Mathematical modeling of complex systems
Part 2. Self-organization vs chaos assumption

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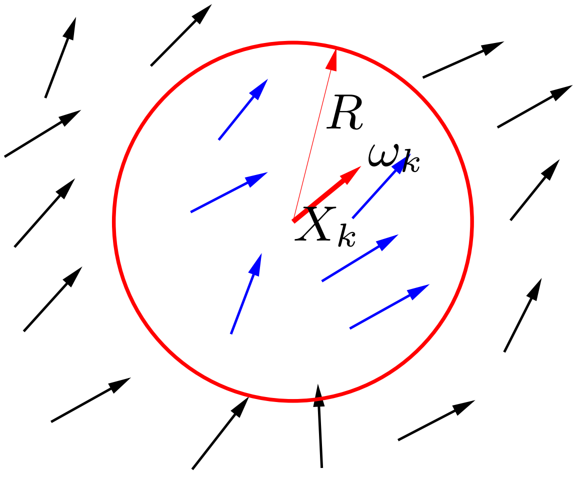
Joint work with E. Carlen and B. Wennberg ;
numerical simulations by R. Chatelin

Summary

1. An example: the Vicsek model

Vicsek model [Vicsek et al, PRL 95]

- Time-discrete model:
  - $t^n = n\Delta t$
  - k-th individual
  - X_k^n: position at t^n
  - ω_k^n: velocity with $|\omega_k^n| = 1$



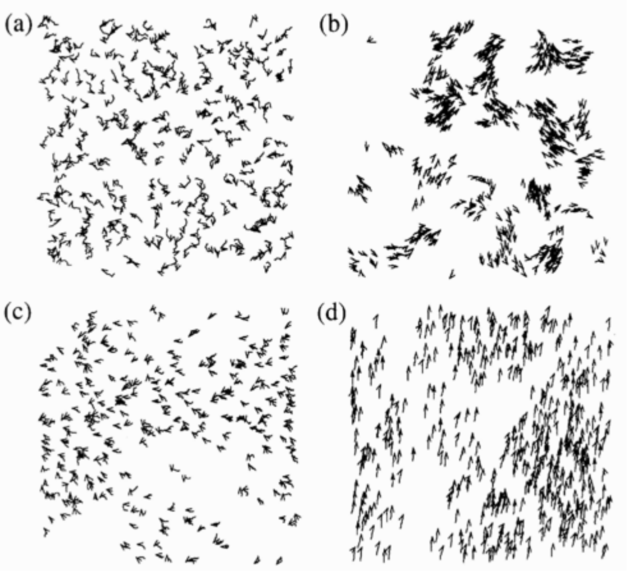
- $$X_k^{n+1} = X_k^n + \omega_k^n \, \Delta t$$

  $$\omega_k^{n+1} = \bar\omega_k^n + \text{ noise (uniform in small angle interval)}$$

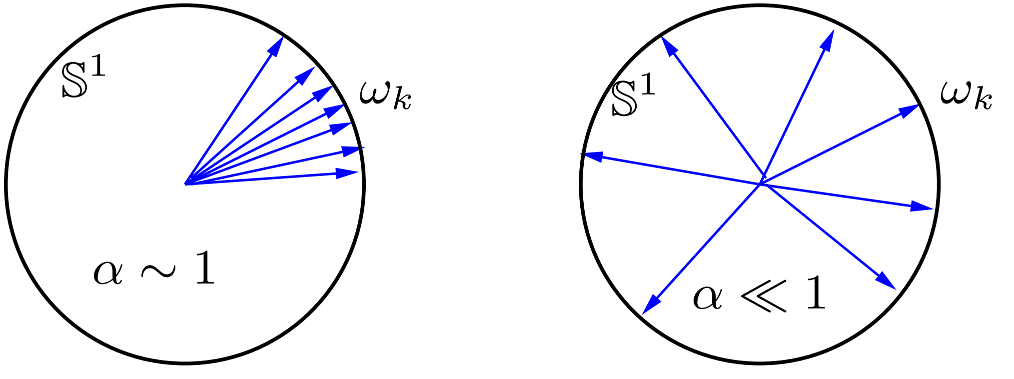
  $$\bar\omega_k^n = \frac{J_k^n}{|J_k^n|}, \quad J_k^n = \sum_{j, |X_j^n - X_k^n| \leq R} \omega_j^n$$

- Alignment to neighbours' mean velocity plus noise

- Phase transition to disorder

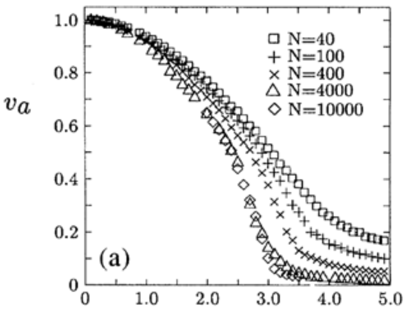


- Order parameter
  - $\alpha = \left| N^{-1} \sum_j \omega_j \right|^2$
  - N = particle number
  - $0 \leq \alpha \leq 1$
- Measures alignment



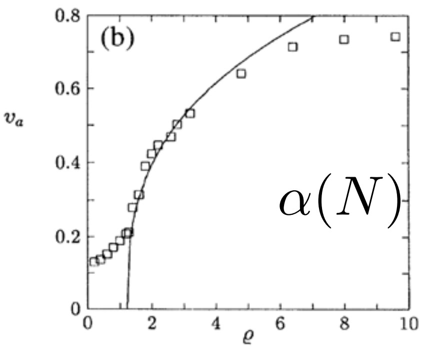
$\alpha \sim 1$: ω aligned $\qquad$ $\alpha \ll 1$: ω random

- As noise decreases [Vicsek et al, PRL 95]

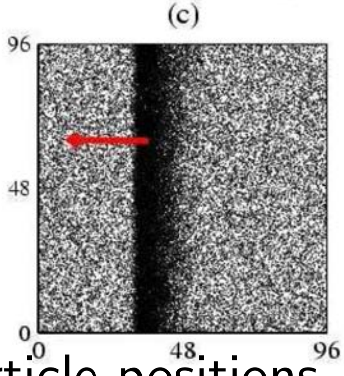


α(noise level)

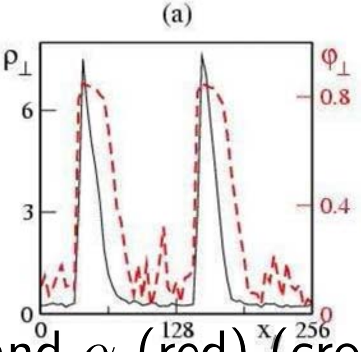
- As density increases [Vicsek et al, PRL 95]



- Band formation [Chaté et al]



Particle positions



ρ (black) and α (red) (cross section)

- Vicsek dynamics exhibits
  - self-organization & emergence of coherent structures
  - supposes the build-up of correlations between particles
- Kinetic and Hydrodynamic models rely on the chaos assumption
  - When N is large, particles are statistically independent
- Question: are kinetic and hydrodynamic models relevant for Complex Systems ?
  - Goal: provide illustrative examples

2. Chaos property in particle systems

Method

- Construct the Master equation
  - Tells us the passage $F_N(t^n) \longrightarrow F_N(t^{n+1})$
  - where $F_N(v_1, \dots, v_N) =$ N-particle probability distribution
  - Note: F_N invariant under permutations of $\{v_1, \dots, v_N\}$
- Compute the marginals

$$F_N^{(j)}(v_1, \dots, v_j) = \int F_N \, dv_{j+1} \dots dv_N$$

  - Master eq. $\Rightarrow$ eq. for the marginals
  - Eqs. for the marginals not closed (BBGKY hierarchy)
  - Marginals: fixed number of variables when $N \to \infty$

- Hierarchy:

$$F_N^{(j)}(t^{n+1}) = \mathcal{J}^{(j)}(F_N^{(j+1)}(t^n))$$

- Taking the limit $N \to \infty$ 'simplifies' the problem
  - If N large, system is not influenced by the state of one given particle

- Particles become independent

$$F^{(j)}(v_1, \ldots, v_j) = \prod_{k=1}^{j} F^{(1)}(v_k)$$

Chaos assumption

Binary interactions (cont)

- Suppose at $t = 0$: particles are independent

$$F^{(j)}(v_1, \dots, v_j)|_{t=0} = \prod F^{(1)}(v_k)|_{t=0}$$

- If N finite: Dynamics builds up correlations instantaneously

- If $N \to \infty$, correlations tend to 0
  - for Hard-Sphere Dynamics [Lanford], $\exists T$ s.t. $\forall t \in [0, T]$

$$F^{(j)}(v_1, \dots, v_j)|_t \to \prod F^{(1)}(v_k)|_t \quad \text{as} \quad N \to \infty$$

  - BBGKY hierarchy 'converges' to the Boltzmann eq.

Related questions

- As $N \to \infty$:
  - Dynamics becomes irreversible
  - $\exists$ entropy functional H which $\searrow$ in time
  - Dissipation
  - Equilibria $=$ states of maximal disorder
- For classical systems (e.g. rarefied gases)
  - strong relation between these concepts
- Is this still true for self-organization processes ?
  - will some of these concepts survive while others won't ?

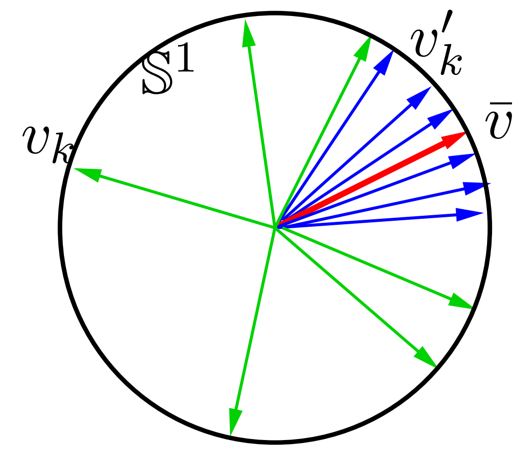
3. Binary particle dynamics on $\mathbb{S}^1$: the CLD & BDG dynamics

Dynamics on $\mathbb{S}^1$

- Setting
  - N particles with velocities $v_k \in \mathbb{S}^1$
  - i.e. $v_k \in \mathbb{R}^2$ with $|v_k| = 1$
  - Space homogeneous problem $\Rightarrow$ kein x !!!
  - All particles can interact
- State of the system at the n-th iterate
  - $Z_N(t^n) = (v_1, \ldots, v_N)(t^n) \in (\mathbb{S}^1)^N$
  - $t^n = n\Delta t$
  - Discrete stochastic dynamics $Z_N(t^n) \longrightarrow Z_N(t^{n+1})$

Ex. 1: Space-homogeneous Vicsek dynamics

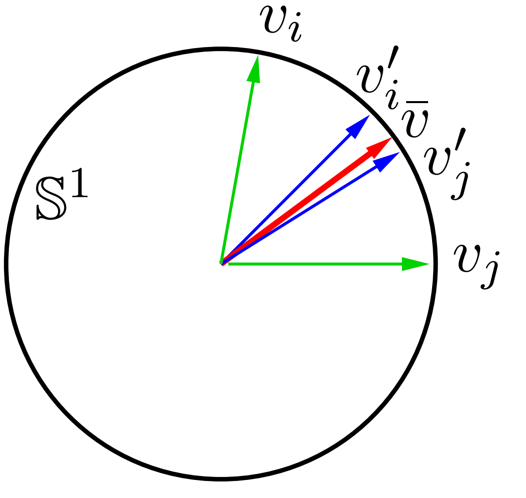
- Compute average direction $\bar v = \sum_k v_k \, / \, | \sum_k v_k|$
- Add independent noise $v'_k = \bar v \, w_k$
  - $g(z)$ proba on $\mathbb{S}^1$, symmetric $g(z) = g(z^*)$
  - w_k: N independent random var. drawn according to g



- Note:
  - Multiplicative group structure of $\mathbb{S}^1$
  - Also use phases θ s.t. $v = e^{i\theta}$
  - All particles interact $\Rightarrow$ no reduction using marginals

Ex 2. A 'binary' Vicsek dynamics: BDG

- After [Bertin, Droz, Gregoire]
- Pick a pair $\{i, j\}$ at random
  - probability $P_{ij} = 2/N(N-1)$
  - average direction: $v_{ij} = (v_i + v_j)/|v_i + v_j|$
- Add independent noise drawn according to g:
  - $v_i' = v_{ij} w_i \qquad v_j' = v_{ij} w_j$
  - All particles but $\{i, j\}$ unchanged
- Variant (acception-rejection)
  - Collision performed with probability $h(v_i v_j^*)$ s.t. $0 \leq h \leq 1$

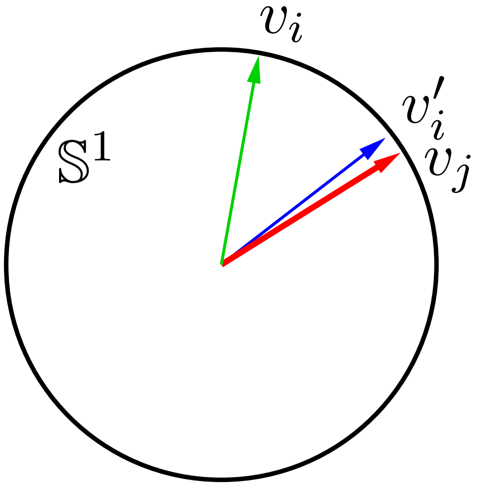


Ex 3. 'Choose the Leader' (CLD)

- Pick an ordered pair (i, j) at random
  - Probability $P_{ij} = 1/N(N-1)$
- Then, i joins j plus noise w drawn according to g

$$v_i' = v_j w$$

  - All particles but i unchanged



4. Chaos property in BDG and CLD dynamics

Noise scaling

- Outline
  - Compute the masters eq. and the marginals
  - Let $N \to \infty$ while scaling noise variance appropriately
- Assumptions on noise distribution as $N \to \infty$:

$$g_N \to \delta(v)$$

$$\text{Var}(g_N) = \frac{\sigma^2}{N} \quad \text{i.e.} \quad \text{MSD}(g_N) = O(\frac{1}{\sqrt{N}})$$

- Goal: find eqs. for the marginals as $N \to \infty$ and $\Delta t = O(\frac{1}{N^2})$ (continuous time limit)

- Take any observable $\phi(v_1, \dots, v_N)$
  - Denote $Z_N(t^n) = (v_1, \dots, v_N)(t^n)$ the state of the system at time t^n
  - Markov transition operator

$$Q^* \phi(v_1, \dots, v_N) = \mathbb{E}\{\phi(Z_N(t^{n+1})) \,|\, Z_N(t^n) = (v_1, \dots, v_N)\}$$

- Denote $F_N(v_1, \dots, v_N)$ = N-particle proba:

$$\mathbb{E}\{\phi(Z_N(t^{n+1}))\} = \int \phi \, F_N(t^{n+1}) \, dZ = \int (Q^* \phi) \, F_N(t^n) \, dZ$$

  - $F_N(t^{n+1}) = Q F_N(t^n)$ where Q = adjoint of Q^*

Example: CLD

$$Q^*\phi(v_1, \dots, v_N) =$$
$$\frac{1}{N(N-1)} \sum_{i \neq j} \int_{\mathbb{S}^1} \phi(v_1, \dots, wv_j, \dots, v_j, \dots, v_N) g(w)\, dw$$

$$QF_N(v_1, \dots, v_N) =$$
$$\frac{1}{N(N-1)} \sum_{i \neq j} g(v_j v\dot{i}_i^*) \int_{\mathbb{S}^1} F_N(v_1, \dots, w_i, \dots, v_N)\, dw_i$$

Example: BDG

$$Q^*\phi(v_1,\ldots,v_N) = \frac{2}{N(N-1)} \sum_{i<j} \Big\{ \int_{\mathbb{S}^1} h(\sqrt{v_i v_j^*}) \times$$
$$\times \phi(v_1,\ldots,v_i',\ldots,v_j',\ldots,v_N)\, g(v_{ij}^* v_i') g(v_{ij}^* v_j')\, dv_i'\, dv_j'$$
$$+ (1 - h(\sqrt{v_i v_j^*}))\phi(v_1,\ldots,v_N) \Big\}$$

with mid-direction v_{ij} defined by

$$v_{ij} = (v_i + v_j)\,/\,|v_i + v_j|$$

- Small noise limit
  - $g_N \to \delta \quad \mathrm{Var}(g_N) = \sigma^2/N \quad \Delta t = O(1/N^2)$

- First marginal:

$$\partial_t f^{(1)} - (\sigma^2/2)\partial^2_{\theta_1} f^{(1)} = 0$$

- Second marginal:

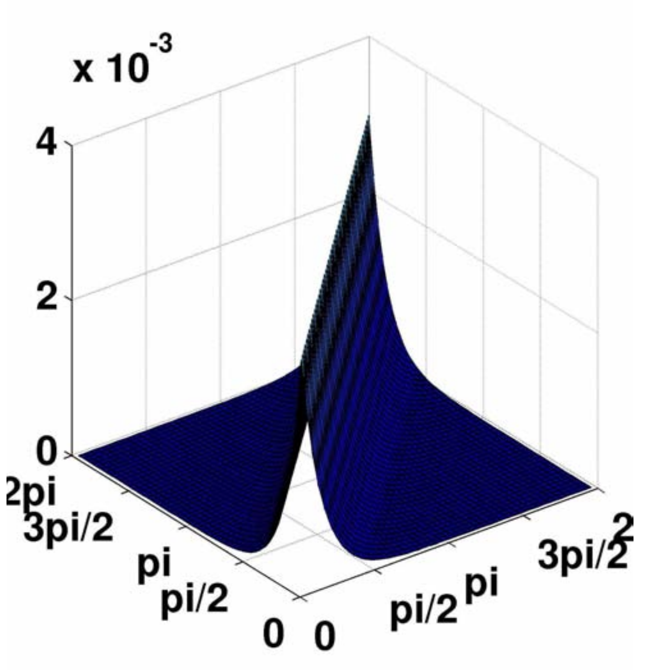
$$\partial_t f^{(2)} - (\sigma^2/2)\Delta_{\theta_1,\theta_2} f^{(2)} + 2 f^{(2)} = (f^{(1)}(\theta_1) + f^{(1)}(\theta_2))\delta(\theta_2 - \theta_1)$$

Stationary states as $t \longrightarrow \infty$

- $f^{(1)} \longrightarrow f^{(1)}_{\text{eq}} = 1$: uniform distribution on $\mathbb{S}^1$
- $f^{(2)} \longrightarrow f^{(2)}_{\text{eq}}$ the unique solution of

$$-(\sigma^2/2)\Delta_{\theta_1,\theta_2} f + 2f = 2\delta(\theta_2 - \theta_1)$$

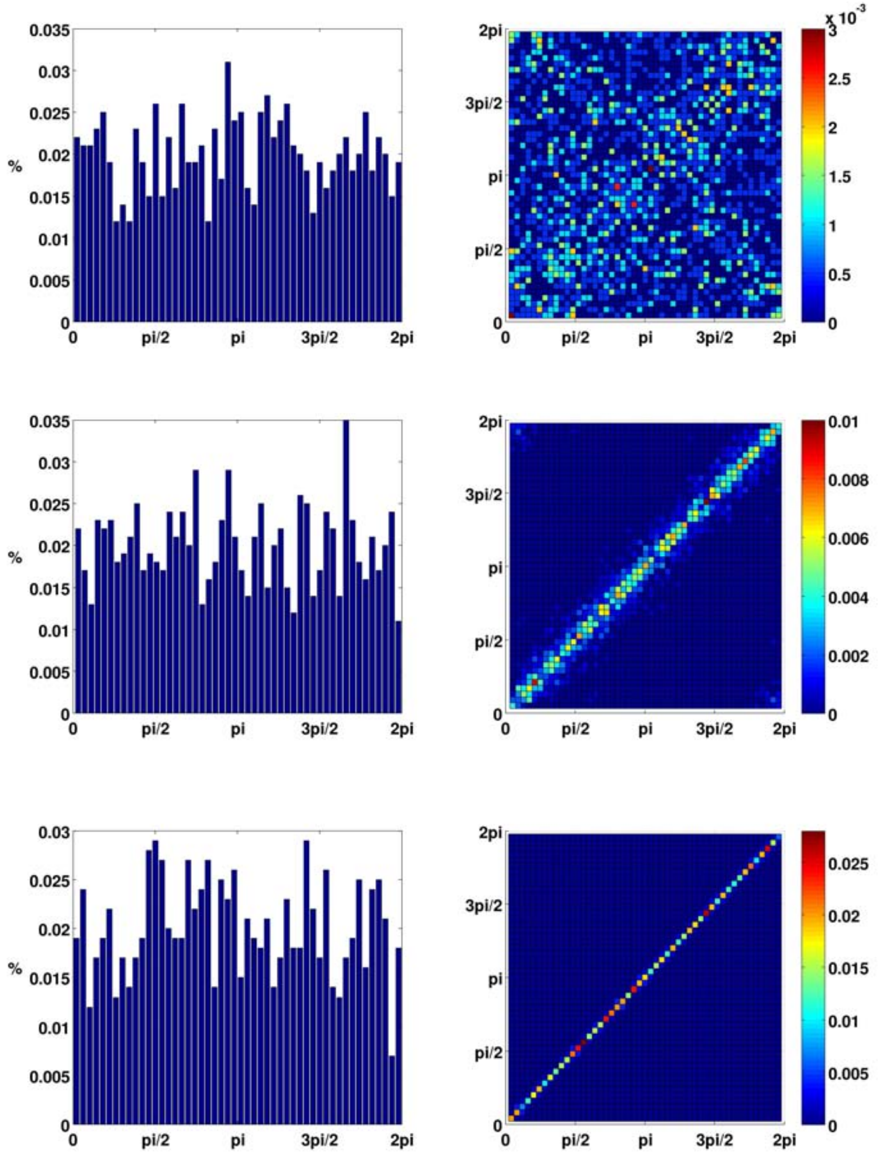
- $f^{(2)}_{\text{eq}}(\theta_1, \theta_2) \neq f^{(1)}_{\text{eq}}(\theta_1)\, f^{(1)}_{\text{eq}}(\theta_2)$
  - Chaos assumption violated
- $f^{(2)}_{\text{eq}}$ peaked at $\theta_1 = \theta_2$
  - coherent motion
  - but no preferred mean direction



Numerical simulations

- Experimental protocol
  - simulations with $N = 10^2$, 10^3, 10^4 & 10^5 particles
  - wait until 'stationary state'
  - Pick one i and a pair (i, j) at random
  - Redo the simulation M times to avoid correlations
  - Plot histograms of θ_1 and (θ_1, θ_2) of these M samples
  - Compare with theoretical $f_{\text{eq}}^{(1)}$ and $f_{\text{eq}}^{(2)}$

$f^{(1)}_{\text{eq}}$ & $f^{(2)}_{\text{eq}}$: experiments $N = 10^3$

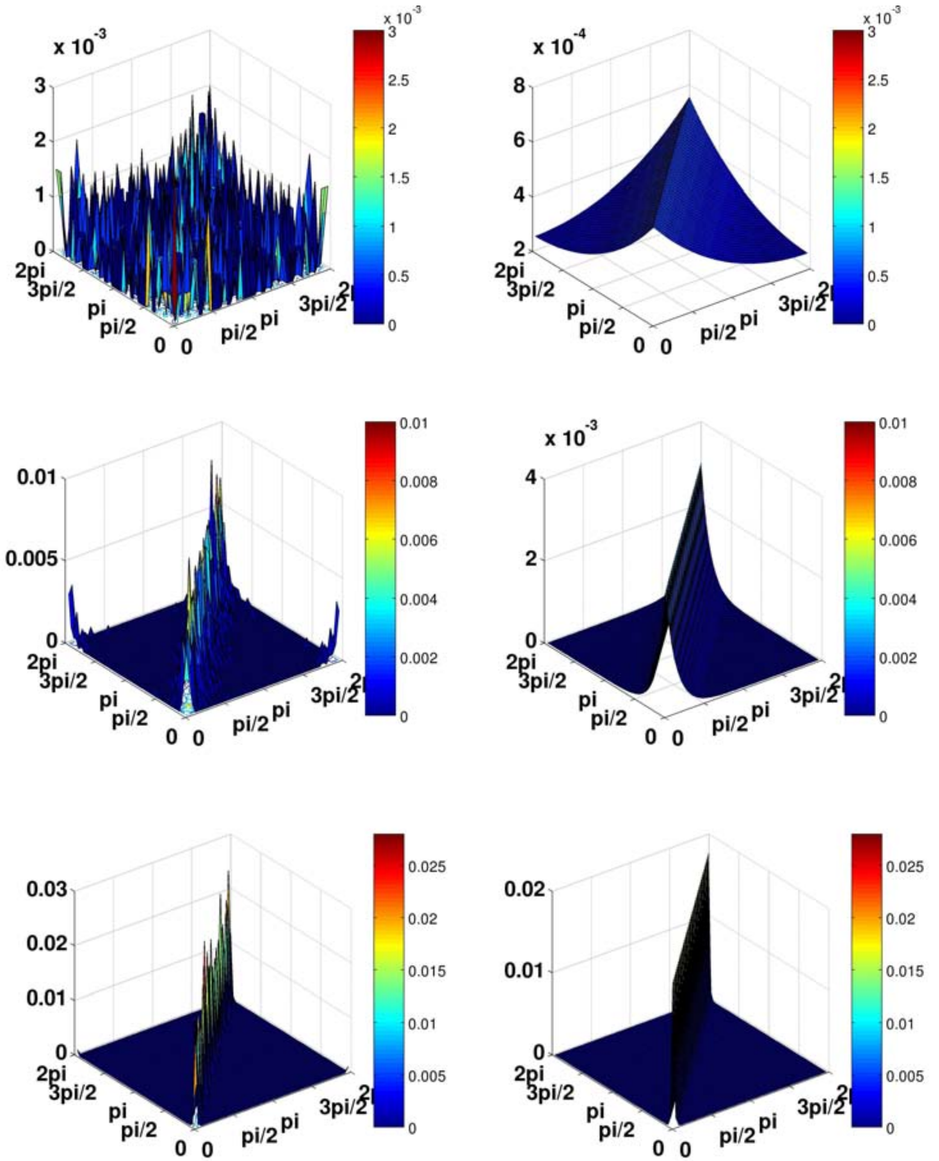


$\sigma = \pi$

$\sigma = \pi/10$

$\sigma = \pi/100$

$f_{\text{eq}}^{(2)}$: experiments vs theory $N = 10^3$



$\sigma = \pi$

$\sigma = \pi/10$

$\sigma = \pi/100$

$N \to \infty$ in BDG

- Small noise limit and continuous time limit
  - $g_N \to \delta \quad \text{Var}(g_N) = \sigma^2/N \quad \Delta t = O(1/N^2)$
- Strong bias ('grazing collisions')
  - $h_N / \int h_N \to \delta \quad \text{Var}(h_N / \int h_N) = \tau^2/N$
- Goal: in the limit $N \to \infty$:
  - Compare the relative influence of the noise σ and the grazing bias τ

Explicit hierarchy

$$\partial_t f^{(1)} = (\sigma^2 - \tau^2)\, \partial_\theta^2 f^{(2)}(\theta, \theta)|_{\theta=\theta_1}$$

$$\partial_t f^{(2)} = (\sigma^2 - \tau^2)(\partial_\theta^2 f^{(3)}(\theta, \theta_2, \theta)|_{\theta=\theta_1} + \partial_\theta^2 f^{(3)}(\theta_1, \theta, \theta)|_{\theta=\theta_2})$$

$$\vdots$$

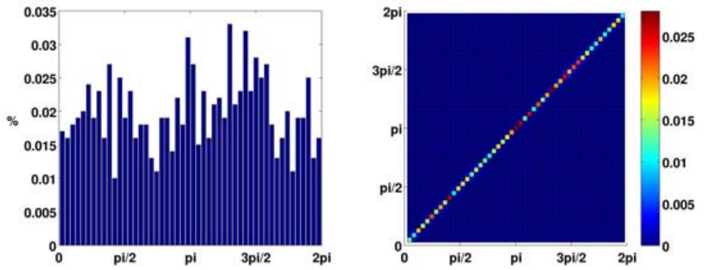
$$\partial_t f^{(j)} = (\sigma^2 - \tau^2) \sum_{k=1}^{j} \partial_\theta^2 f^{(j+1)}(\theta_1, \ldots, \theta_{k-1}, \theta, \theta_{k+1}, \ldots, \theta_j, \theta)|_{\theta=\theta_k}$$

- If chaos assumption holds, $f^{(1)}(\theta)$ satisfies

$$\partial_t f = (\sigma^2 - \tau^2)\,(f^2)" = 2(\sigma^2 - \tau^2)\,(f\,f')'$$

  - nonlinear heat equation
  - $\sigma > \tau$: well-posed ; noise added wider than initial spread
  - $\sigma < \tau$: ill-posed ; noise added narrower: concentration ?

- BUT: Chaos assumption does not hold



- Existence for hierarchy ?
  - infinitely many stationary states

5. Conclusion

Observations & Future work

- 'Simple' dynamics of aggregation do not satisfy chaos assumption
  - How can kinetic theory survive this situation ?
  - Requires rethinking of classical concepts (entroypy, dissipation, irreversibility, equilibria, . . .)
- Spatialization
  - Kinetic & fluid models
  - application to practical systems (swarming, trail formation, construction, . . .)