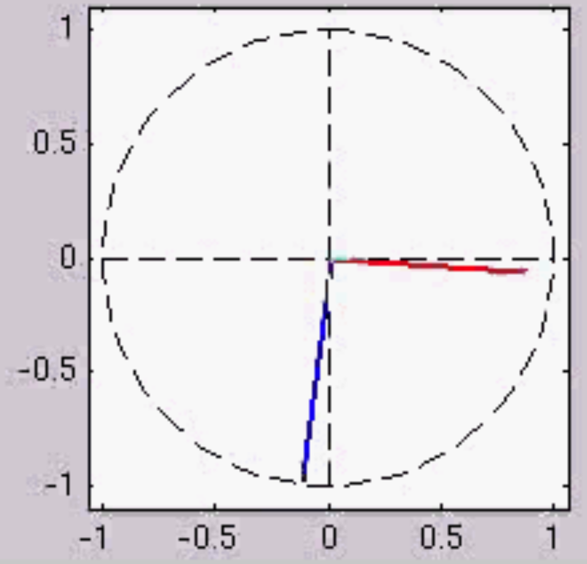
Reconstructed L(1,0) and P(1,0) modes: Q space only

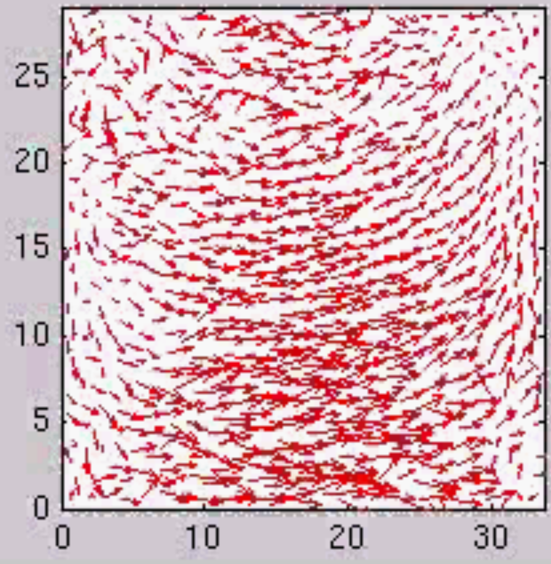


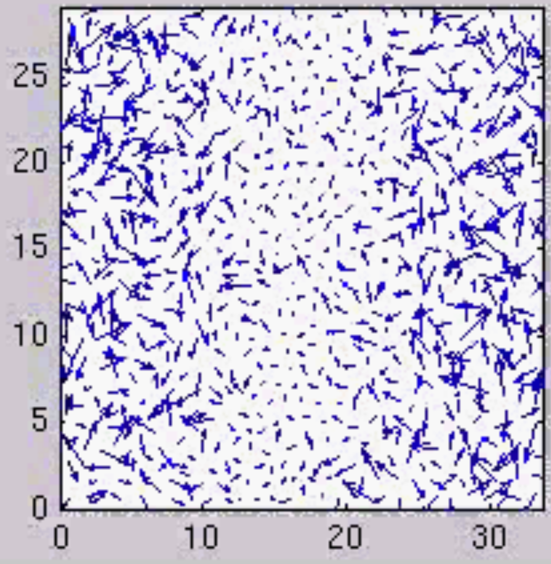
Reconstructed L(1,0) and P(1,0) modes: P space only



Gram-Schmidt mode LP(1,0)
N = 780 hard disks, rho = 0.8, A = 0.867
reflecting boundaries







$$\begin{pmatrix}\varphi_x^{\mathrm{L}}\\ \varphi_y^{\mathrm{L}}\end{pmatrix} = \frac{1}{z_1}\begin{pmatrix}s_x\\ 0\end{pmatrix}, \quad \begin{pmatrix}\varphi_x^{\mathrm{P}}\\ \varphi_y^{\mathrm{P}}\end{pmatrix} = \frac{1}{z_2}\begin{pmatrix}p_x\\ p_y\end{pmatrix} c_x, \quad k_x = \frac{\pi}{L_x}$$

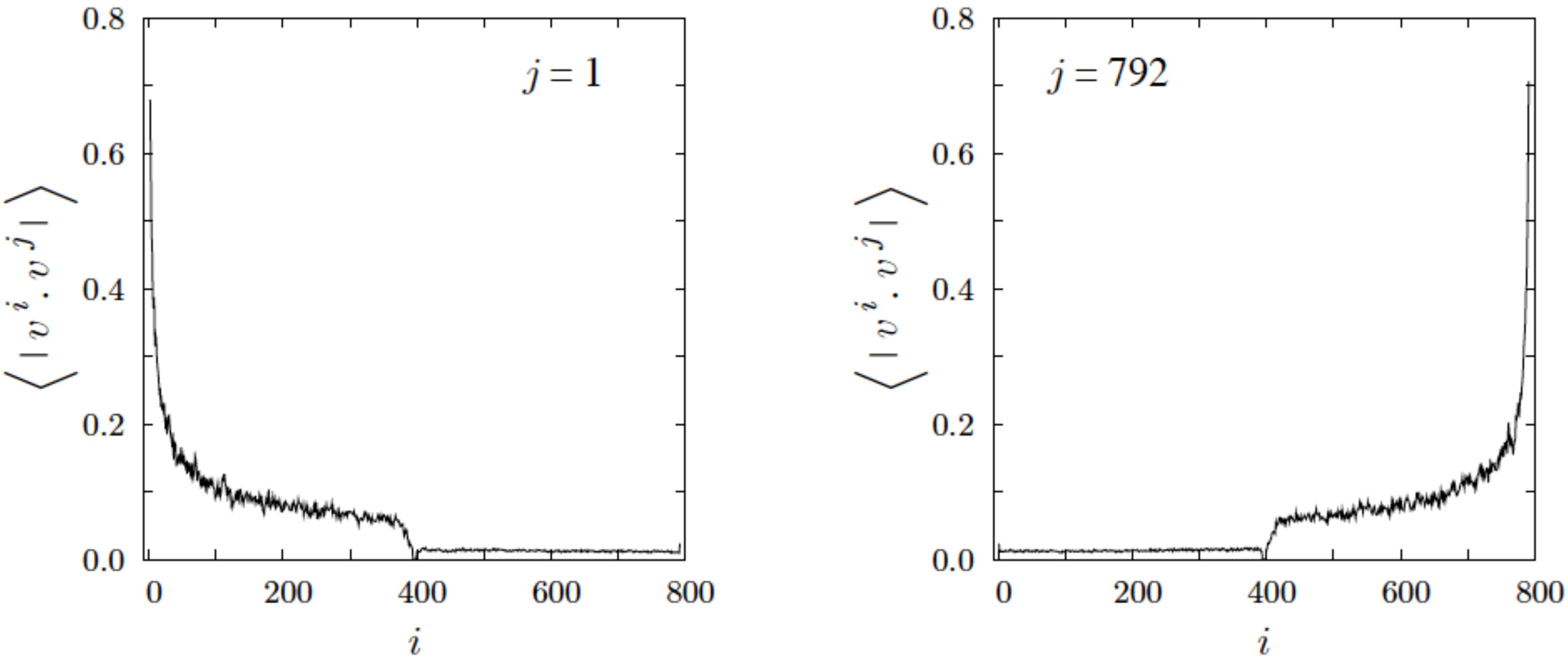
$$\varphi^{\mathrm{L}} = \psi^1 a + \psi^2 b$$
$$\varphi^{\mathrm{P}} = \psi^1 c + \psi^2 d$$

$d \simeq a$, and $a^2 + b^2 \simeq 1$

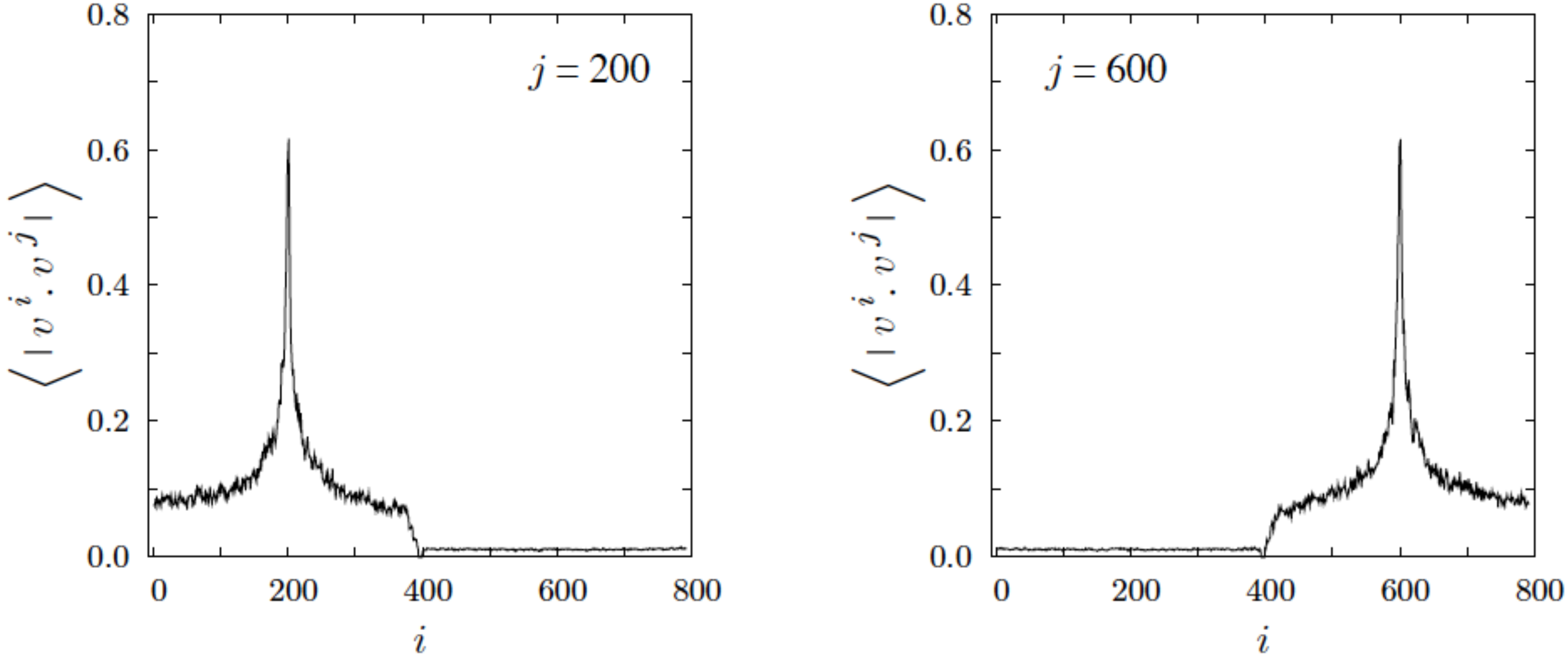
$c \simeq -b$,

$\phi(t) = \arctan(b(t)/a(t))$

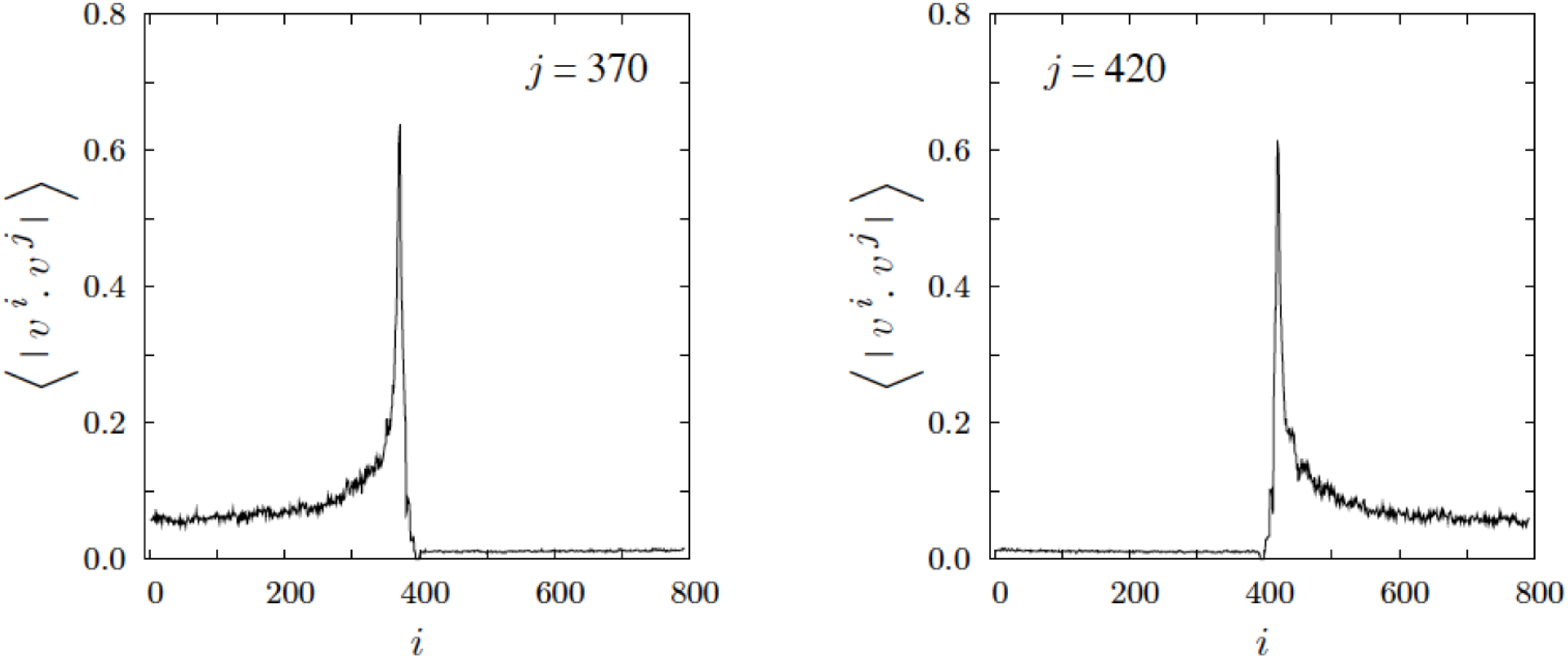
Transversality I



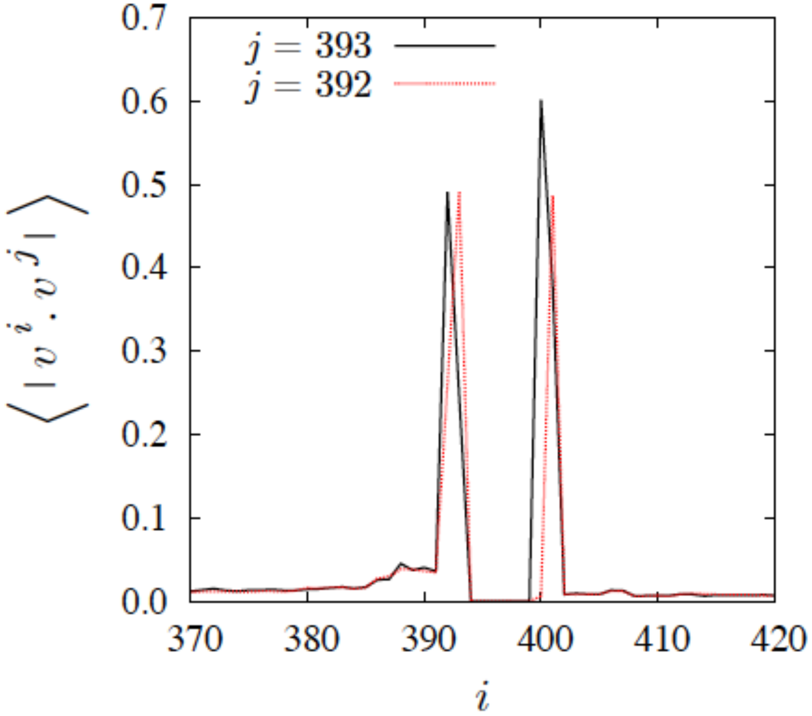
Transversality II

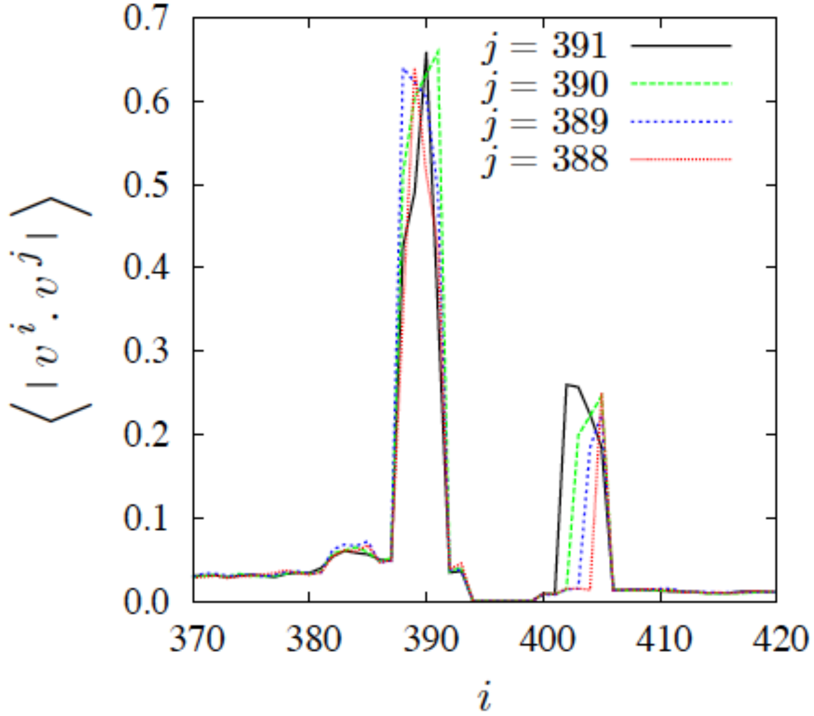


Transversality III

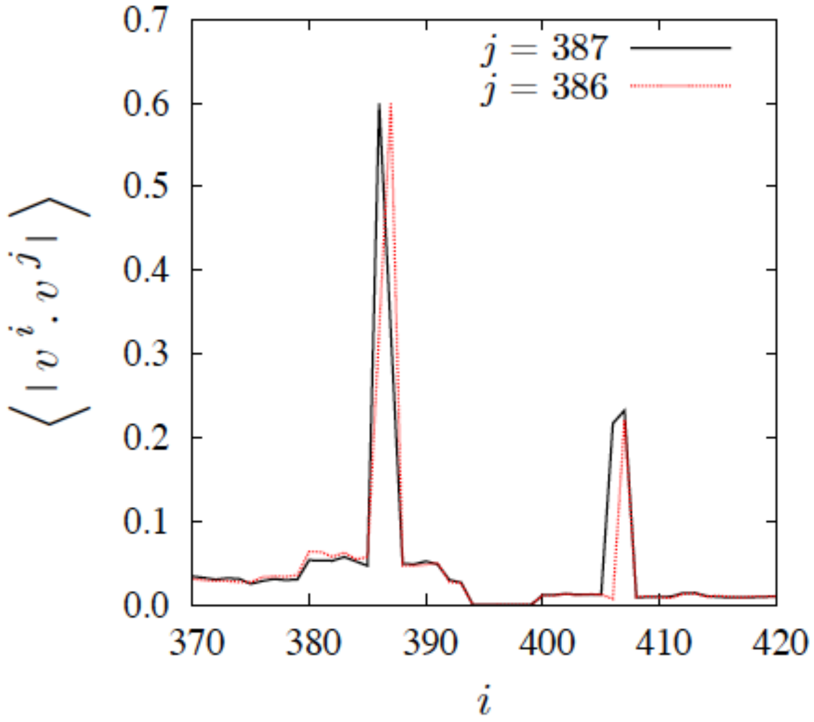


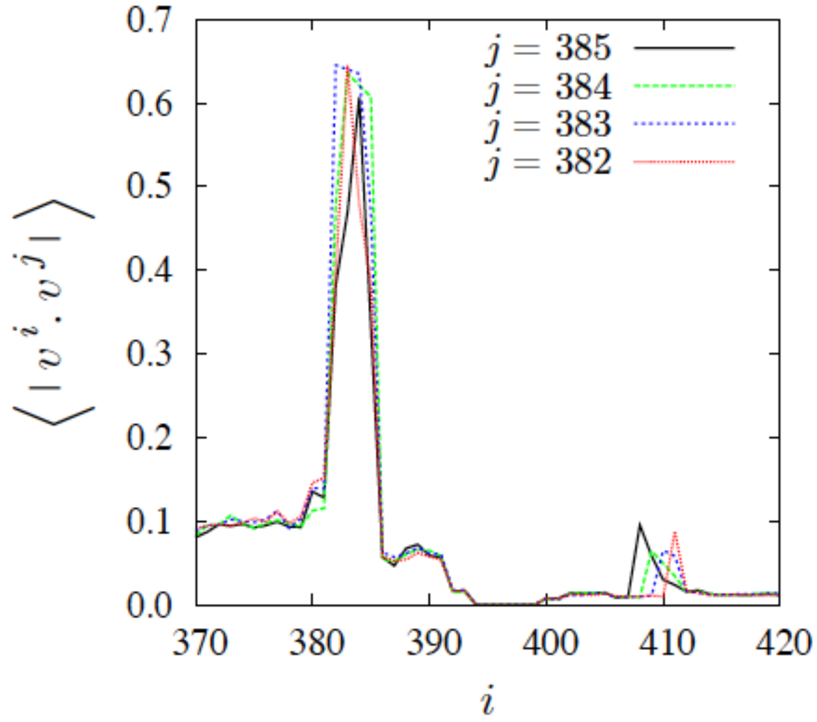
Transversality in the mode domain I



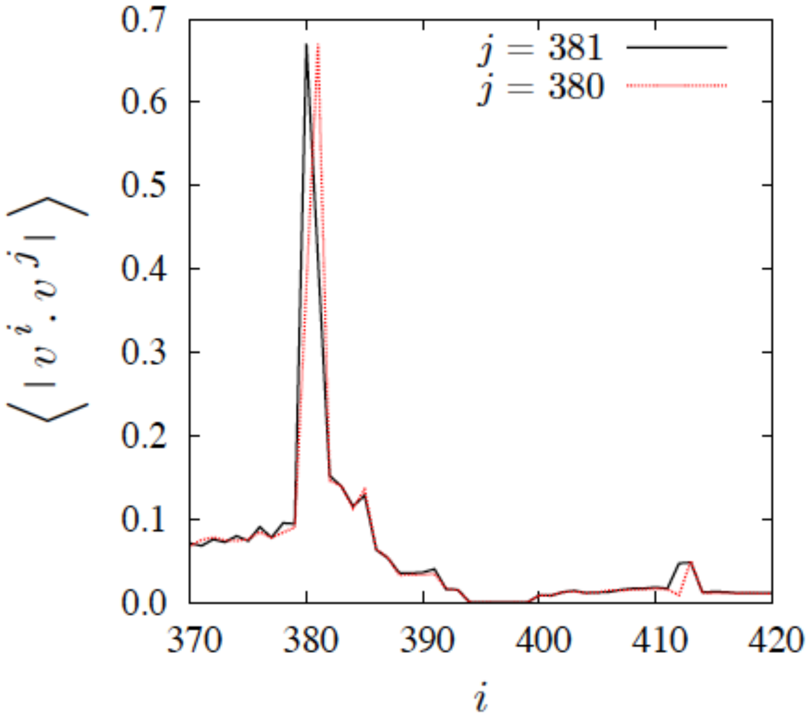


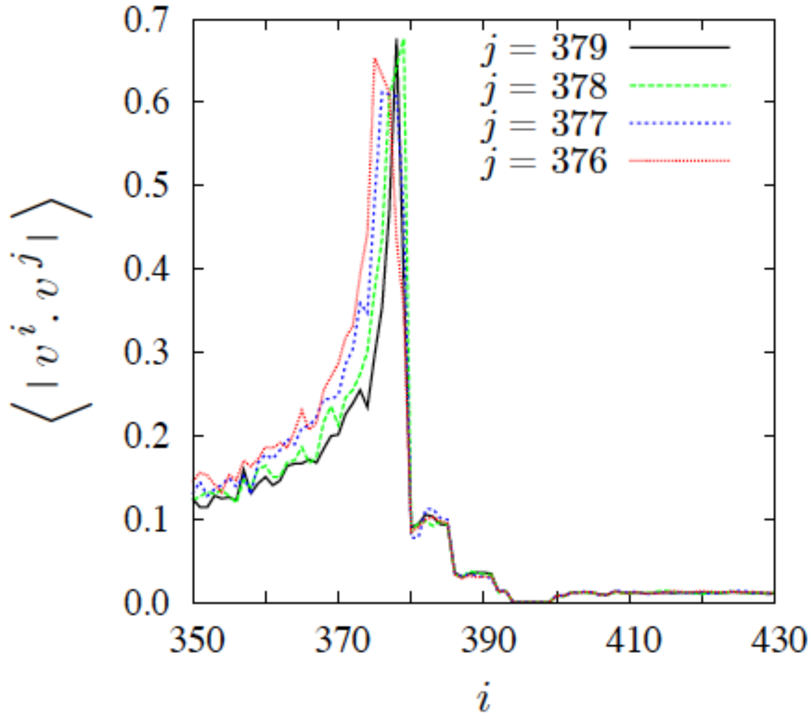
Transversality in the mode domain II



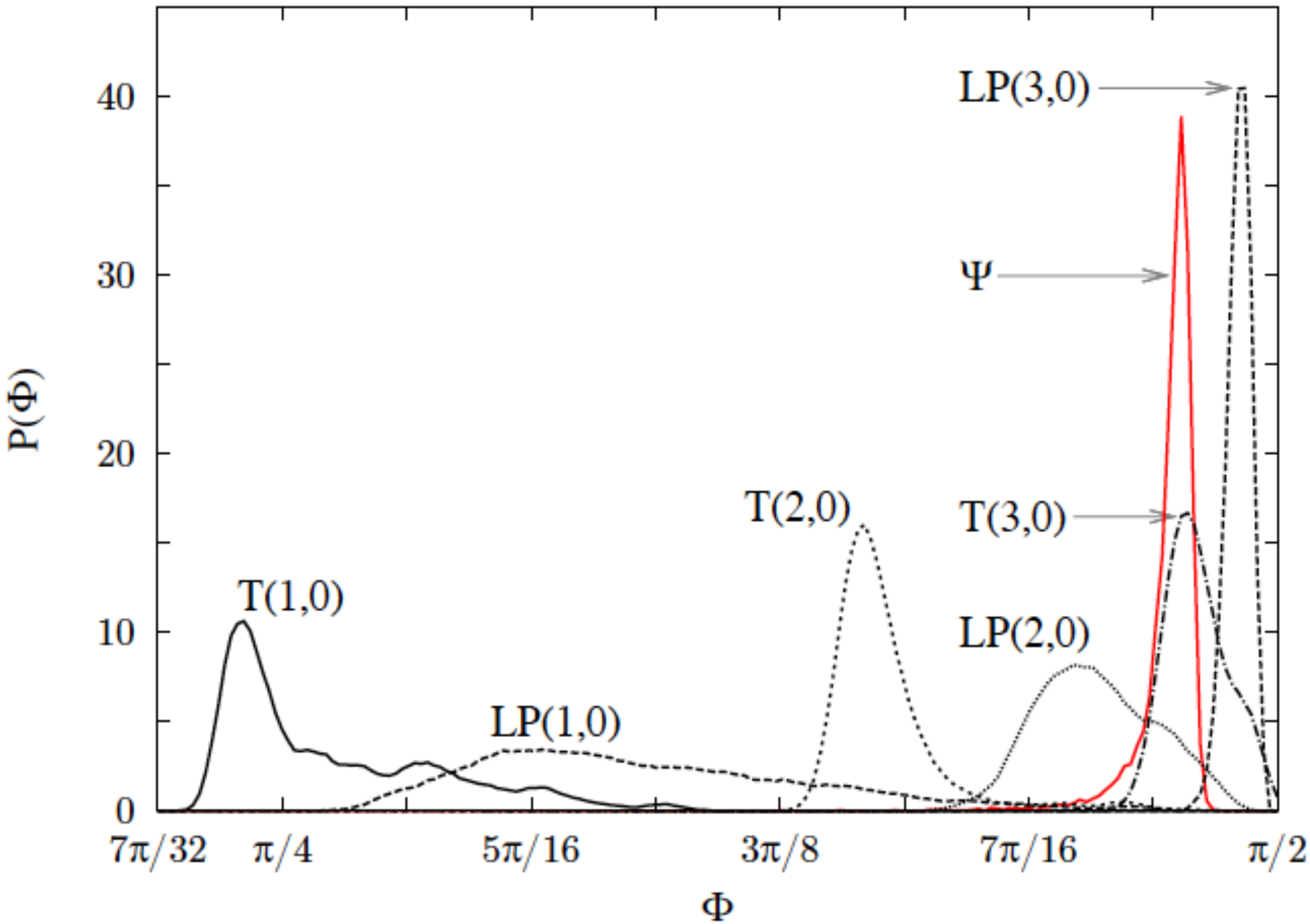


Transversality in the mode domain III

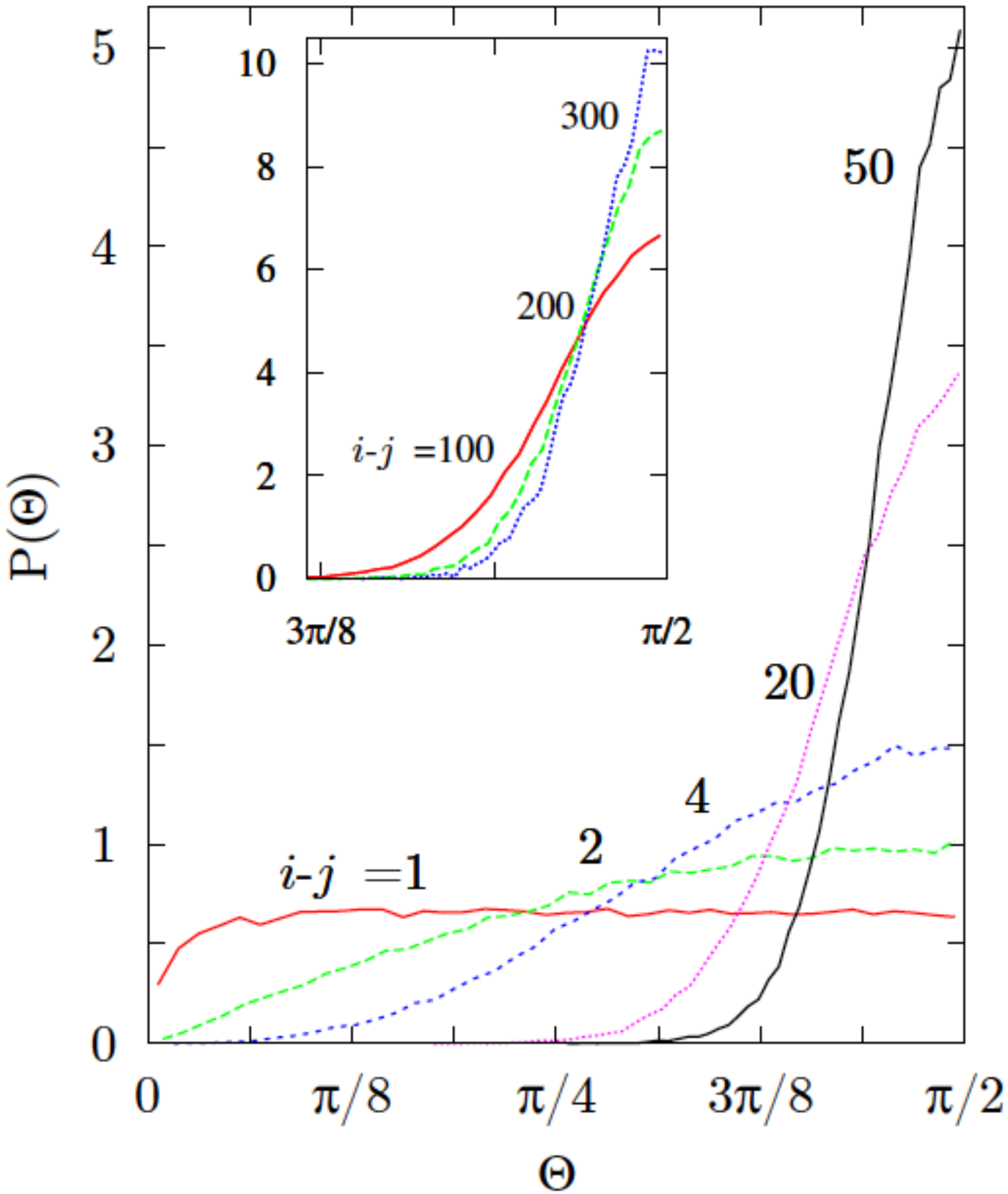




Distribution of Minimum angle between conjugate subspaces



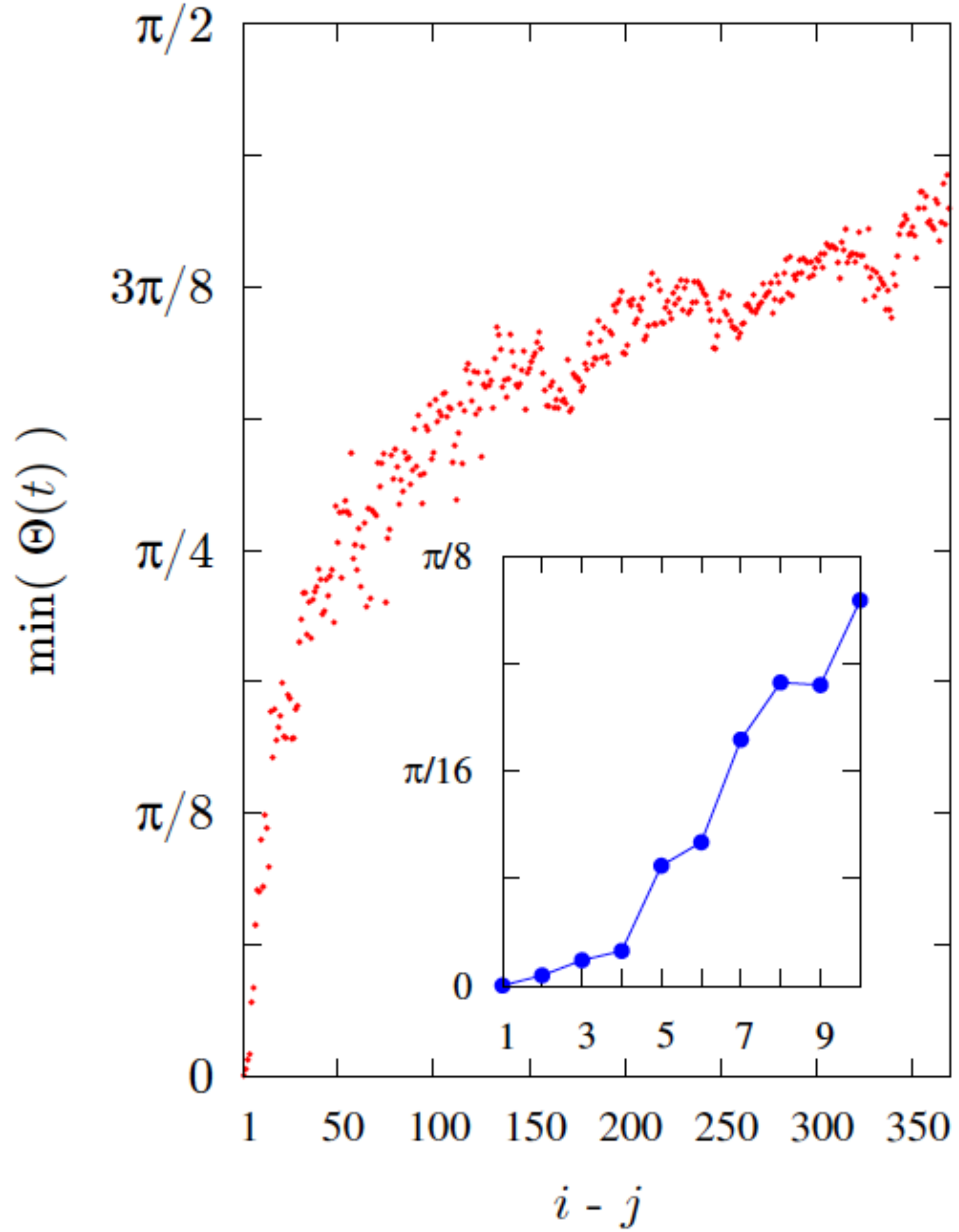
Transversality of adjacent covariant vectors



$$\Theta = \cos^{-1} \left| \boldsymbol{v}^i \cdot \boldsymbol{v}^j \right|$$

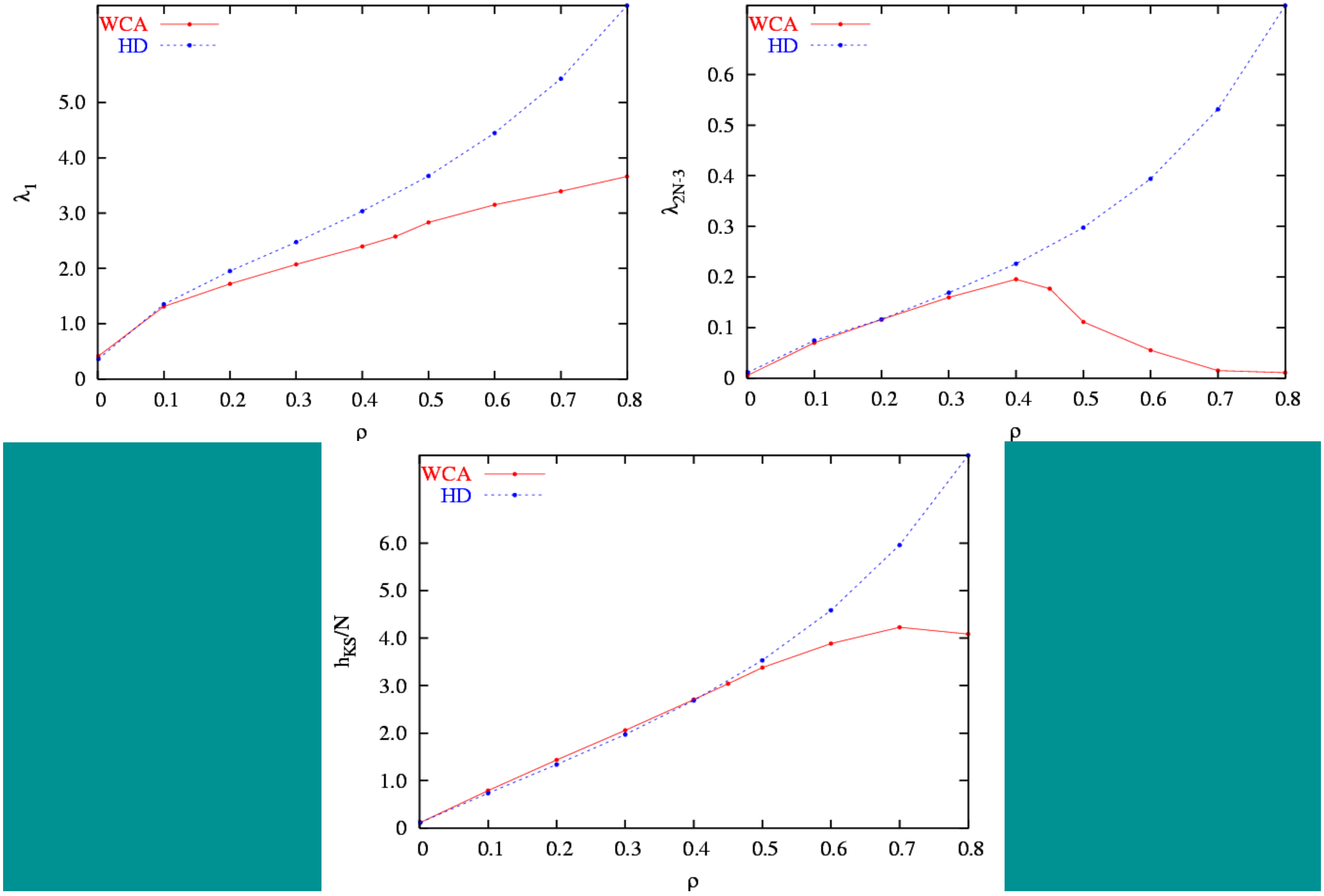
$\boldsymbol{v}^i \in \boldsymbol{V}^{(J)}$ and $\boldsymbol{v}^j \in \boldsymbol{V}^{(J)}$

$$\boldsymbol{V}^{(J)} = \boldsymbol{v}^1 \oplus \cdots \oplus \boldsymbol{v}^J$$



π/2
3π/8
π/4
π/8
0
min(Θ(t))
1
50
100
150
200
250
300
350
i - j
π/8
π/16
0
1
3
5
7
9

Density dependence: hard and soft disks

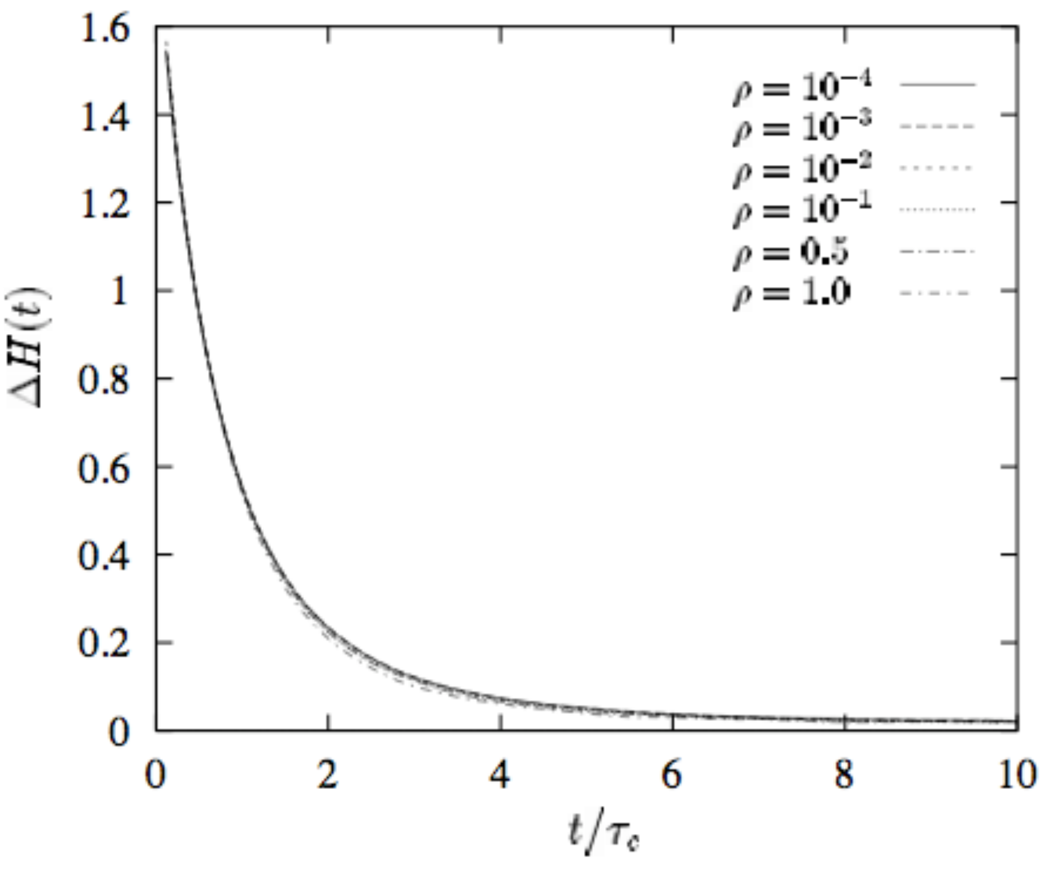


Relaxation to equilibrium (Ch. Dellago, and HAP, PRE 55, R9 (1997)

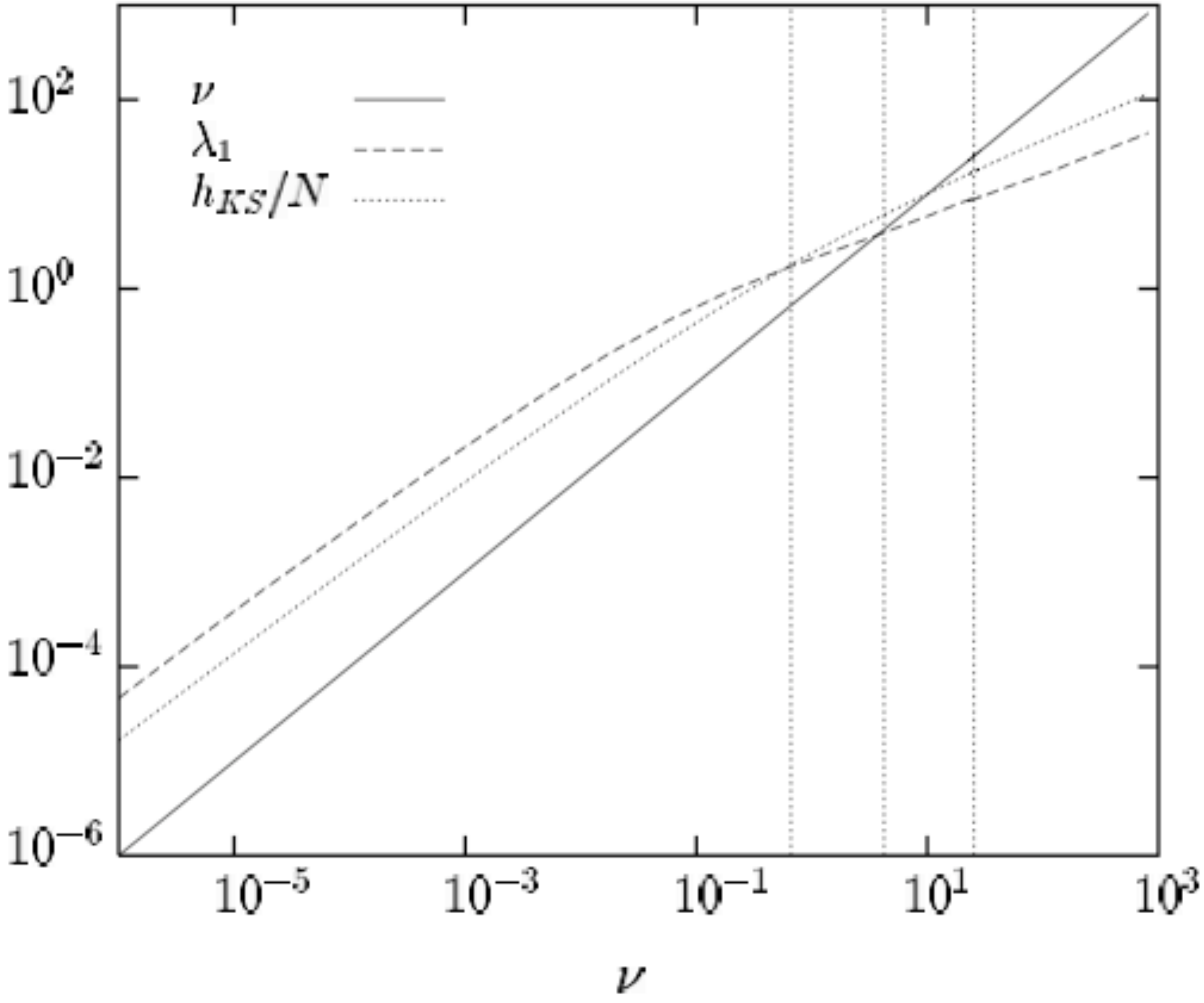
$$t = 0: \quad |p_i| = const, \quad i = 1, 108$$

$$H(t) = \int_0^\infty f(p,t) \ln f(p,t)\, dp,$$

$$\Delta H(t) = H(t) - H_0$$



Ch. Dellago and H.A.Posch, Phys. Rev. E 55, R9 (1997)



$$\Delta\Gamma_t = \Delta\Gamma_0 \exp(h_{KS} t)$$

$$t_0 = \frac{1}{h_{KS}} \ln \frac{1}{\Delta\Gamma_0}$$

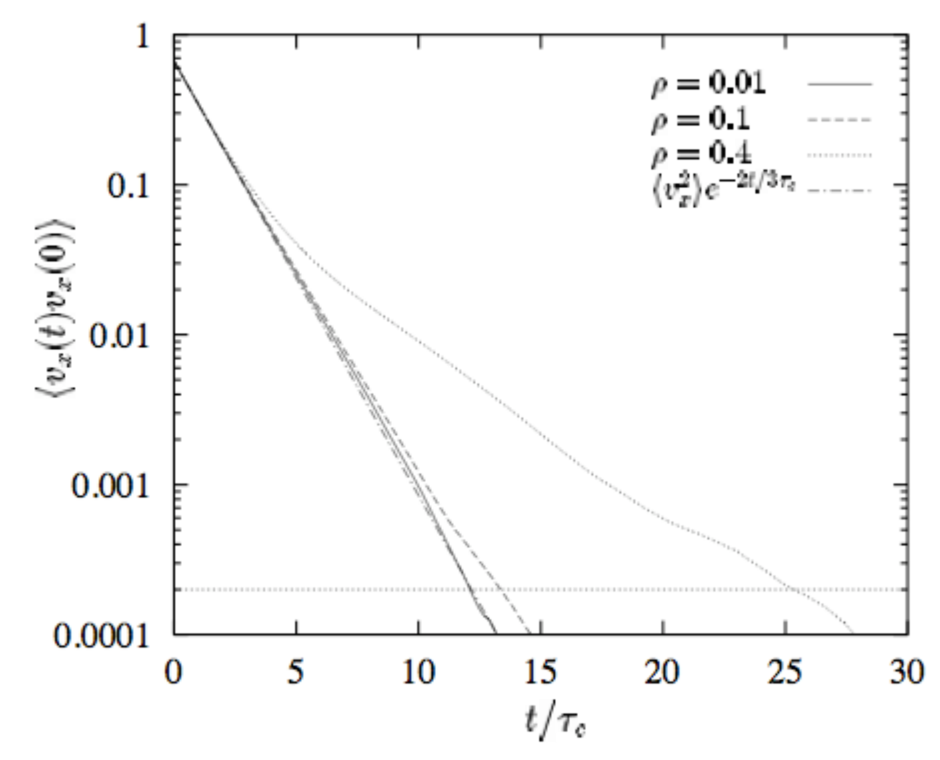
$$\text{Small } \rho: \quad \frac{\tau_\lambda}{\tau_c} \propto \frac{\rho}{|\rho \log \rho|}$$

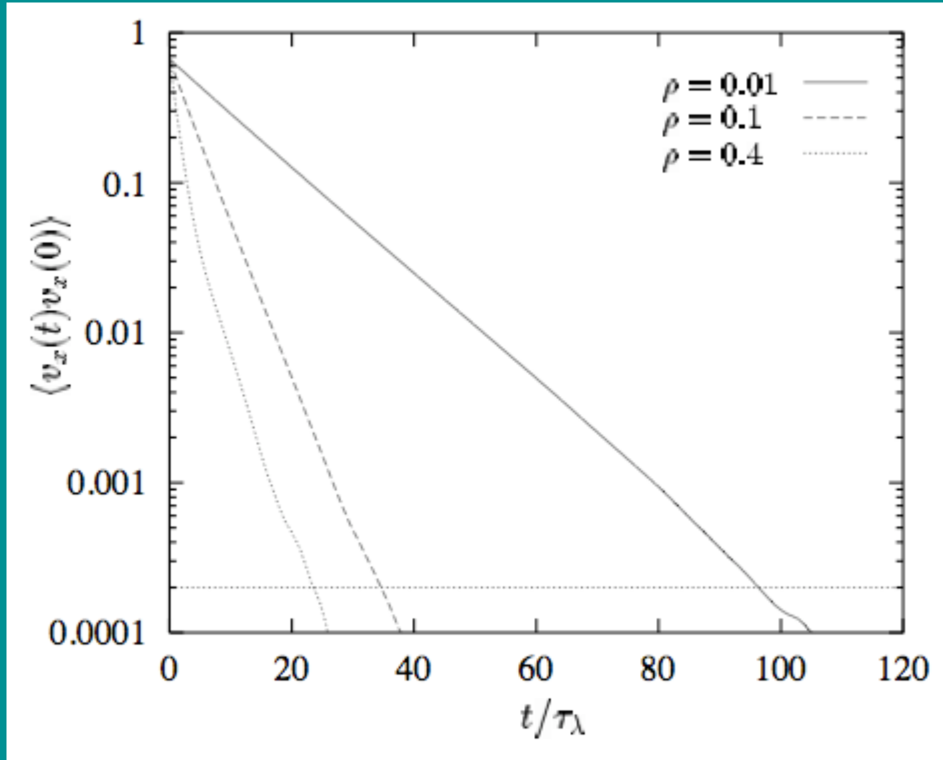
$$\text{Large } \rho: \quad \frac{\tau_\lambda}{\tau_c} \propto \frac{\nu}{\nu^b} \approx \nu^{0.54}$$

$$\lim_{\rho \to 0} \frac{\tau_\lambda}{\tau_c} = 0$$

$$\lim_{\rho \to \rho_{cp}} \frac{\tau_\lambda}{\tau_c} = \lim_{\nu \to \infty} \frac{\nu}{\nu^{0.46}} = \infty$$

Reliability of correlation functions (single particle correlations)





$$\epsilon_t \sim \epsilon_0 \exp(\lambda_1 t)$$

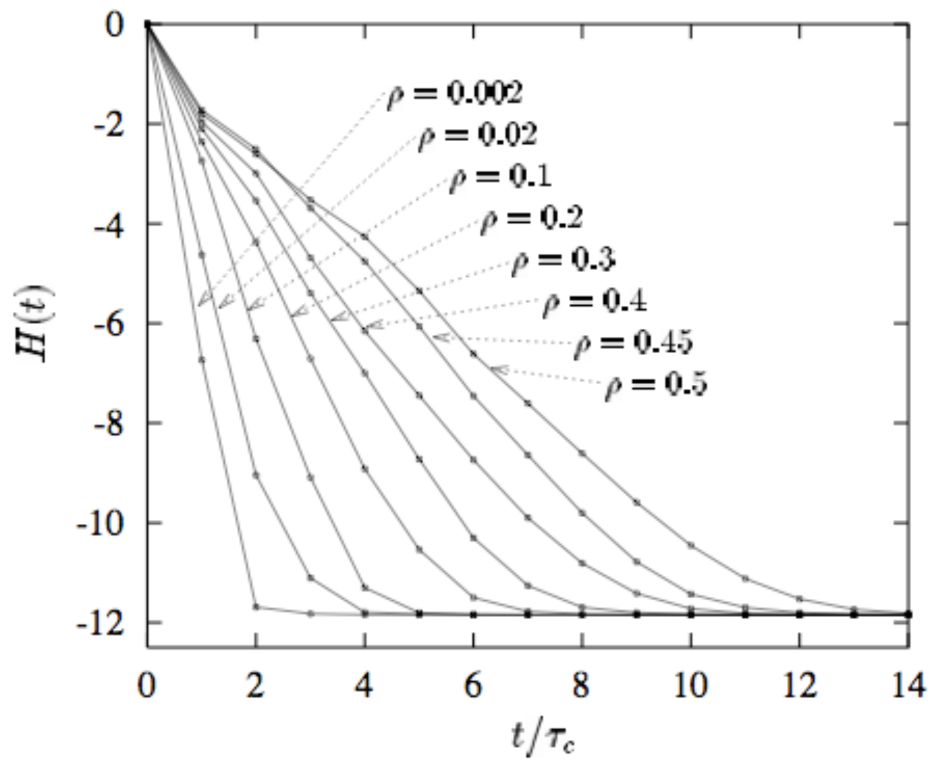
$$\epsilon_0 \approx 10^{-15}; \quad t/\tau_\lambda \approx 35$$

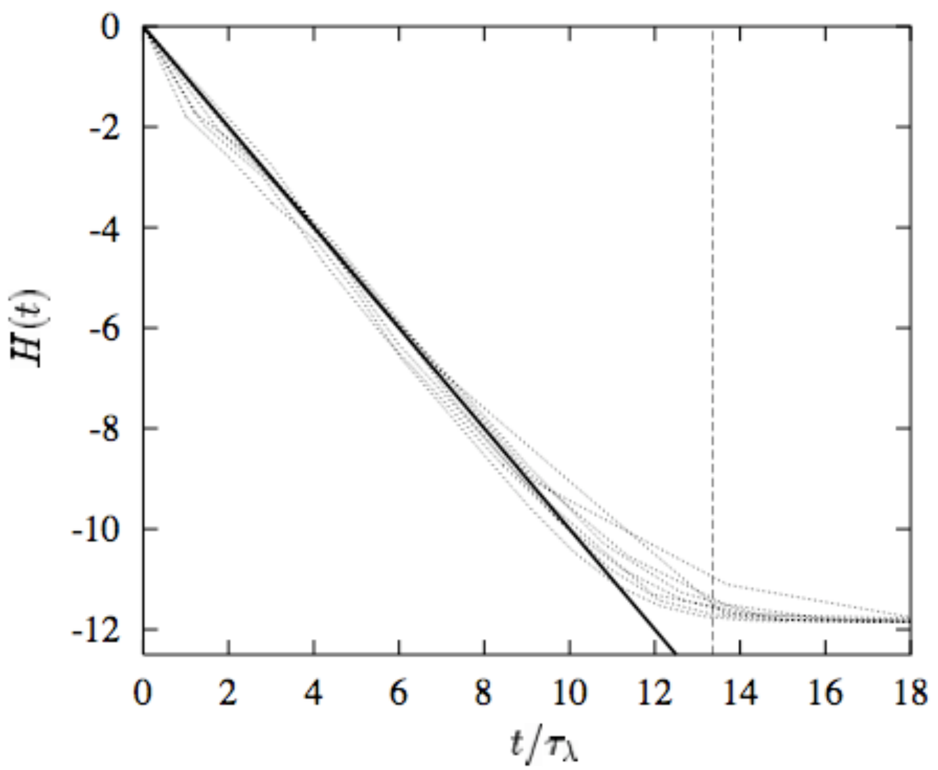
Collective properties

Partitioning of phase space for the periodic Lorentz gas:

$$f_i = n_i / \sum_i n_i; \quad H_k = \sum_{i=1}^{N} f_i \ln f_i$$

$$t = 0: \quad n_1 = n; \quad n_i = 0 \text{ for } i > 1$$





Rough Hard Disks and Spheres

$$\vec{q} = \vec{q}_j - \vec{q}_i; \quad \vec{n} = \frac{1}{\sigma}\vec{q}; \quad \vec{v} = \vec{v}_j - \vec{v}_i; \quad \vec{\Omega} = \vec{\omega}_j + \vec{\omega}_i$$

$$\vec{g} = \vec{v} + \frac{\sigma}{2}\vec{n} \times \vec{\Omega}$$

$$\begin{aligned}
\vec{q}_i{}' &= \vec{q}_i \\
\vec{q}_j{}' &= \vec{q}_j \\
\vec{v}_i{}' &= \vec{v}_i + \gamma\vec{g} + \beta\,\vec{n}(\vec{n}\cdot\vec{v}) \\
\vec{v}_j{}' &= \vec{v}_j - \gamma\vec{g} - \beta\,\vec{n}(\vec{n}\cdot\vec{v}) \\
\vec{\omega}_i{}' &= \vec{\omega}_i + (2\beta/\sigma)\,\vec{n} \times \vec{g} \\
\vec{\omega}_j{}' &= \vec{\omega}_j + (2\beta/\sigma)\,\vec{n} \times \vec{g}
\end{aligned}$$

$$\kappa = \frac{4I}{m\sigma^2}; \qquad \gamma = \frac{\kappa}{\kappa+1}; \qquad \beta = \frac{1}{\kappa+1}$$

$\kappa = 0$, mass concentrated in the center.
$\kappa = \frac{1}{2}$, mass uniformly distributed.
$\kappa = 1$, mass concentrated on the disk boundary.

Rough particles: collision map in tangent space

$$\delta\tau_c = -\frac{\delta\vec{q}\cdot\vec{n}}{\vec{v}\cdot\vec{n}}; \qquad \delta\vec{q}_c = \delta\vec{q}+\vec{v}\,\delta\tau_c$$

$$\delta\vec{q} = \delta\vec{q}_j - \delta\vec{q}_i; \quad \delta\vec{v} = \delta\vec{v}_j - \delta\vec{v}_i; \quad \delta\vec{\Omega} = \delta\vec{\omega}_j + \delta\vec{\omega}_i$$

$$\delta\vec{g} = \delta\vec{v} + \frac{1}{2}\left[\delta\vec{q}_c\times\vec{\Omega} + \vec{q}\times\delta\vec{\Omega}\right]$$

$$\delta\vec{q}_i{}' = \delta\vec{q}_i - \left[\gamma\vec{g} + \frac{\beta}{\sigma^2}\vec{q}(\vec{q}\cdot\vec{v})\right]\delta\tau_c$$

$$\delta\vec{q}_j{}' = \delta\vec{q}_j + \left[\gamma\vec{g} + \frac{\beta}{\sigma^2}\vec{q}(\vec{q}\cdot\vec{v})\right]\delta\tau_c$$

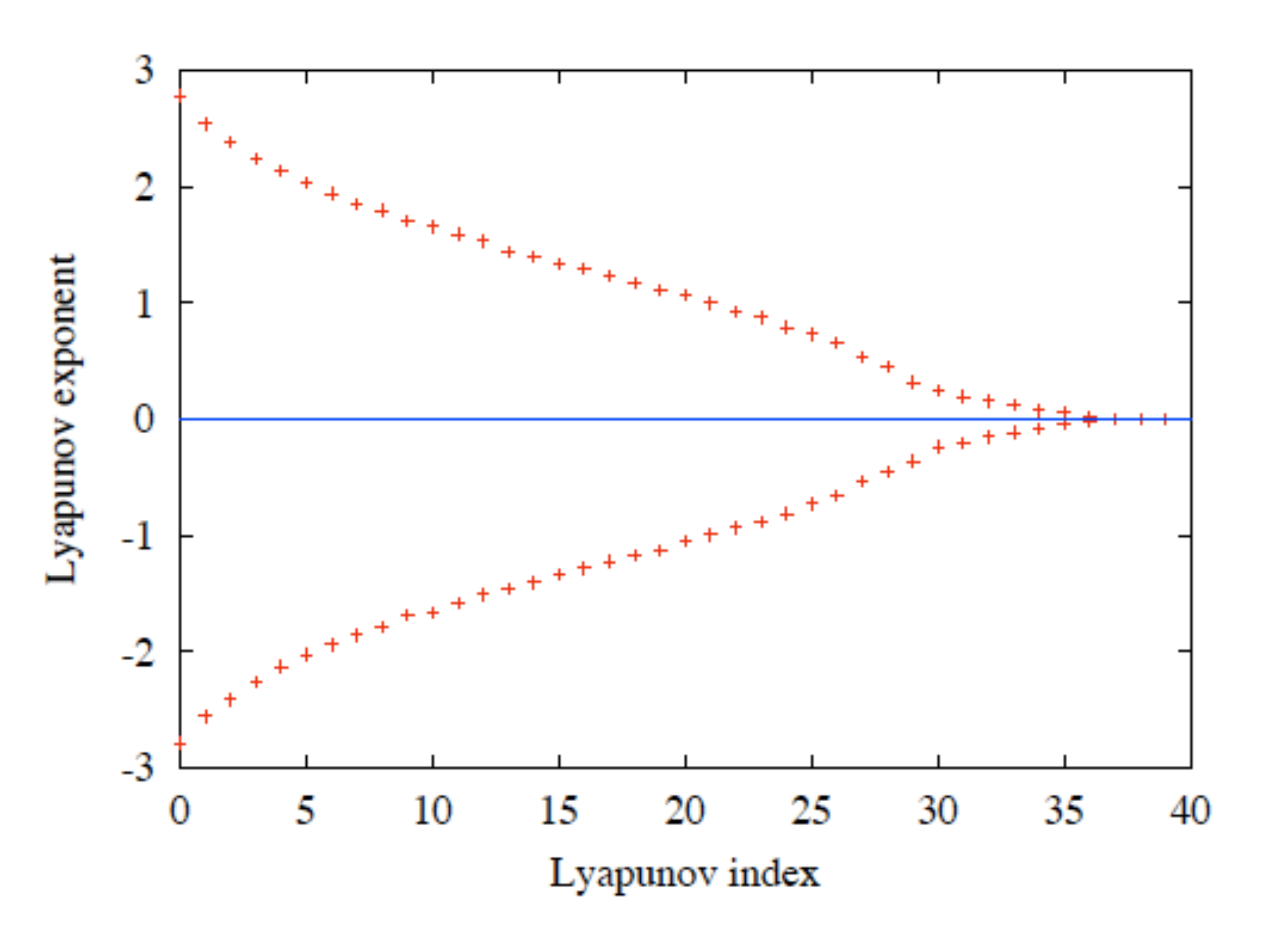
$$\delta\vec{v}_i{}' = \delta\vec{v}_i + \gamma\,\delta\vec{g} + \frac{\beta}{\sigma^2}\left[\delta\vec{q}_c(\vec{q}\cdot\vec{v}) + \vec{q}(\vec{v}\cdot\delta\vec{q}_c) + \vec{q}(\vec{q}\cdot\delta\vec{v})\right]$$

$$\delta\vec{v}_j{}' = \delta\vec{v}_j - \gamma\,\delta\vec{g} - \frac{\beta}{\sigma^2}\left[\delta\vec{q}_c(\vec{q}\cdot\vec{v}) + \vec{q}(\vec{v}\cdot\delta\vec{q}_c) + \vec{q}(\vec{q}\cdot\delta\vec{v})\right]$$

$$\delta\vec{\omega}_i{}' = \delta\vec{\omega}_i + \frac{2\beta}{\sigma^2}\left[\delta\vec{q}_c\times\vec{g} + \vec{q}\times\delta\vec{g}\right]$$

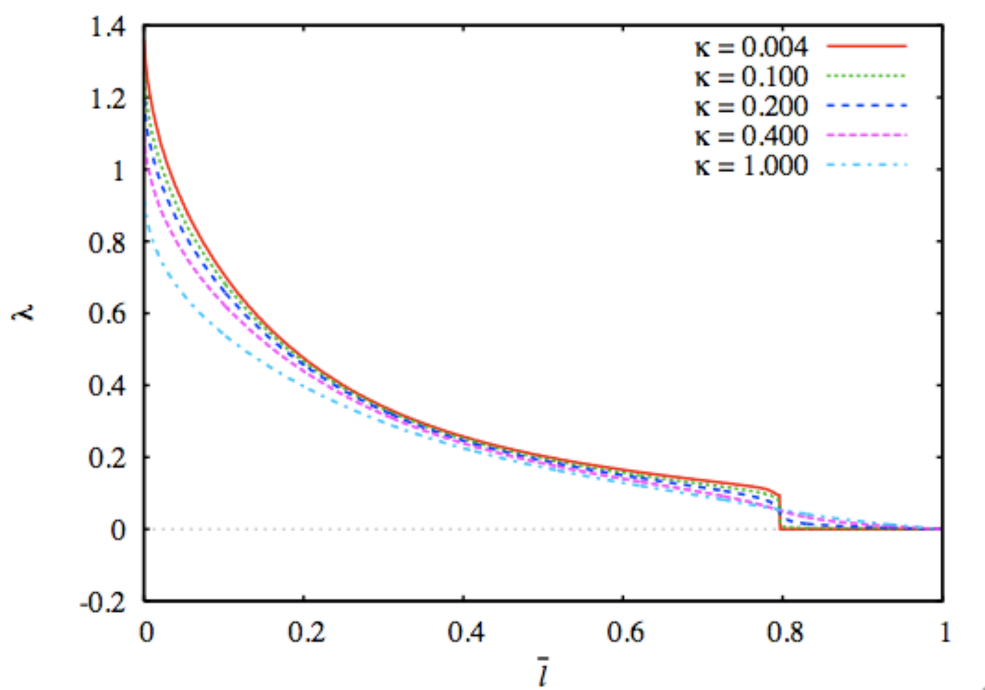
$$\delta\vec{\omega}_j{}' = \delta\vec{\omega}_j + \frac{2\beta}{\sigma^2}\left[\delta\vec{q}_c\times\vec{g} + \vec{q}\times\delta\vec{g}\right]$$

N = 16, N/V = 0.5, l = 0.1

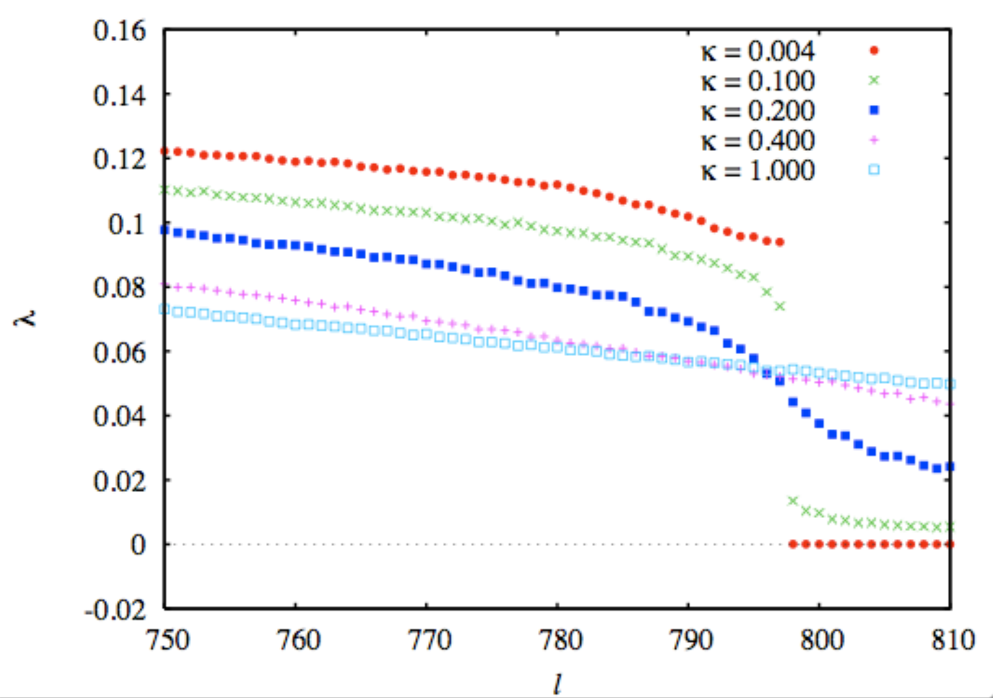


Lyapunov exponent
Lyapunov index
3
2
1
0
-1
-2
-3
0
5
10
15
20
25
30
35
40

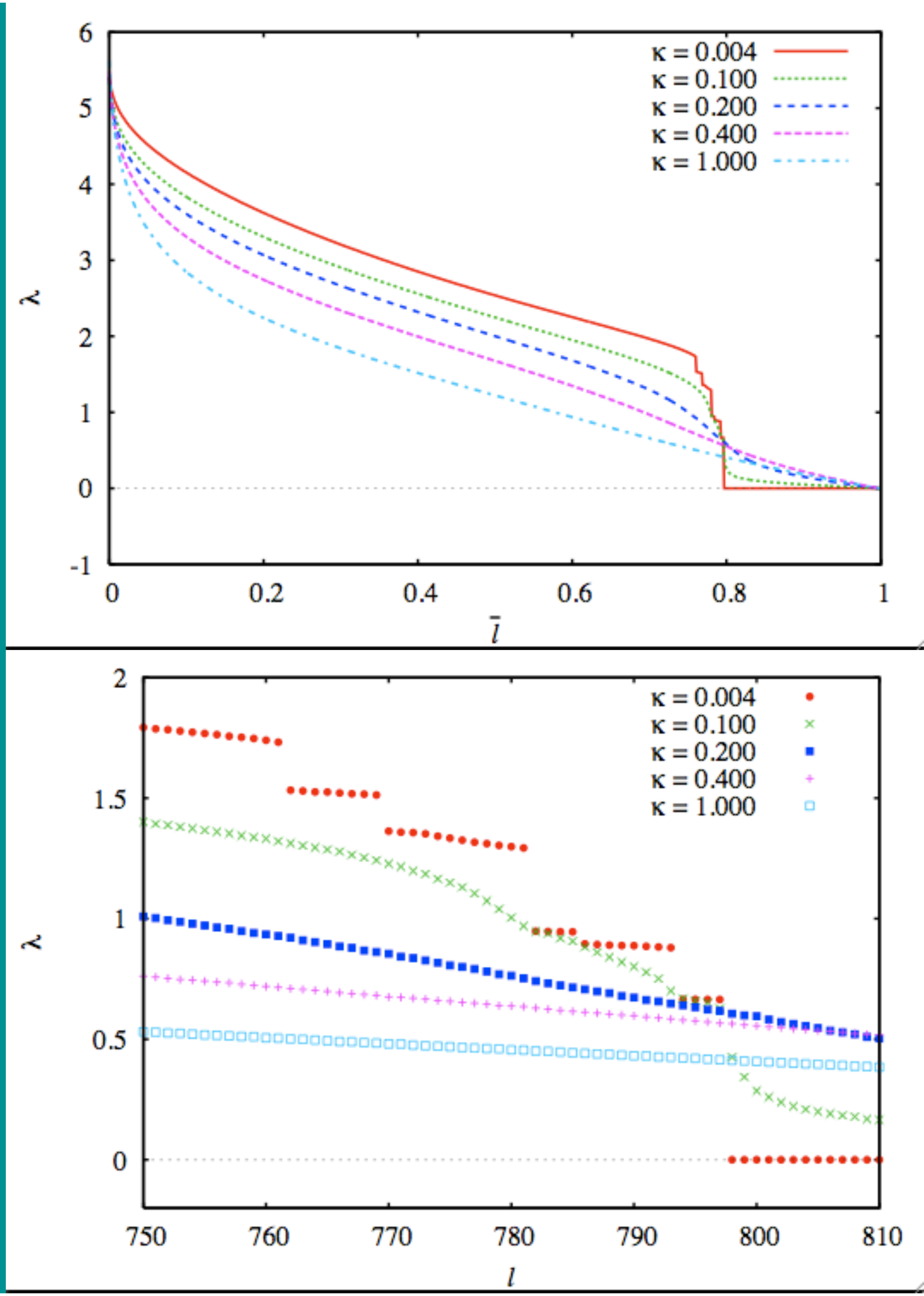
$\rho = 0.1$



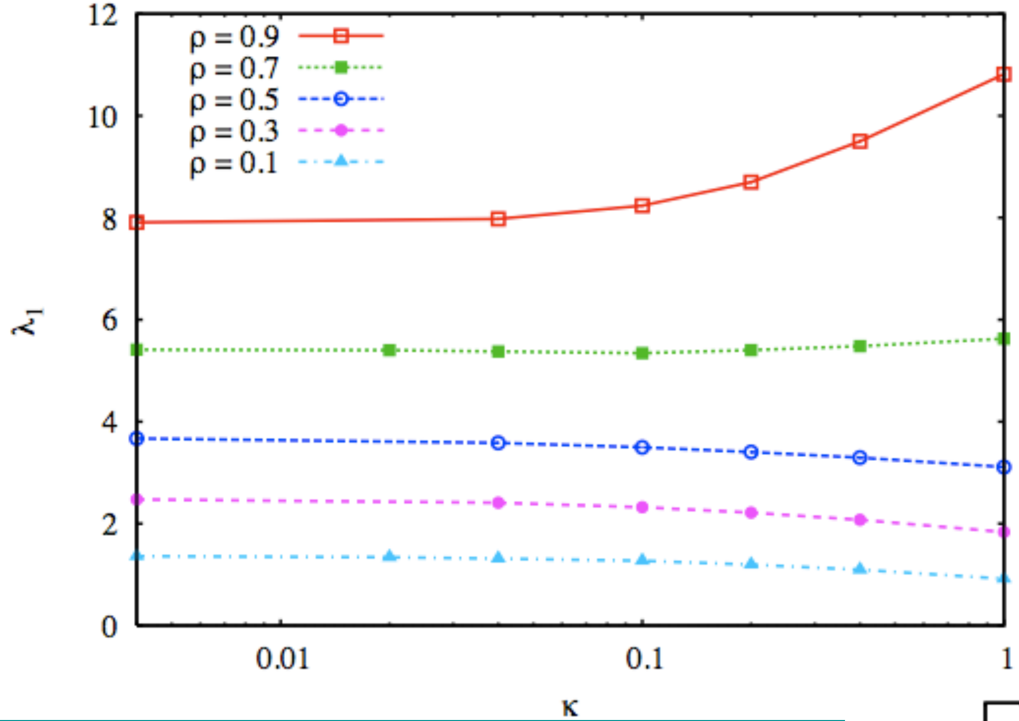
κ = 0.004
κ = 0.100
κ = 0.200
κ = 0.400
κ = 1.000
λ
$\bar{l}$



κ = 0.004
κ = 0.100
κ = 0.200
κ = 0.400
κ = 1.000
λ
l

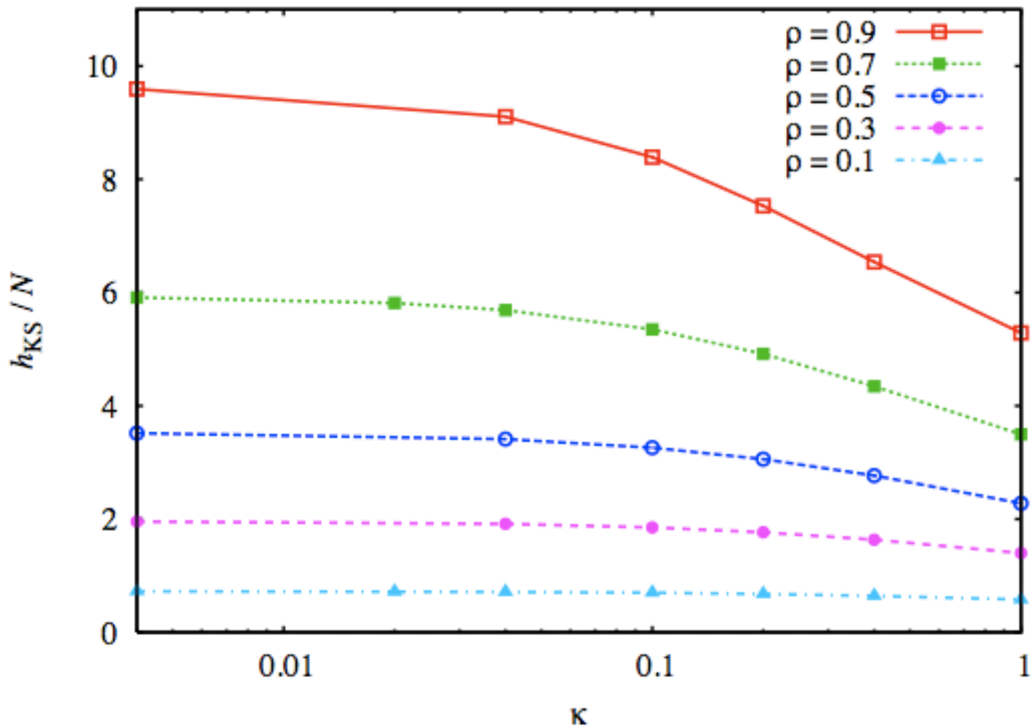

κ = 0.004
κ = 0.100
κ = 0.200
κ = 0.400
κ = 1.000
λ
$\bar{l}$
κ = 0.004
κ = 0.100
κ = 0.200
κ = 0.400
κ = 1.000
λ
l

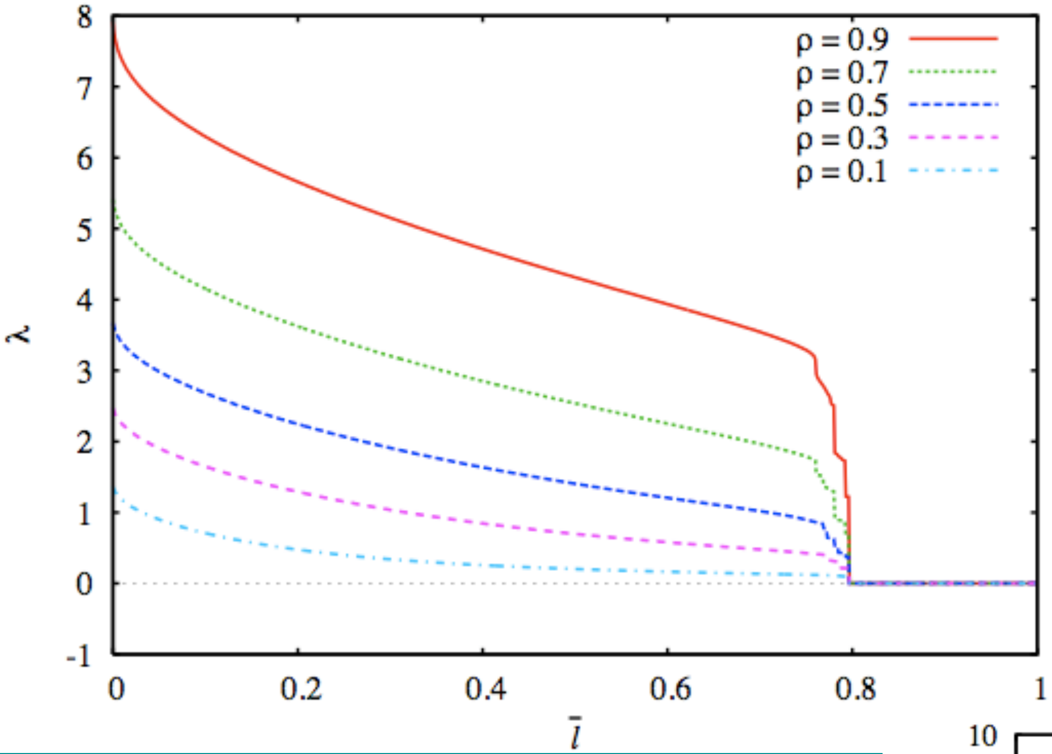
$\rho = 0.7$



$N = 400$

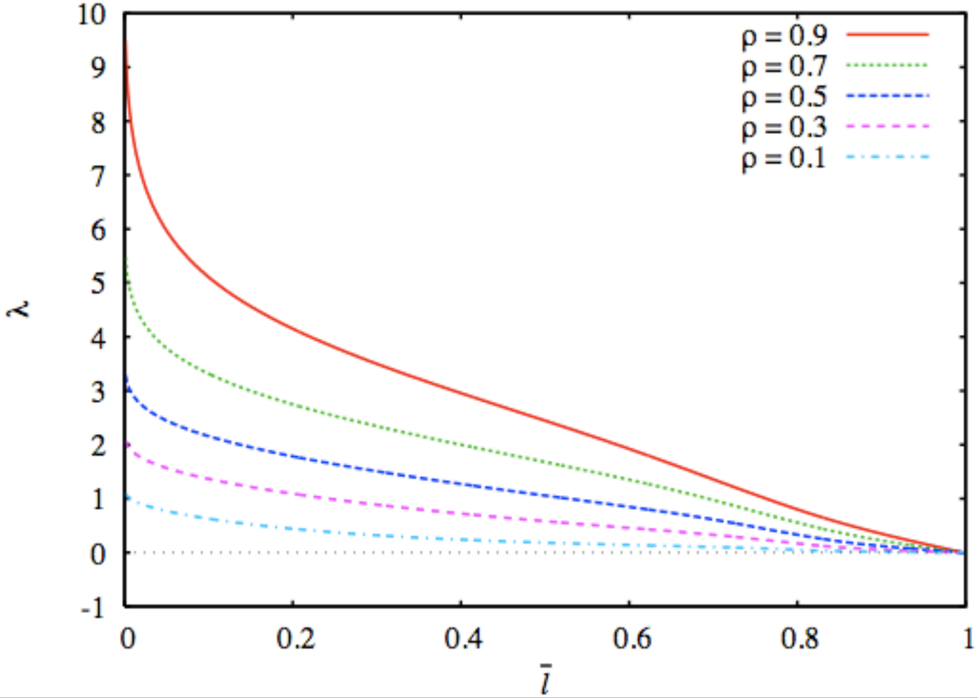
$kT = 1$

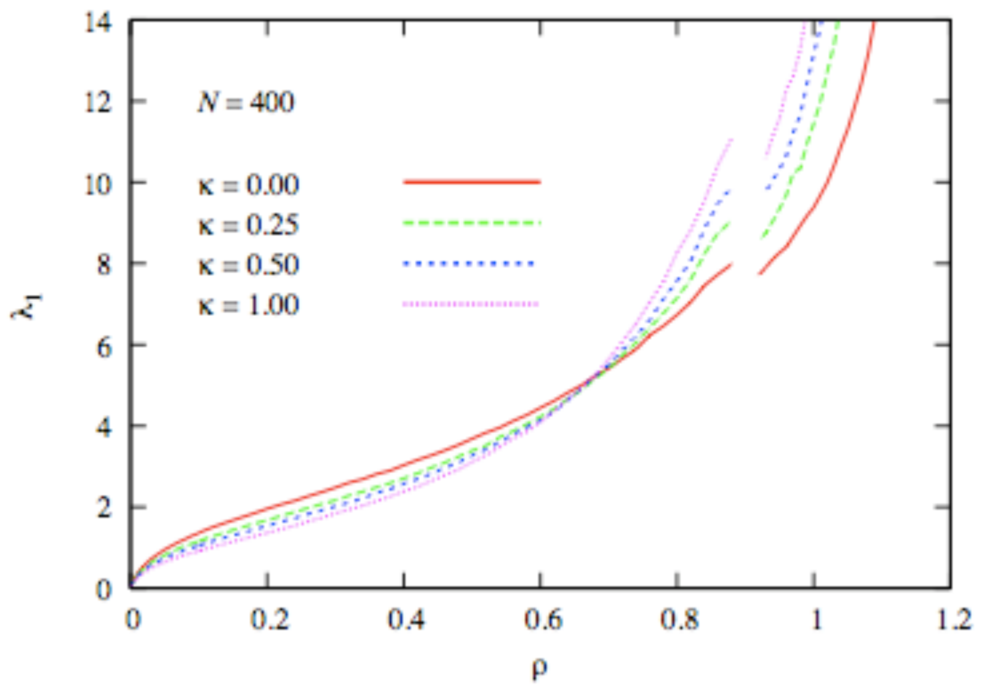




$\kappa = 4I = 0.004$

$\kappa = 0.4$





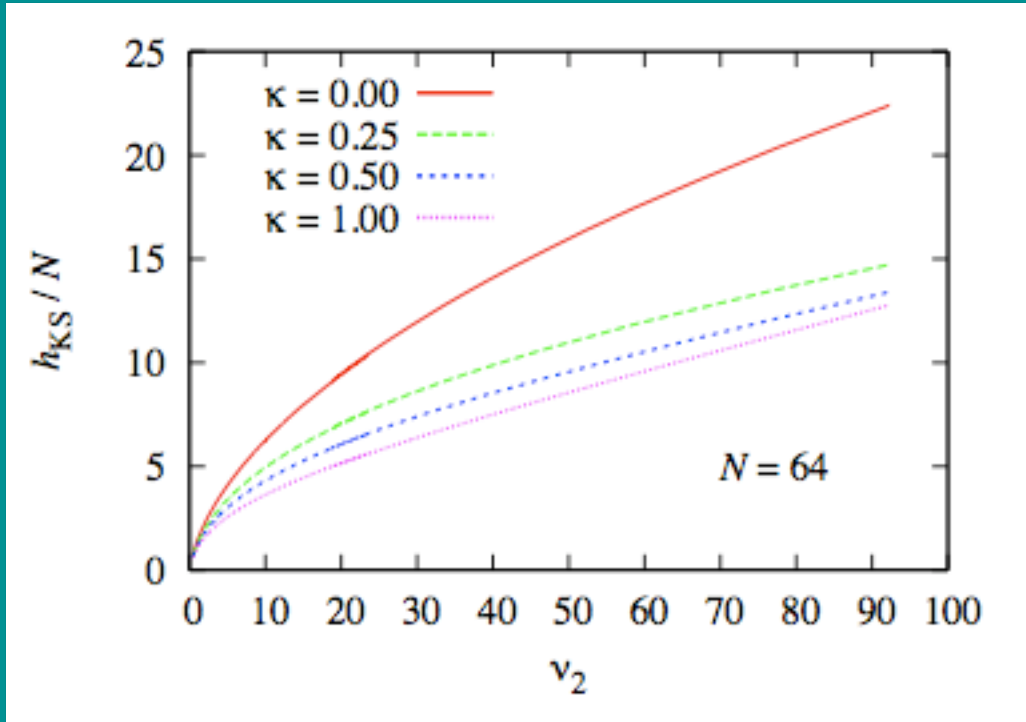
$\kappa = 0:$

$$\lambda_1 = A\nu_2\left[-\ln\rho - B + \mathcal{O}(1/\ln\rho)\right]$$

$$\nu_2 = 2\pi^{1/2}\rho\sigma\,(kT/m)\,g(\sigma)$$

$$A = 1.473, B = 2.48$$

R. van Zon and H. van Beijeren, J. Stat. Phys. **109**, Nos. 3/4, 641 (2002).



$$h_{KS}/N = A'\nu_2\left[-\ln\rho + B' + \mathcal{O}(\rho)\right]$$

$\kappa = 0$:

$$A' = 0.5, B' = 1.47 \pm 0.11 \text{ for} \rho < 10^{-3}$$

A.S. de Wijn Phys. Rev. E **71**, 046211 (2005)

Localization (G-S vectors):

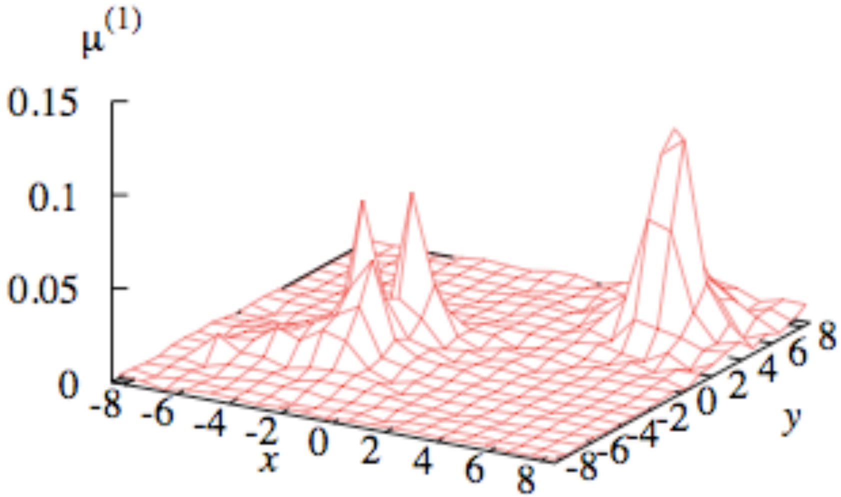
rho = 0.5

$$\mu_i^{(l)} = \left(\delta\vec{q}_i^{\,(l)}\right)^2 + \left(\delta\vec{v}_i^{\,(l)}\right)^2 + \left(\delta\omega_i^{(l)}\right)^2$$

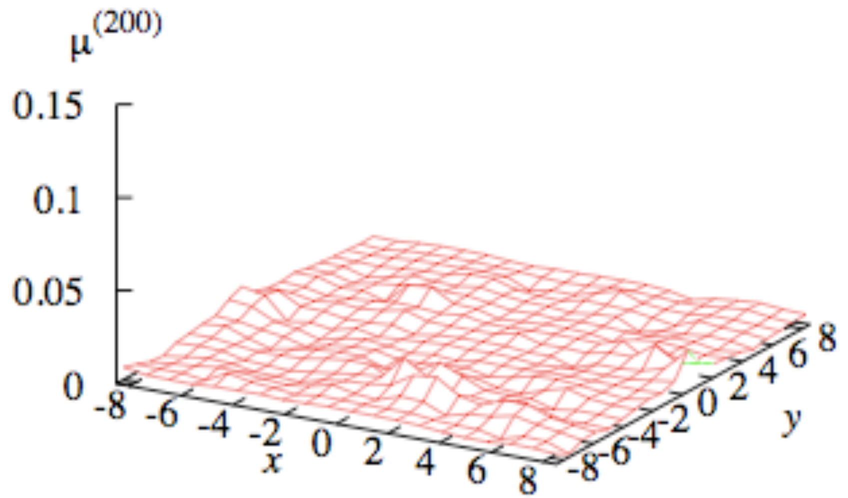
$$\sum_i^N \mu_i^{(l)} = 1\,; \quad S^{(l)} = \left\langle -\sum_{i=1}^N \mu_i^{(l)} \ln \mu_i^{(l)} \right\rangle$$

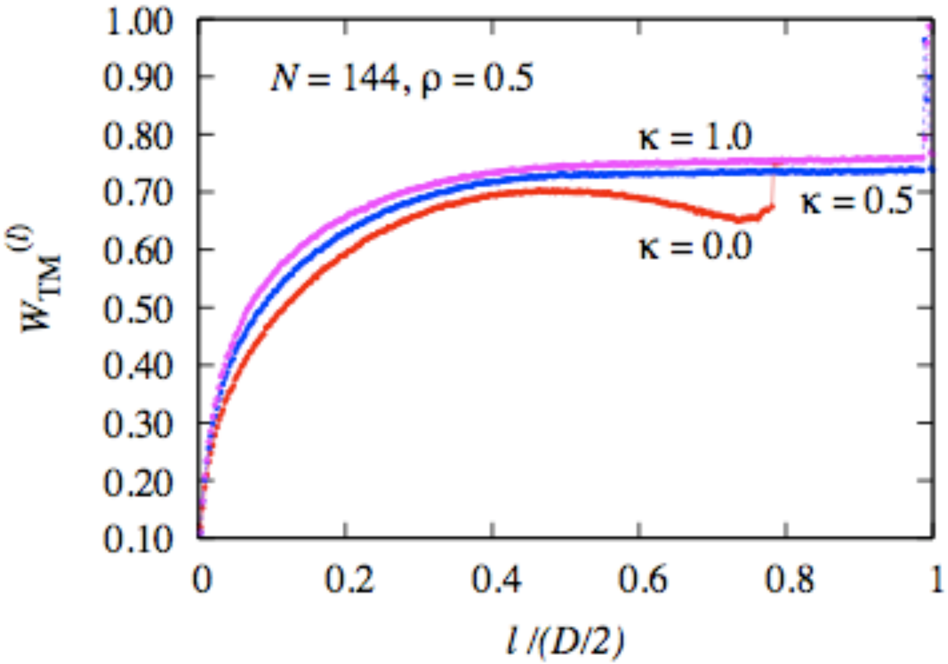
$$W_{TM}^{(l)} = \exp[S^{(l)}]/N, \quad 1/N \le W_{TM}^{(l)} \le 1$$

T. Taniguchi and G. P. Morriss, Phys. Rev. E **68**, 046203 (2003).

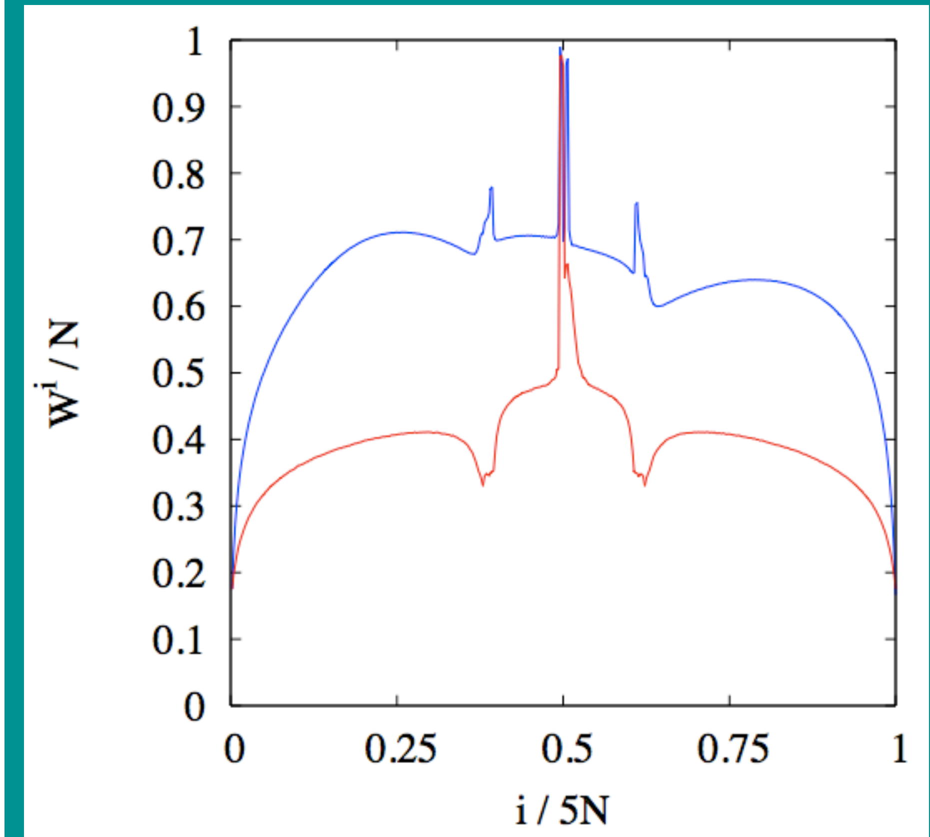


$$S_F^{(l)} = \left\langle \sum_{i=1}^N \mu_i^{(l)}(1-\mu_i^{(l)}) \right\rangle$$

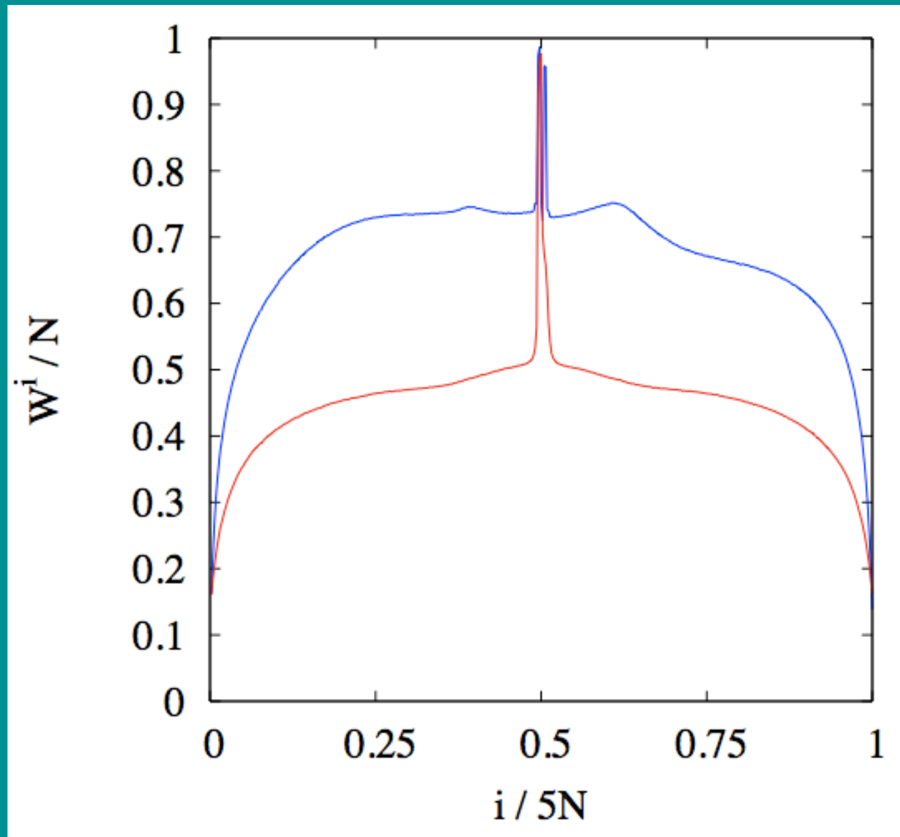




Localization: G-S (blue) and covariant (red) vectors
N = 88, A = 2/11, N/V = 0.7

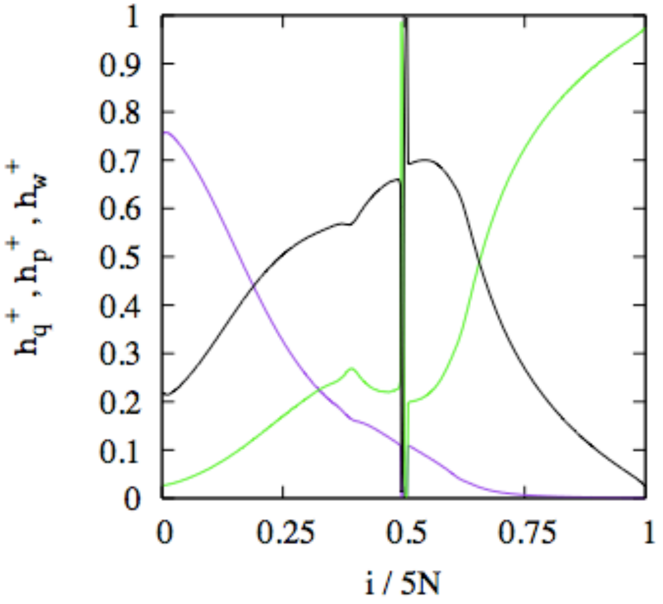


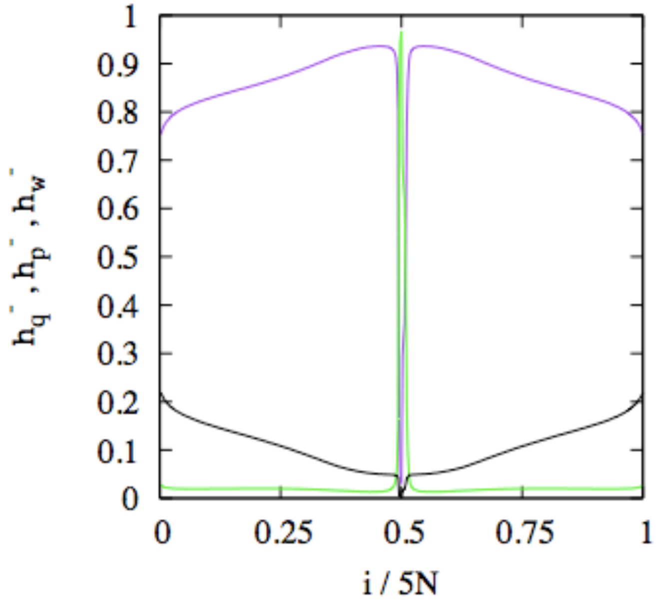
$\kappa = 0.1$



$\kappa = 0.4$

Rough disks: comparson G-S and covariant vectors





$$\eta_q = \langle(\delta q)^2\rangle$$

$$\eta_p = \langle(\delta p)^2\rangle$$

$$\eta_\omega = \langle(\delta \omega)^2\rangle$$

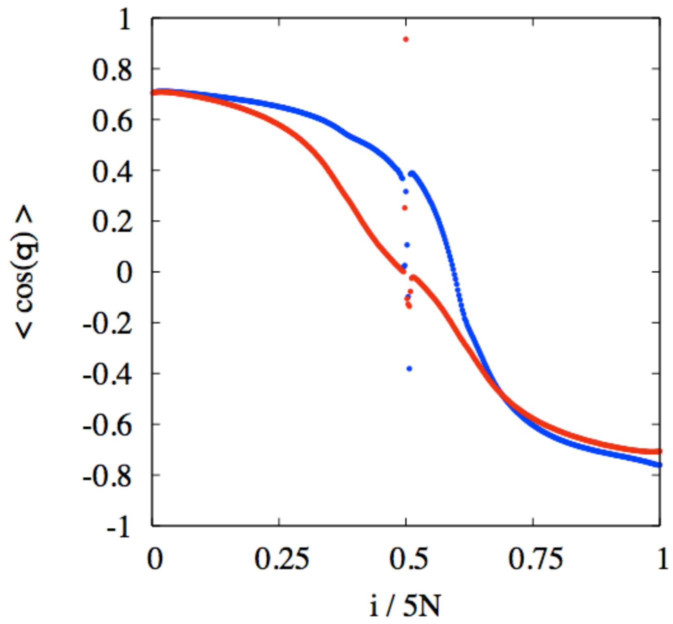
$$\kappa = 0.4$$

$+$: G-S vectors

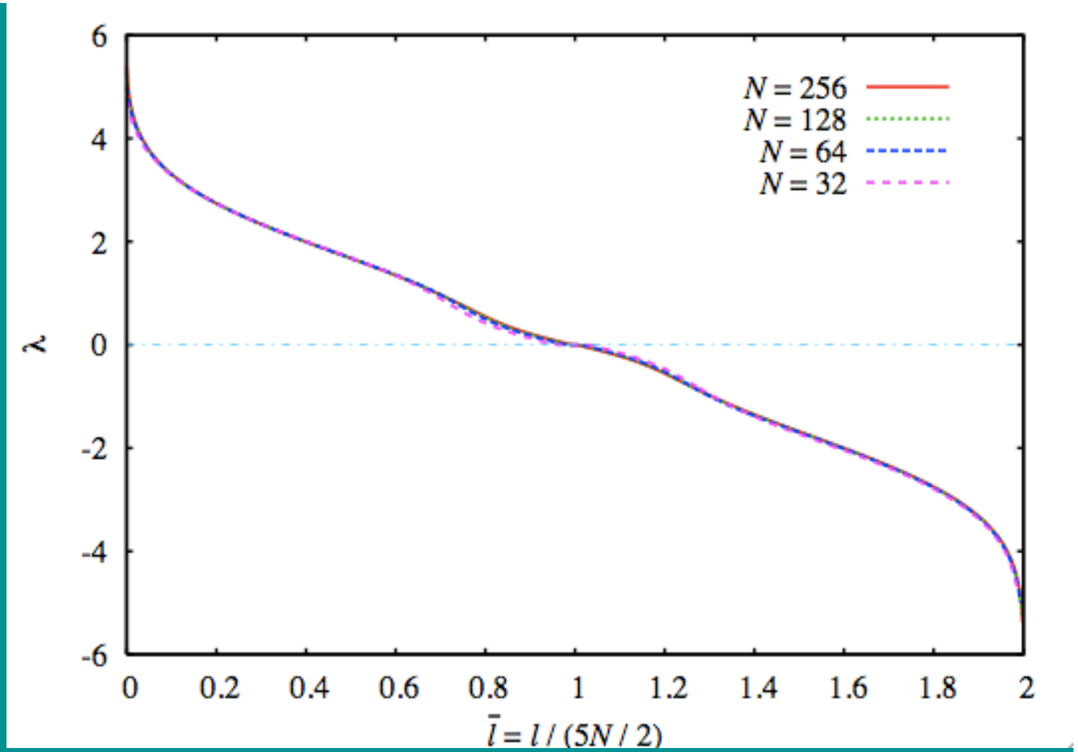
$-$: covariant vectors

$$\langle \cos(\Theta) = (\delta\mathbf{q} \cdot \delta\mathbf{p})/(|\delta\mathbf{q}| \cdot |\delta\mathbf{p}|)$$

$$\kappa = 0.4$$



Convergence
(G_S vectors)

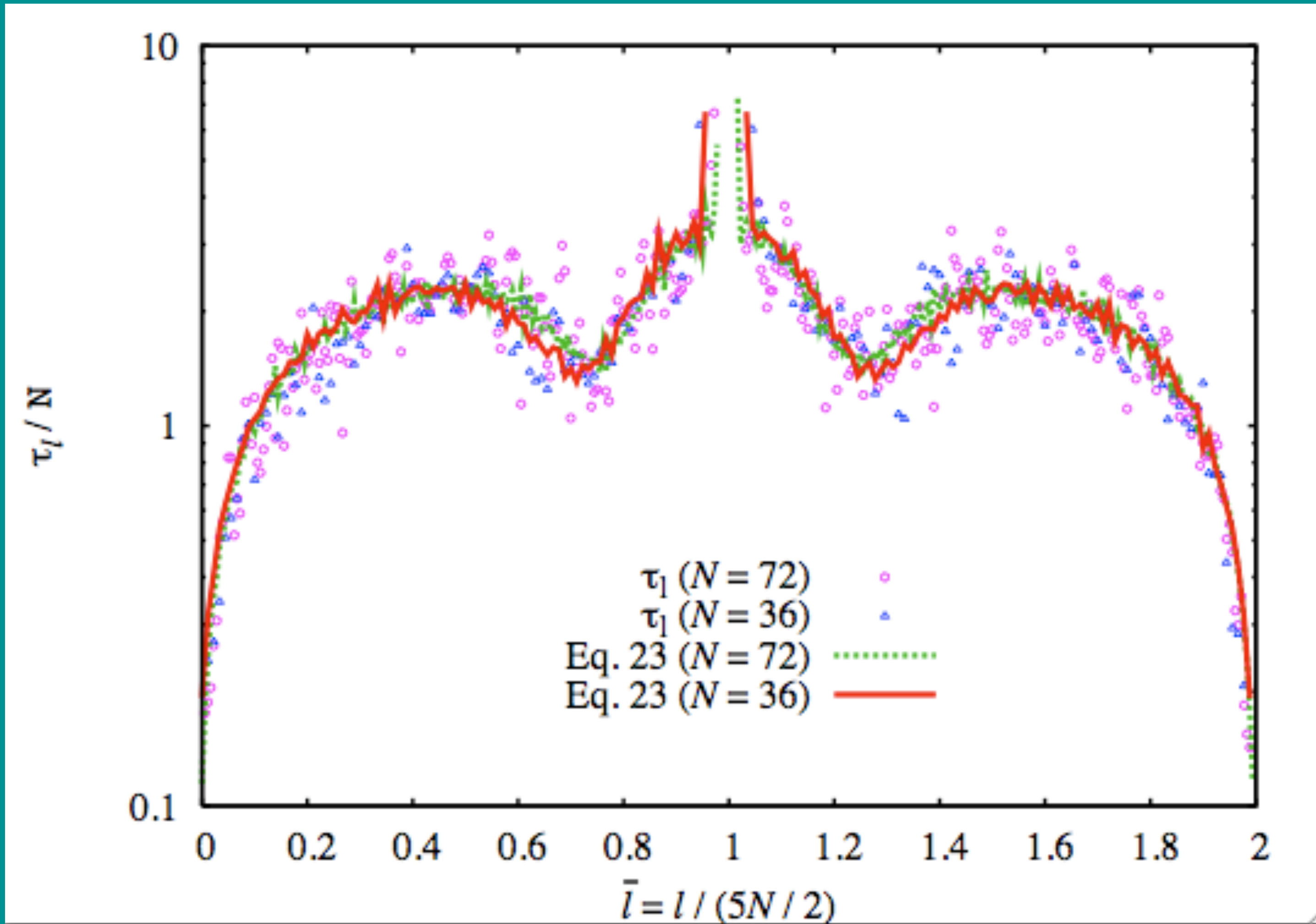


$$\chi_l(t) = \frac{2}{M(M-1)} \sum_{m=1}^{M-1} \sum_{m'=m+1}^{M} \left| \delta\vec{\Gamma}_m^{(l)} \cdot \delta\vec{\Gamma}_{m'}^{(l)} \right|$$

$$\chi_l(\tau_l) = \theta = 0.9$$

$$\tau_l = \frac{A(\Theta)}{|\lambda_{l+1} - \lambda_l|} = \frac{A}{|\Delta\lambda(\bar{l})/\Delta\bar{l}|\,\Delta\bar{l}} \approx \frac{5NA}{2} \left| \frac{d\lambda(\bar{l})}{d\bar{l}} \right|^{-1}$$

Convergence (G-S vectors)



$$\rho = 0.7, \quad \kappa = 0.4$$

Summary I: Equilibrium systems with short-range forces

- Lyapunov modes: formally similar to the modes of fluctuating hydrodynamics
- Broken continuous symmetries give rise to modes
- Unbiased mode decomposition
- Hard dumbbells, ...
- Applications to phase transitions (with transition
- path sampling), particles in narrow channels, translation-rotation coupling, ...