Generalized Collision Rules in Interacting Particle Systems: Lyapunov Exponents and Measures of Chaos

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Motivation

This poster presents the dynamics of generalized binary collisions and the associated results for quantitative measures of chaos reduction, relative to the elastic collision rule [Del96, Eck05], in interacting particle systems. These results lend credence to the idea that such generalized collisions can indeed lead to self-organization in these systems.

Dellago et. al proposed a method for computing the Lyapunov exponents of continuous-time systems that undergo elastic collisions [Del96]. We extend these results to the case of generalized binary collision rules between particles in two-dimensions. We present the computation of the Lyapunov spectra for these generalized collision rules, along with the associated modes.

Highlights

$\beta = 0$	velocity swap ($\mathbf{M} = \mathbf{M}^{-1}$)
$0 < \beta < 1$	not time-reversible ($\mathbf{M} \neq \mathbf{M}^{-1}$)
$\beta = 1$	elastic collision rule ($\mathbf{M} = \mathbf{M}^{-1}$)

Table 1: Description of dynamics for different β; $\mathbf{M}$ is the collision rule; see "Dynamics in the Presence of a Generalized Collision" section.

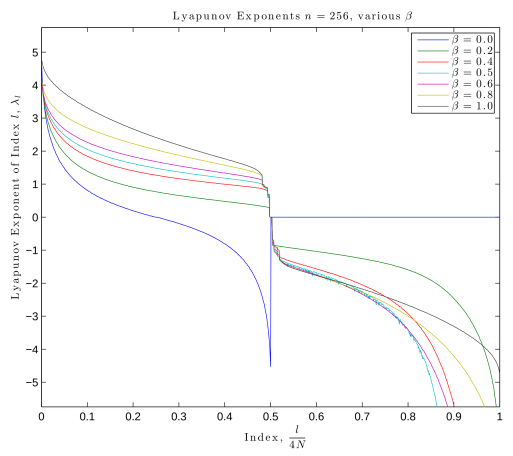

Figure 1: Lyapunov spectra for various β. For $0 < \beta < 1$, spectra are asymmetric about the center-index, indicating the collision rule is not time-reversible.

- **As β changes, so to do measures of intrinsic chaos within the system: the maximal Lyapunov exponent, λ_1, and the Kolmogorov-Sinai entropy per particle, h_{KS}/N.**
- **Cumulative effect of collisions is different from elastic case. Even though all events happen locally in space, changing β has global effect on the dynamics.**

Visualization of a Binary Collision

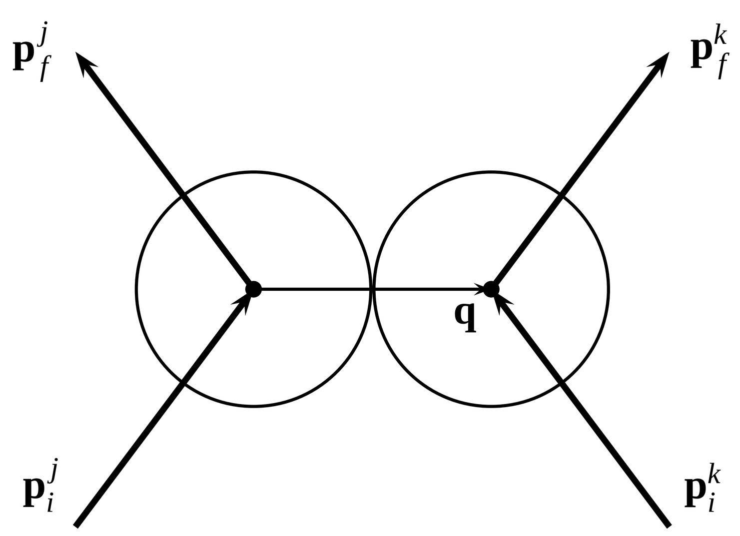

Figure 2: Binary collision in forward- time. Disks j and k, each with diameter $\sigma = \|\mathbf{q}\|_2$, undergo a collision. The vectors $\mathbf{p}_i^j, \mathbf{p}_f^j$ represent the momenta of particle j before and after collision, respectively. At impact, each particle maintains a weighted portion of the component of its momentum that is normal to $\mathbf{q}$, the vector connecting the particles' centers, while a repulsive force (anti-)parallel to $\mathbf{q}$ is applied to each particle such that (i) the particles move away from each other after collision and (ii) total kinetic energy is conserved.

Dynamics in the Presence of a Generalized Collision

The dynamics for N particles of equal mass m and diameter σ moving on the 2-torus $\mathbb{T}^2 = \{(x \bmod L_x, y \bmod L_y)^\top | L_x, L_y \in \mathbb{R}\}$ is represented by the state $\mathbf{\Gamma}$. To compute Lyapunov exponents, we are interested in the dynamics of the perturbation vector $\delta\mathbf{\Gamma}$,

$$\mathbf{\Gamma} := \begin{pmatrix}\mathbf{Q}\\ \mathbf{P}\end{pmatrix} = \begin{pmatrix}\mathbf{q}^1\\ \vdots\\ \mathbf{q}^N\\ \mathbf{p}^1\\ \vdots\\ \mathbf{p}^N\end{pmatrix}, \quad \delta\mathbf{\Gamma} := \begin{pmatrix}\delta\mathbf{Q}\\ \delta\mathbf{P}\end{pmatrix} = \begin{pmatrix}\delta\mathbf{q}^1\\ \vdots\\ \delta\mathbf{q}^N\\ \delta\mathbf{p}^1\\ \vdots\\ \delta\mathbf{p}^N\end{pmatrix}.$$

where $\mathbf{q}^j := (q^{1j}\ q^{2j})^\top$ and $\mathbf{p}^j := (p^{1j}\ p^{2j})^\top$ are the position and momentum of particle j, respectively, and $\delta\mathbf{q}^j := (\delta q^{1j}\ \delta q^{2j})^\top$ and $\delta\mathbf{p}^j := (\delta p^{1j}\ \delta p^{2j})^\top$ are the associated perturbations. $\mathbf{\Gamma}, \delta\mathbf{\Gamma}$ are $4N$-dimensional vectors. The dynamics are described by two alternating stages: free flight and collision.

1. *Phase-space dynamics*
   - *Free-flight: Motion absent an external force (continuous-time)*

$$\frac{d\mathbf{\Gamma}(t)}{dt} = \mathbf{F}(\mathbf{\Gamma}(t)) = \begin{pmatrix}\frac{\mathbf{P}}{m}\\ \mathbf{0}\end{pmatrix},$$

   - *Collision: Instantaneous change in momenta of colliding particles (discrete-time). All particle positions and momenta of non-colliding particles are invariant under the collision transformation. The value α ensures conservation of total kinetic energy at collision. The collision map, $\mathbf{M}$, takes the state before collision, $\mathbf{\Gamma}_i$, to the final state $\mathbf{\Gamma}_f$:*

$$\begin{aligned}
\mathbf{Q}_f &= \mathbf{Q}_i,\\
\mathbf{p}_f^l &= \mathbf{p}_i^l, \quad l \neq j, k\\
\mathbf{p}_f^j &= \beta\mathbf{p}_i^j + (1-\beta)\mathbf{p}_i^k + \alpha d\mathbf{p},\\
\mathbf{p}_f^k &= (1-\beta)\mathbf{p}_i^j + \beta\mathbf{p}_i^k - \alpha d\mathbf{p},\\
\beta &\in [0,1], \ \alpha = \frac{2\beta-1}{2} + \frac{\sqrt{(2\beta-1)^2(\mathbf{q}\cdot\mathbf{p})^2 - 4\beta(\beta-1)(\mathbf{p}\cdot\mathbf{p})\sigma^2}}{2|\mathbf{q}\cdot\mathbf{p}|},
\end{aligned}$$

$d\mathbf{p} := (\mathbf{q}\cdot\mathbf{p})\mathbf{q}/\sigma^2$; $\mathbf{q} := \mathbf{q}_i^k - \mathbf{q}_i^j$ and $\mathbf{p} := \mathbf{p}_i^k - \mathbf{p}_i^j$ are the relative position and momentum of particles j and k before collision. Terms due to the generalized collision rule that are not present in the elastic case are highlighted in red.

2. *Linearized Dynamics of Perturbations*
   - *Free-flight:*

$$\frac{d(\delta\mathbf{\Gamma})}{dt} = J_{\mathbf{F}}(\mathbf{\Gamma})\delta\mathbf{\Gamma} = \begin{pmatrix}\frac{\delta\mathbf{P}}{m}\\ \mathbf{0}\end{pmatrix},$$

   - *Collision: Perturbations introduce a time offset ($\delta\tau_c$) between collision in the reference trajectory (at τ_c) and a perturbed trajectory (at $\tau_c + \delta\tau_c$) [Del96]. Again assuming that particles j and k undergo collision ($l \neq j, k$):*

$$\begin{aligned}
\delta\mathbf{q}_f^l &= \delta\mathbf{q}_i^l, \ \delta\mathbf{p}_f^l = \delta\mathbf{p}_i^l,\\
\delta\mathbf{q}_f^j &= \delta\mathbf{q}_i^j + \left[(1-\beta)\mathbf{p} + \frac{\alpha(\mathbf{q}\cdot\mathbf{p})\mathbf{q}}{\sigma^2}\right]\left(\frac{\delta\mathbf{q}\cdot\mathbf{q}}{\mathbf{p}\cdot\mathbf{q}}\right),\\
\delta\mathbf{q}_f^k &= \delta\mathbf{q}_i^k - \left[(1-\beta)\mathbf{p} + \frac{\alpha(\mathbf{q}\cdot\mathbf{p})\mathbf{q}}{\sigma^2}\right]\left(\frac{\delta\mathbf{q}\cdot\mathbf{q}}{\mathbf{p}\cdot\mathbf{q}}\right),\\
\delta\mathbf{p}_f^j &= \beta\delta\mathbf{p}_i^j + (1-\beta)\delta\mathbf{p}_i^k + \left(\frac{\alpha}{\sigma^2} + \kappa|\mathbf{p}|^2\right)(\delta\mathbf{p}\cdot\mathbf{q} + \delta\mathbf{q}_c\cdot\mathbf{p})\mathbf{q}\\
&\quad + \frac{\alpha}{\sigma^2}(\mathbf{q}\cdot\mathbf{p})\delta\mathbf{q}_c - \kappa(\mathbf{q}\cdot\mathbf{p})(\delta\mathbf{p}\cdot\mathbf{p})\mathbf{q},\\
\delta\mathbf{p}_f^k &= (1-\beta)\delta\mathbf{p}_i^j + \beta\delta\mathbf{p}_i^k - \left(\frac{\alpha}{\sigma^2} + \kappa|\mathbf{p}|^2\right)(\delta\mathbf{p}\cdot\mathbf{q} + \delta\mathbf{q}_c\cdot\mathbf{p})\mathbf{q}\\
&\quad - \frac{\alpha}{\sigma^2}(\mathbf{q}\cdot\mathbf{p})\delta\mathbf{q}_c + \kappa(\mathbf{q}\cdot\mathbf{p})(\delta\mathbf{p}\cdot\mathbf{p})\mathbf{q},\\
\kappa &:= \frac{2\beta(\beta-1)}{(\mathbf{q}\cdot\mathbf{p})^2(2(\alpha-\beta)+1)}.
\end{aligned}$$

In the above expressions, $\delta\mathbf{p} = \delta\mathbf{p}_i^k - \delta\mathbf{p}_i^j$ and $\delta\mathbf{q} = \delta\mathbf{q}_i^k - \delta\mathbf{q}_i^j$. The offset between the reference trajectory relative position vector before collision, $\mathbf{q}$, and a perturbed trajectory relative position vector before collision, $\mathbf{q} + \delta\mathbf{q}_c$, is $\delta\mathbf{q}_c := \delta\mathbf{q} + \mathbf{p}/m\delta\tau_c$.

Lyapunov Spectra and Modes

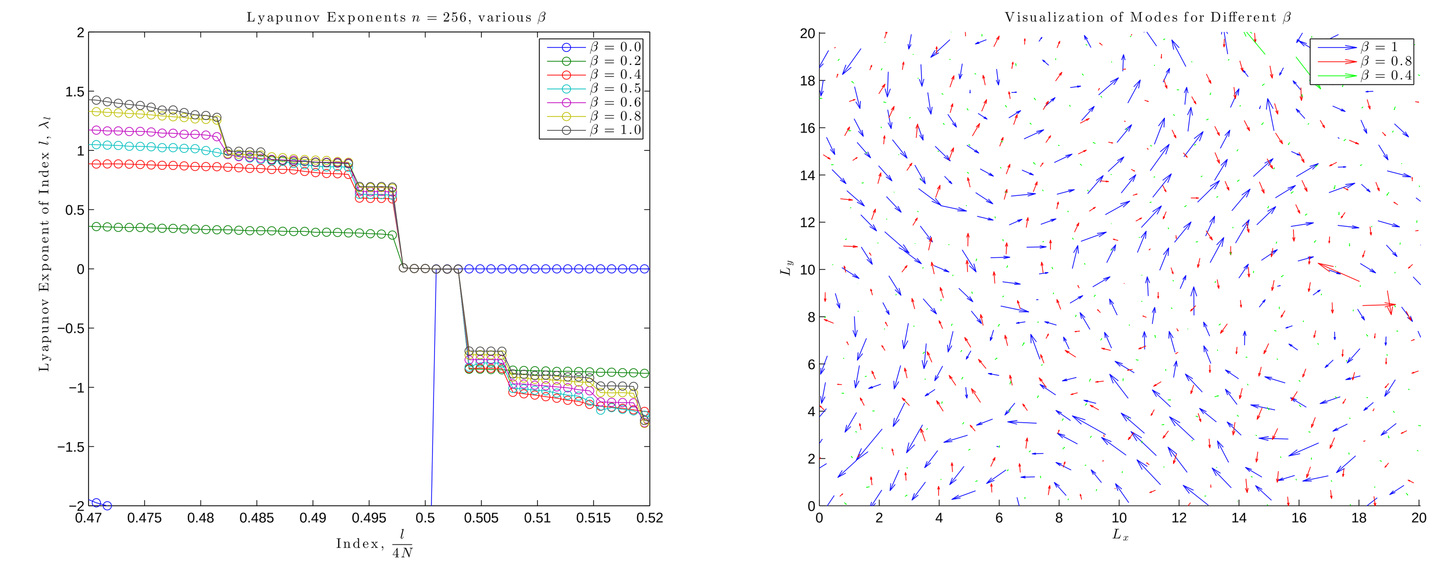

Figure 3: Left: Blown-up picture of Lyapunov spectra at density $\rho = 0.5$, aspect ratio $A = 1$ for $\beta = 0, 0.2, 0.4, 0.5, 0.6, 0.8$ and 1. Step structure of spectra indicate the presence of "Lyapunov modes" associated with degenerate exponents for $\beta >\approx 0.4$. For $0.2 < \beta < 0.4$ the step structure is diminished and degenerate exponents are no longer observed. Right: Picture of superposition of modes associated with index l such that $0.494 < \frac{l}{4N} < 0.498$ for $\beta = 0.4, 0.8$ and 1.0. The Lyapunov modes present for $\beta < 1$ show breakdown of structure apparent in $\beta = 1$ case (elastic collisions).

Measures of Chaos

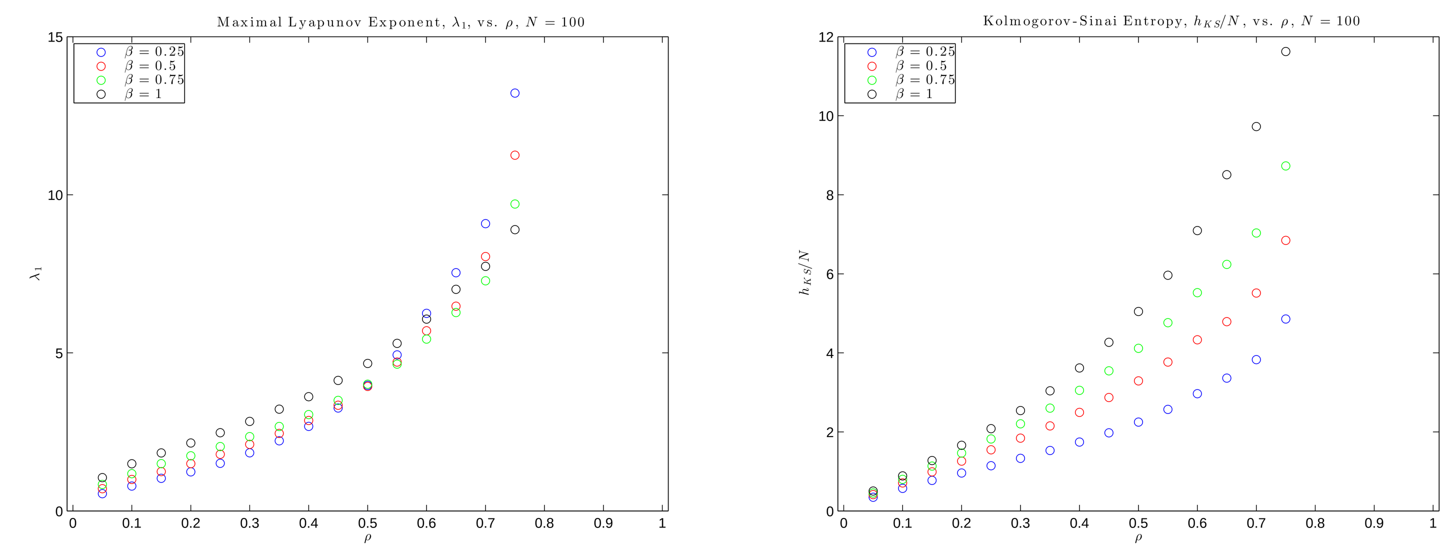

Figure 4: Left: Maximal Lyapunov exponent, λ_1, for $\beta = 0.25, 0.5, 0.75$, and 1.0 as a function of volume density (packing fraction) ρ with aspect ratio $A = 1$. Right: Kolmogorov-Sinai entropy, $h_{KS}/N = \sum_{\{l:\lambda_l>0\}} \lambda_l$. As ρ increases, the maximal exponent is larger for smaller β, while the Kolmogorov-Sinai entropy shows the opposite trend.

Conclusions and Future Work

- **Changing β changes the microscopic dynamics and affects macroscopic order (e.g. entropy is reduced)**
- **Generalized collision rule: (i) is not time-reversible (except for $\beta = 0, 1$) and (ii) modes can no longer be specified entirely by position perturbations (some proportion of momentum perturbations needs to be considered).**
- Further investigation is needed:
  - Classify structure of Lyapunov modes. **How is this structure related to the phase space dynamics?**
  - Since forward- and reverse-time dynamics are different, there should be some observable measure of the phase space dynamics that indicates whether or not the generalized collision rule induces self-organizing behavior. **What are the appropriate measures to show this self-organization?**

[Del96] Dellago, Ch., H.A. Posch, and W.G. Hoover. Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states. *Phys. Rev. E*, 53(2):1485, 1996.

[Eck05] Eckmann, J.P., C. Forster, H.A. Posch, and E. Zabey. Lyapunov Modes in Hard-Disk Systems. *J. Stat. Phys.*, 118(5/6):813, 2005.

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