# **Aggregation model and related topics**



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## **Aggregation model**

We consider a simple model of particle interaction,

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1...N\\k\neq j}} F\left(|x_j - x_k|\right) \frac{x_j - x_k}{|x_j - x_k|}, \ \ j = 1...N$$
(1)

- Models insect aggregation [Edelstein-Keshet et al, 1998] such as locust swarms [Topaz et al, 2008]; robotic motion [Gazi, Passino, 2004].
- Interaction force F(r) is of *attractive-repelling type*: the insects repel each other if they are too close, but attract each-other at a distance.
- Note that acceleration effects are ignored as a first-order approximation.
- Mathematically F(r) is positive for small r, but negative for large r.
- Alternative formulation: (1) is a gradient flow of the minimization problem

min 
$$E(x_1, \ldots x_N)$$
 where  $E = \sum \sum P(|x_i - x_j|)$  with  $F(r) = -P'(r)$ .

#### Confining vs. spreading

• Consider a *Morse interaction force*:

$$F(r) = \exp(-r) - G \exp(-r/L); \quad G < 1, L > 1$$

• If  $GL^3 > 1$ , the morse potential is *confining* (or catastrophic): doubling N doubles the density but cloud volume is unchanged:



• If  $GL^3 < 1$ , the system is *non-confining* (or h-stable): doubling N doubles the cloud volume but density is unchanged:

$$G = 0.5, \quad L = 1.2$$

#### **Continuum limit**

- For confining potentials, we can take the continuum limit as the number of particles  $N \to \infty.$
- We define the *density*  $\rho$  as

$$\int_D \rho(x) dx \approx \frac{\# \text{particles inside domain } D}{N}$$

• The flow is then characterized by density  $\rho$  and velocity field v:

$$\rho_t + \nabla \cdot (\rho v) = 0; \qquad v(x) = \int_{\mathbb{R}^n} F\left(|x - y|\right) \frac{x - y}{|x - y|} \rho(y) dy. \tag{3}$$

• Variational formulation: Let

$$E\left[\rho\right] := \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \rho(x)\rho(y)P(|x-y|)dxdy; \quad P'(r) = -F(r) \tag{4}$$

Then (3) is the gradient flow of E; minima of E are stable equilibria of (3).

- Questions
  - 1. Describe the equilibrium cloud shape in the limit  $t \to \infty$
  - 2. What about dynamics?

#### **Turing analysis in 1D:**

$$\rho_t + \nabla \cdot (v\rho) = 0; \qquad v = K * \rho, \quad K(x) = F(|x|) \operatorname{sign}(x).$$
(5)

- Note that K \* 1 = 0 (since kernel K is odd) so that  $\rho \equiv 1$  is a steady state.
- Linearize around homogeneous state  $\rho=1$  :

$$\rho(x,t) = 1 + \phi(x,t), \quad \phi \ll 1$$
$$\phi_t + (K * \phi)_x = 0$$

• Plug in  $\phi = e^{\lambda t} e^{imx}$  :

$$K * \exp(imx) = \int_{-\infty}^{\infty} F(|y|) \operatorname{sign}(y) \exp(imx - imy) dy$$
$$= \exp(imx) \int_{-\infty}^{\infty} \underbrace{F(|y|) \operatorname{sign}(y)}_{odd} \left\{ \underbrace{\cos(imy)}_{even} - i \underbrace{\sin(imy)}_{odd} \right\} dy$$
$$= -2i \exp(imx) \int_{0}^{\infty} F(y) \sin(my) dy$$
$$\lambda = -2m \int_{0}^{\infty} F(y) \sin(my) dy$$

- Conclusion: The homogeneous state is stable if and only if  $\int_0^\infty F(y) \sin(my) dy > 0$  for all m > 0.
- In particular, *patterns form* (w.r.t. low frequencies) if  $\int_0^\infty F(y)ydy < 0$ .
- Patterns form when the constant state is unstable!
- In the case of the repulsive-attractive morse potential:

$$F(r) = \exp(-r) - G \exp(-r/L); \ G < 1, L > 1$$

$$\begin{split} \lambda(m) &= -2m^2 \left( \frac{1}{m^2 + 1} - \frac{G}{m^2 + \left(\frac{1}{L}\right)^2} \right) \\ \lambda(0) &= -2(1 - GL^2) \end{split}$$

- Conclusions:
  - Homogenous state is unstable iff  $GL^2 > 1$
  - Confining potential [i.e. "catostrophic case" iff  $GL^2 > 1$ ].

## Turing in any dimension $\boldsymbol{d}$

- Exercise: In dimension d, homogeneous state is unstable (wrt small m) when  $\int_0^\infty F(r) r^d dr < 0.$
- For Morse force, confining potential if  $GL^{d+1} > 1$ .

#### **Complex patterns:**



#### **PW-linear force:** $F(r) = \min(ar + b, 1 - r)$



#### **Ring-type steady states**

- Seek steady state of the form  $x_j = r \left( \cos \left( 2\pi j/N \right), \sin \left( 2\pi j/N \right) \right), \ j = 1 \dots N.$
- $\bullet$  In the limit  $N \to \infty$  the radius of the ring must be the root of

$$I(r) := \int_0^{\frac{\pi}{2}} F(2r\sin\theta)\sin\theta d\theta = 0.$$
 (6)

- For Morse force  $F(r) = \exp(-r) G \exp(-r/L)$ , such root exists whenever  $GL^2 > 1$  [coincides with 1D catastrophic regime]
- For general repulsive-attractive force F(r), a ring steady state exists if  $F(r) \le C < 0$  for all large r.
- Even if the ring steady-state exists, the time-dependent problem can be ill-posed!

#### **Continuum limit for curve solutions**

 $\bullet$  If particles concentrate on a curve, in the limit  $N \to \infty$  we obtain

$$\rho_t = \rho \frac{\langle z_\alpha, z_{\alpha t} \rangle}{|z_\alpha|^2}; \quad z_t = K * \rho$$
(7)

where  $z\left( lpha;t
ight)$  is a parametrization of the solution curve;  $ho\left( lpha;t
ight)$  is its density and

$$K * \rho = \int F\left(|z(\alpha') - z(\alpha)|\right) \frac{z(\alpha') - z(\alpha)}{|z(\alpha') - z(\alpha)|} \rho(\alpha', t) dS(\alpha').$$
(8)

- Depending on F(r) and initial conditions, the curve evolution may be *ill-defined!* 
  - For example a circle can degenerate into an annulus, gaining a dimension.
- We used a Lagrange particle-based numerical method to resolve (7).
  - Agrees with direct simulation of the ODE system (1):



#### Local stability of a ring

- Turing-type analysis (linearization around the ring solution)
- Direct approach for ODE linearization:

$$x_k = r_0 \exp\left(2\pi i k/N\right) \left(1 + \exp(t\lambda)\phi_k\right), \quad \phi_k \ll 1.$$

• After some algebra:

$$\lambda \phi_j = \frac{1}{N} \sum_{k \neq j} G_+ \left( \frac{\pi(k-j)}{N} \right) \left( \phi_j - \phi_k \exp\left( \frac{2\pi i(k-j)}{N} \right) \right) + G_- \left( \frac{\pi(k-j)}{N} \right) \left( \bar{\phi}_k - \bar{\phi}_j \exp\left( \frac{2\pi i(k-j)}{N} \right) \right),$$
$$G_+ = \frac{1}{2} F'(2r_0 |\sin\theta|) + \frac{F(2r_0 |\sin\theta|)}{4r_0 |\sin\theta|}; \quad G_- = \frac{1}{2} F'(2r_0 |\sin\theta|) - \frac{F(2r_0 |\sin\theta|)}{4r_0 |\sin\theta|}$$

• Anzatz:

$$\phi_j = b_+ e^{2m\pi i j/N} + b_- e^{-2m\pi i j/N}$$

$$\lambda \begin{pmatrix} b_+ \\ b_- \end{pmatrix} = M(m) \begin{pmatrix} b_+ \\ b_- \end{pmatrix}, \qquad M(m) := \begin{bmatrix} I_1(m) & I_2(m) \\ I_2(m) & I_1(-m) \end{bmatrix}; \quad m = 1, 2, \dots; \quad (9)$$

$$I_1(m) = \frac{4}{N} \sum_{l=1}^{N/2} G_+ \left(\frac{\pi l}{N}\right) \sin^2 \left((m+1)\frac{\pi l}{N}\right);$$
$$I_2(m) = \frac{4}{N} \sum_{l=1}^{N/2} G_- \left(\frac{\pi l}{N}\right) \left[\sin^2 \left(\frac{\pi l}{N}\right) - \sin^2 \left(m\frac{\pi l}{N}\right)\right].$$

• Taking the limit  $N \to \infty,$  we obtain

$$I_1(m) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \left[ \frac{F(2r\sin\theta)}{2r\sin\theta} + F'(2r\sin\theta) \right] \sin^2\left((m+1)\theta\right) d\theta;$$
(10a)

$$I_2(m) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \left[ \frac{F(2r\sin\theta)}{2r\sin\theta} - F'(2r\sin\theta) \right] \left[ \sin^2\left(m\theta\right) - \sin^2(\theta) \right] d\theta.$$
 (10b)

• Eigenfunction is a pure fourier mode when projected to the curvilinear coordinates of

the circle.



# Quadratic force $F(r) = r - r^2$

• Computing explicitly,

$$\operatorname{tr} M(m) = -\frac{\left(4m^4 - m^2 - 9\right)}{(4m^2 - 1)(4m^2 - 9)} < 0, \quad m = 2, 3, \dots$$
$$\det M(m) = \frac{3m^2(2m^2 + 1)}{(4m^2 - 9)(4m^2 - 1)^2} > 0, \quad m = 2, 3, \dots$$

- Conclusion: ring pattern corresponding to  $F(r) = r r^2$  is locally stable
- For large m, the two eigenvalues are  $\lambda \sim -\frac{1}{4}$  and  $\lambda \sim -\frac{3}{8m^2} \rightarrow 0$  as  $m \rightarrow \infty$ . The presence of arbitrary small eigenvalues implies the existence of very slow dynamics near the ring equilibrium.



#### **General power force**

 $F(r) = r^p - r^q, \ 0$ 

- The mode  $m = \infty$  is stable if and only if pq > 1 and p < 1.
- Stability of other modes can be expressed in terms of Gamma functions.
- The dominant unstable mode corresponds to m = 3; the boundary is given by  $0 = 723 - 594(p+q) - 27(p^2 + q^2) - 431pq + 106(pq^2 + p^2q) + 19(p^3q + pq^3) + 10(p^3q^2 + p^2q^3) + 6(p^3 + q^3) + p^3q^3;$
- Boundaries for  $m=4,5,\ldots$  are similarly expressed in terms of higher order polynomials in p,q.



## Weakly nonlinear analysis

- Near the instability threshold, higher-order analysis shows a supercritical pitchfork bifurcation, whereby a ring solution bifurcates into an *m*-symmetry breaking solution
- This shows existence of nonlocal solutions.
- Example:  $F(r) = r^{1.5} r^q$ ; bifurcation m = 3 occurs at  $q = q_c \approx 4.9696$ ; nonlinear analysis predicts



#### **Point-concentration (hole) solutions**

$$F(r) = \min(ar, r - r^2)$$

Solutions consist of K "clusters", where each cluster has N/K points inside. The number K depends on a :



#### Spots: "degenerate" holes

 $F(r) = \min(ar + \delta, 1 - r); \quad \delta \ll 1$ 

• Points degenerate into spots of size  $O(\delta)$ . eg.  $a = 0.3, \delta = 0.05$ :



Inside each of the cluster, the *reduced* problem is:

$$\phi_l' = \sum_{j \neq l}^n \frac{\phi_l - \phi_j}{|\phi_l - \phi_j|} - n \begin{bmatrix} \alpha & 0\\ 0 & \beta \end{bmatrix} \phi_l$$

•  $\alpha, \beta$  depend only on F(r) not on N.

#### (In)stability of $m \gg 1 \mod s$

- If  $\lambda(m) > 0$  for all sufficiently large m, then we call the ring solution **ill-posed**. Otherwise we call it **well-posed**.
- For ill-posed problems, the ring can degenerate into either an annulus (eg.  $F(x) = 0.5 + x x^2$ ) or discrete set of points (eg  $F(x) = x^{1.3} x^2$ )
- , if F(r) is  $C^4$  on [0, 2r], then the necessary and sufficient conditions for well-posedness of a ring are:

$$F(0) = 0, \quad F''(0) < 0 \text{ and}$$

$$\int_0^{\pi/2} \left( \frac{F(2r\sin\theta)}{2r\sin\theta} - F'(2r\sin\theta) \right) d\theta < 0.$$
(11)
(12)

• Ring solution for the morse force  $F(r) = \exp(-r) - G \exp(-r/L)$  is always ill-posed since F(0) > 0.

#### **Bifurcation to annulus:**

Consider

$$F(r) = r - r^2 + \delta, \qquad 0 \le \delta \ll 1.$$

- A ring is stable of radius  $R \sim \frac{3\pi}{16} + \frac{2}{\pi}\delta + O(\delta^2)$  if  $\delta = 0$  but *high modes* become unstable for  $\delta > 0$
- The most unstable mode in the *discrete* system is m = N/2 and can be stable even if the continuous model is ill-posed!
- Proposition: Let

$$N_c \sim \frac{\pi}{4} e^{4-\gamma} \exp\left(\frac{3\pi^2}{64\delta}\right).$$

The ring is stable if  $N < N_c$ .

• For  $N>N_c$  but  $N\sim N_c$ , solution consists of two radii  $R\pm \varepsilon$  where

$$R = \frac{3\pi}{32} \left( 1 + \sqrt{1 + \frac{128}{3\pi^2} \delta} \right); \quad \varepsilon \sim 4Re^{-2} \exp\left(\frac{-4R^2 + R\pi/2}{\delta}\right)$$

• Example:  $\delta = 0.35 \implies N_c \sim 90, \ 2\varepsilon \sim 0.033$ . Numerically, we obtain  $2\varepsilon \approx 0.036$ . Good agreement!



• Increasing N further, more rings appear until we get a thin annulus of width  $O(\varepsilon)$ .



#### Annulus: continuum limit $N \gg N_c$ :

• 
$$F(r) = r - r^2 + \delta$$
,  $0 < \delta \ll 1$ 

• Main result: In the limit  $\delta \to 0$ , the annulus inner and outer radii  $R_1, R_2$  are given by

$$R \sim \frac{3\pi}{16} + \frac{2}{\pi}\delta;$$
  $R_1 \sim R - \beta,$   $R_2 \sim R + \beta$ 

where

$$\beta \sim 3\pi e^{-5} \exp\left(-\frac{3\pi^2}{64}\frac{1}{\delta}\right) \ll \delta \ll 1.$$

The radial density profile inside the annulus is

$$\rho(x) \sim \begin{cases} \frac{c}{\sqrt{\beta^2 - \left(R - |x|\right)^2}}, & |R - x| < \beta \ll 1 \\ 0, & \text{otherwise} \end{cases}$$

• Annulus is *exponentially thin in*  $\delta$ ... note the 1/sqrt singularity near the edges!



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#### Key steps for computing annulus profile

• For radially symmetric density, the velocity field reduces to a 1D problem:

$$v(r) = \int_0^\infty K(s,r)\rho(s)sds$$

where

$$K(s,r) := \int_0^{2\pi} \left(r - s\cos\theta\right) f\left(\sqrt{r^2 + s^2 - 2rs\cos\theta}\right) d\theta; \quad f(r) = 1 - r + \frac{\delta}{r}$$

• Assume thin annulus; expand all integrals. *It boils down to integral equation* 

$$\int_{-\beta}^{\beta} \ln |\eta - \xi| \, \varrho(\eta) d\eta = 1 \text{ for all } \xi \in (\alpha, \beta)$$

• *Explicit solution* is a special case of Formula 3.4.2 from "Handbook of integral equations" A.Polyanin and A.Manzhirov:

$$\varrho\left(\xi\right) = \frac{C}{\sqrt{\beta^2 - \xi^2}}$$

#### **3D sphere instabilities**

- Radius satisfies:  $\int_0^{\pi} F(2r_0 \sin \theta) \sin \theta \sin 2\theta = 0$
- Instability can be done using spherical harmonics



#### Stability of a spherical shell

Define

$$g(s) := \frac{F(\sqrt{2s})}{\sqrt{2s}};$$

The spherical shell has a radius given implicitly by

$$0 = \int_{-1}^{1} g(R^2(1-s))(1-s) \mathrm{d}s.$$

Its stability is given by a sequence of 2x2 eigenvalue problems

$$\lambda \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \alpha + \lambda_l(g_1) & l(l+1)\lambda_l(g_2) \\ \lambda_l(g_2) & \frac{l(l+1)}{R^2}\lambda_l(g_3) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \quad l = 2, 3, 4, \dots$$

where

$$\lambda_l(f) := 2\pi \int_{-1}^1 f(s) P_l(s) \, \mathrm{d}s;$$

with  $P_l(s)$  the Legendre polynomial and

$$\begin{split} \alpha &:= 8\pi g(2R^2) + \lambda_0 (g(R^2(1-s^2))) \\ g_1(s) &:= R^2 g'(R^2(1-s))(1-s)^2 - g(R^2(1-s))s \\ g_2(s) &:= g(R^2(1-s))(1-s); \qquad g_3(s) := \int_0^{R^2(1-s)} g(z) dz \end{split}$$

#### Well-posedness in 3D

Suppose that g(s) can be written in terms of the generalized power series as

$$g(s) = \sum_{i=1}^{\infty} c_i s^{p_i}, \quad p_1 < p_2 < \cdots \text{ with } c_1 > 0.$$

Then the ring is well-posed [i.e.  $\lambda < 0$  for all sufficiently large l] if

(i)  $\alpha < 0$  and (ii)  $p_1 \in (-1, 0) \bigcup (1, 2) \bigcup (3, 4) \dots$ 

The ring is **ill-posed** [i.e.  $\lambda > 0$  for all sufficiently large l] if either  $\alpha > 0$  or  $p_1 \notin [-1,0] \bigcup [1,2] \bigcup [3,4] \ldots$ 

#### Key identity to prove well-posedness:

$$\int_{-1}^{1} (1-s)^{p} P_{l}(s) \, \mathrm{d}s = \frac{2^{p+1}}{p+1} \frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)} \\ \sim -\frac{1}{\pi} \sin(\pi p) \, \Gamma^{2}(p+1)2^{p+1} l^{-2p-2} \quad \text{as } l \to \infty.$$

Proof:

- Use hypergeometric representation:  $P_l(s) = {}_2F_1\left( \begin{array}{c} l+1, -l \\ 1 \end{array}; \frac{1-s}{2} \right).$
- Use generalized Euler transform:

$${}_{A+1}F_{B+1}\left(\begin{array}{c}a_1,\ldots,a_A,c\\b_1,\ldots,b_B,d\end{array};z\right) = \frac{\Gamma(d)}{\Gamma(c)\Gamma(d-c)}\int_0^1 t^{c-1}(1-t)^{d-c-1}{}_AF_B\left(\begin{array}{c}a_1,\ldots,a_A,c\\b_1,\ldots,b_B,d\end{array}\right)$$
  
to get  $\int_{-1}^1(1-s)^p P_l(s) \,\mathrm{d}s = \frac{2\pi 2^{p+1}}{p+1}{}_3F_2\left(\begin{array}{c}p+1,l+1,-l\\p+2,1\end{array};1\right).$ 

• Apply the Saalschütz Theorem to simplify

$${}_{3}F_{2}\left(\begin{array}{c}p+1,l+1,-l\\p+2,1\end{array};1\right) = \frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)}$$

# **Generalized Lennard-Jones interaction**

$$g(s) = s^{-p} - s^{-q}; \qquad 0 < p, q < 1; \ p > q$$

• Well posed if  $q < \frac{2p-1}{2p-2}$ ; ill-posed if  $q > \frac{2p-1}{2p-2}$ .



Example: steady state with N = 1000 particles. (a) (p,q) = (1/3, 1/6). Particles concentrate uniformly on a surface of the sphere, with no particles in the interior. (b) (p,q) = (1/2, 1/4). Particles fill the interior of a ball. The particles are color-coded according to their distance from the center of mass.

#### **Custom-designed kernels**

- In 3D, we can design force F(r) which is stable for all modes except specified mode.
- EXAMPLE: Suppose we want only mode m = 5 to be unstable. Using our algorithm, we get

$$F(r) = \left\{ 3\left(1 - \frac{r^2}{2}\right)^2 + 4\left(1 - \frac{r^2}{2}\right)^3 - \left(1 - \frac{r^2}{2}\right)^4 \right\} r + \varepsilon; \quad \varepsilon = 0.1.$$



Particle simulation



Linearized solution

#### Part II: Constant-density swarms

- Biological swarms have sharp boundaries, relatively constant internal population.
- Question: What interaction force leads to such swarms?
- More generally, can we deduce an interaction force from the swarm density?





#### **Bounded states of constant density**

Claim. Suppose that

$$F(r) = \frac{1}{r^{n-1}} - r, \quad \text{where } n \equiv \text{dimension}$$

Then the aggregation model

$$\rho_t + \nabla \cdot (\rho v) = 0; \quad v(x) = \int_{\mathbb{R}^n} F\left(|x - y|\right) \frac{x - y}{|x - y|} \rho(y) dy.$$

admits a steady state of the form

$$\rho(x) = \begin{cases} 1, & |x| < R \\ 0, & |x| > R \end{cases}; \quad v(x) = \begin{cases} 0, & |x| < 1 \\ -ax, & |x| > 1 \end{cases}$$

where R = 1 for n = 1, 2 and a = 2 in one dimension and  $a = 2\pi$  in two dimensions.



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#### **Proof for two dimensions**

Define

$$G(x) := \ln |x| - \frac{|x|^2}{2}; \quad M = \int_{\mathbb{R}^n} \rho(y) dy$$

Then we have:

$$\nabla G = F(|x|) \frac{x}{|x|}$$
 and  $\Delta G(x) = 2\pi \delta(x) - 2$ .

so that

$$v(x) = \int_{\mathbb{R}^n} \nabla_x G(x-y) \rho(y) dy.$$

Thus we get:

$$\nabla \cdot v = \int_{\mathbb{R}^n} (2\pi\delta(x-y) - 2)\rho(y)dy$$
$$= 2\pi\rho(x) - 2M$$
$$= \begin{cases} 0, & |x| < R\\ -2M, & |x| > R \end{cases}$$

The steady state satisfies  $\nabla \cdot v = 0$  inside some ball of radius R with  $\rho = 0$  outside such a ball but then  $\rho = M/\pi$  inside this ball and  $M = \int_{\mathbb{R}^n} \rho(y) dy = MR^2 \implies R = 1$ .

#### Dynamics in 1D with F(r) = 1 - r

Assume WLOG that

$$\int_{-\infty}^{\infty} x \rho(x) = 0; \quad M := \int_{-\infty}^{\infty} \rho(x) \, dx$$

Then

$$\begin{split} v(x) &= \int_{-\infty}^{\infty} F\left(|x-y|\right) \frac{x-y}{|x-y|} \rho(y) dy \\ &= \int_{-\infty}^{\infty} \left(1 - |x-y|\right) \operatorname{sign}(x-y) \rho(y) \\ &= 2 \int_{-\infty}^{x} \rho(y) dy - M(x+1). \end{split}$$

and continuity equations become

$$\rho_t + v\rho_x = -v_x\rho$$
$$= (M - 2\rho)\rho$$

Define the characteristic curves  $X(t,x_0)$  by

$$\frac{d}{dt}X(t;x_0) = v; \quad X(0,x_0) = x_0$$

Then along the characteristics, we have  $\rho=\rho(X,t);$ 

$$\frac{d}{dt}\rho = \rho(M - 2\rho)$$

Solving we get:

$$\rho(X(t,x_0),t) = \frac{M}{2 + e^{-Mt}(M/\rho_0 - 2)}; \quad \rho(X(t,x_0),t) \to M/2 \text{ as } t \to \infty$$

#### Solving for characteristic curves

Let

$$w:=\int_{-\infty}^x\rho(y)dy$$

then

$$v = 2w - M(x+1); \quad v_x = 2\rho - M$$

and integrating  $\rho_t + (\rho v)_x = 0$  we get:

$$w_t + vw_x = 0$$

Thus w is constant along the characteristics X of  $\rho,$  so that characteristics  $\frac{d}{dt}X=v$  become

$$\frac{d}{dt}X = 2w_0 - M(X+1); \quad X(0;x_0) = x_0$$

### Summary for F(r) = 1 - r in 1D:

$$X = \frac{2w_0(x_0)}{M} - 1 + e^{-Mt} \left( x_0 + 1 - \frac{2w_0(x_0)}{M} \right)$$
$$w_0(x_0) = \int_{-\infty}^{x_0} \rho_0(z) dz; \quad M = \int_{-\infty}^{\infty} \rho_0(z) dz$$
$$\rho(X, t) = \frac{M}{2 + e^{-tM} (M/\rho_0(x_0) - 2)}$$

Example:  $\rho_0(x) = \exp(-x^2) / \sqrt{\pi}; M = 1:$ 



#### **Global stability**

In limit  $t \to \infty$  we get:

$$X = \frac{2w_0}{M} - 1; \quad w_0 = 0 \dots M; \quad \rho(X, \infty) = \frac{M}{2}$$

We have shown that as  $t \to \infty$ , the steady state is

$$\rho(x,\infty) = \begin{cases} M/2, & |x| < 1\\ 0, & |x| > 1 \end{cases}$$
(13)

- This proves the global stability of (13)!
- Characteristics intersect at  $t = \infty$ ; solution forms a shock at  $x = \pm 1$  at  $t = \infty$ .

# Dynamics in 2D, $F(r) = \frac{1}{r} - r$

• Similar to 1D,

$$\nabla \cdot v = 2\pi\rho(x) - 4\pi M;$$

$$\rho_t + v \cdot \nabla \rho = -\rho \nabla \cdot v$$
$$= -\rho \left(\rho - 2M\right) 2\pi$$

• Along the characterisitics:

$$\frac{d}{dt}X(t;x_0) = v; \quad X(0,x_0) = x_0$$

we still get

$$\frac{d}{dt}\rho = 2\pi\rho(2M - \rho);$$

$$\rho(X(t;x_0),t) = \frac{2M}{1 + \left(\frac{2M}{\rho(x_0)} - 1\right)\exp\left(-4\pi Mt\right)}$$
(14)

• Continuity equations yield:

$$\rho(X(t;x_0),t) \det \nabla_{x_0} X(t;x_0) = \rho_0(x_0)$$

• Using (14) we get

$$\det \nabla_{x_0} X(t; x_0) = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp\left(-4\pi M t\right).$$

• If  $\rho$  is radially symmetric, characteristics are also radially symmetric, i.e.

$$X(t;x_0) = \lambda(|x_0|, t) x_0$$

then

$$\det \nabla_{x_0} X(t; x_0) = \lambda(t; r) \left( \lambda(t; r) + \lambda_r(t; r) r \right), \quad r = |x_0|$$

so that

$$\lambda^2 + \lambda_r \lambda r = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp\left(-4\pi M t\right)$$
$$\lambda^2 r^2 = \frac{1}{M} \int_0^r s\rho_0(s) ds + 2\exp\left(-4\pi M t\right) \int_0^r s\left(1 - \frac{\rho\left(s\right)}{2M}\right) ds$$

So characteristics are fully solvable!!

- $\bullet$  This proves global stability in the space of radial initial conditions  $\rho_0(x)=\rho_0(|x|).$
- More general global stability is still open.

# The force $F(r) = \frac{1}{r} - r^{q-1}$ in 2D

- If q = 2, we have explicit ode and solution for characteristics.
- For other *q*, no explicit solution is available but we have **differential inequalities**: Define

$$ho_{\max} := \sup_{x} 
ho(x,t); \quad R(t) := ext{ radius of support of } 
ho(x,t)$$

Then

$$\begin{aligned} \frac{d\rho_{\max}}{dt} &\leq (aR^{q-2} - b\rho_{\max})\rho_{\max} \\ \frac{dR}{dt} &\leq c\sqrt{\rho_{\max}} - dR^{q-1}; \end{aligned}$$

where a, b, c, d are some [known] positive constants.

- It follows that if R(0) is sufficiently big, then  $R(t), \rho_{\max}(t)$  remain bounded for all t. [using bounding box argument]
- **Theorem:** For  $q \ge 2$ , there exists a bounded steady state [uniqueness??]

#### Inverse problem: Custom-designer kernels: 1D

Theorem. In one dimension, conisder a radially symmetric density of the form

$$\rho(x) = \begin{cases} b_0 + b_2 x^2 + b_4 x^4 + \ldots + b_{2n} x^{2n}, & |x| < R \\ 0, & |x| \ge R \end{cases}$$
(15)

Define the following quantities,

$$m_{2q} := \int_0^R \rho(r) r^{2q} dr.$$
 (16)

Then  $\rho(r)$  is the steady state corresponding to the kernel

$$F(r) = 1 - a_0 r - \frac{a_2}{3} r^3 - \frac{a_4}{5} r^5 - \dots - \frac{a_{2n}}{2n+1} r^{2n+1}$$
(17)

where the constants  $a_0, a_2, \ldots, a_{2n}$ , are computed from the constants  $b_0, b_2, \ldots, b_{2n}$  by solving the following linear problem:

$$b_{2k} = \sum_{j=k}^{n} a_{2j} \begin{pmatrix} 2j \\ 2k \end{pmatrix} m_{2(j-k)}, \quad k = 0 \dots n.$$
 (18)

#### **Example: custom kernels 1D**

**Example 1**:  $\rho = 1 - x^2$ , R = 1, then  $F(r) = 1 - 9/5r + 1/2r^3$ .

**Example 2**:  $\rho = x^2$ , R = 1, then  $F(r) = 1 + 9/5r - r^3$ .

Example 3:  $\rho = 1/2 + x^2 - x^4$ , R = 1; then  $F(r) = 1 + \frac{209425}{336091}r - \frac{4150}{2527}r^3 + \frac{6}{19}r^5$ .



#### Inverse problem: Custom-designer kernels: 2D

**Theorem.** In two dimensions, conisder a radially symmetric density  $\rho(x) = \rho(|x|)$  of the form

$$\rho(r) = \begin{cases} b_0 + b_2 r^2 + b_4 r^4 + \ldots + b_{2n} r^{2n}, & r < R \\ 0, & r \ge R \end{cases}$$
(19)

Define the following quantities,

$$m_{2q} := \int_0^R \rho(r) r^{2q} dr.$$
 (20)

Then  $\rho(r)$  is the steady state corresponding to the kernel

$$F(r) = \frac{1}{r} - \frac{a_0}{2}r - \frac{a_2}{4}r^3 - \dots - \frac{a_{2n}}{2n+2}r^{2n+1}$$
(21)

where the constants  $a_0, a_2, \ldots, a_{2n}$ , are computed from the constants  $b_0, b_2, \ldots, b_{2n}$  by solving the following linear problem:

$$b_{2k} = \sum_{j=k}^{n} a_{2j} \left( \begin{array}{c} j \\ k \end{array} \right)^2 m_{2(j-k)+1}; \quad k = 0 \dots n.$$
 (22)

This system always has a unique solution for provided that  $m_0 \neq 0$ .

#### **Numerical simulations, 1D**

• First, use standard ODE solver to integrate the corresponding discrete particle model,

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1...N\\k \neq j}} F\left(|x_j - x_k|\right) \frac{x_j - x_k}{|x_j - x_k|}, \ \ j = 1 \dots N.$$

- How to compute  $\rho(x)$  from  $x_i$ ? [Topaz-Bernoff, 2010]
  - Use  $x_i$  to approximate the cumulitive distribution,  $w(x) = \int_{-\infty}^{x} \rho(z) dz$ .
  - Next take derivative to get  $\rho(x)=w^\prime(x)$



[Figure taken from Topaz+Bernoff, 2010 preprint]

#### **Numerical simulations, 2D**

- Solve for  $x_i$  using ODE particle model as before [2N variables]
- Use x<sub>i</sub> to compute Voronoi diagram;
- Estimate  $\rho(x_j) = 1/a_j$  where  $a_j$  is the area of the voronoi cell around  $x_j$ .
- Use **Delanay triangulation** to generate smooth mesh.
- Example: Take

$$o(r) = \begin{cases} 1 + r^2, r < 1 \\ 0, r > 0 \end{cases}$$

Then by Custom-designed kernel in 2D is:

$$F(r) = \frac{1}{r} - \frac{8}{27}r - \frac{r^3}{3}.$$

Running the particle method yeids...



# Numerical solutions for radial steady states for $F(r) = \frac{1}{r} - r^{q-1}$

- Radial steady states of radius R satisfy  $\rho(r) = 2q \int_0^R (r'\rho(r')I(r,r')dr')$ where c(q) is some constant and  $I(r,r') = \int_0^\pi (r^2 + r'^2 - 2rr'\sin\theta)^{q/2-1}d\theta$ .
- To find  $\rho$  and R, we adjust R until the operator  $\rho \to c(q) \int_0^R (r'\rho(r')K(r,r')dr') dr'$  has eigenvalue 1; then  $\rho$  is the corresponding eigenfunction.



#### **Vortex dynamics**

• Equations first given by Helmholtz (1858): each vortex generates a rotational velocity field which advects all other vortices. *Vortex model:* 

$$\frac{dz_j}{dt} = i \sum_{k \neq j} \gamma_k \frac{z_j - z_k}{|z_j - z_k|^2}, \quad j = 1 \dots N.$$

- Classical problem; observed in many physical experiments: floating magnetized needles (Meyer, 1876); Malmberg-Penning trap (Durkin & Fajans, 2000), Bose-Einstein Condensates (Ketterle et.al. 2001); magnetized rotating disks (Whitesides et.al, 2001)
- Conservative, hamiltonian system
- General initial conditions lead to chaos: movie chaos
- Certain special configurations are "stable" in hamiltonial sense: movie stable
- Rigidly rotating steady states are called *relative equilibria*:

$$z_j(t) = e^{\omega i t} \xi_j \quad \Longleftrightarrow \quad 0 = \sum_{k \neq j} \gamma_k \frac{\xi_j - \xi_k}{|\xi_j - \xi_k|^2} - \omega \xi_j$$

#### PHYSICAL REVIEW E, VOLUME 64, 011603

#### Dynamic, self-assembled aggregates of magnetized, millimeter-sized objects rotating at the liquid-air interface: Macroscopic, two-dimensional classical artificial atoms and molecules

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**ure 1** Experimental set-up and magnetic force profiles. **a**, A scheme of the erimental set-up. A bar magnet rotates at angular velocity ω below a dish filled with iid (typically ethylene glycol/water or glycerine/water solutions). Magnetically doped is are placed on the liquid–air interface, and are fully immersed in the liquid except for ir top surface. The disks spin at angular velocity ω around their axes. A magnetic force attracts the disks the area to a budrodwamic force E pushes.



**Figure 2** Dynamic patterns formed by various numbers (*n*) of disks rotating at the ethylene glycol/water-air Interface. This interface is 27 mm above the plane of the external magnet. The disks are composed of a section of polyethylene tube (white) of outer diameter 1.27 mm, filled with poly(dimethylsiloxane), PDMS, doped with 25 wt% of magnetite (black centre). All disks spin around their centres at  $\omega = 700 \text{ r.p.m.}$ , and the entire aggregate slowly ( $\Omega < 2 \text{ r.p.m.}$ ) precesses around its centre. For n < 5, the aggregates do not have a 'nucleus'—all disks are precessing on the rim of a circle. For n > 5, nucleated structures appear. For n = 10 and n = 12, the patterns are bistable in the sense that the two observed patterns interconvert irregularly with time. For n = 19, the hexagonal pattern (left) appears only above  $\omega \approx 800 \text{ r.p.m.}$ , but can be 'annealed' down

#### Observation of Vortex Lattices in Bose-Einstein Condensates

J. R. Abo-Shaeer, C. Raman, J. M. Vogels, W. Ketterle

Fig. 1. Observation of vortex lattices. The examples shown contain approximately (A) 16, (B) 32, (C) 80, and (D) 130 vortices. The vortices have "crystallized" in a triangular pattern. The diameter of the cloud in (D) was 1 mm after ballistic expansion, which represents a magnification of 20.



Slight asymmetries in the density distribution were due to absorption of the optical pumping light.

• Campbell and Ziff (1978) classified many stable configurations for *small* (eg. N = 18) number of vortices of equal strength.



• Goal: describe the stable configuration in the continuum limit of a *large* number of vortices N (eg. N = 100, 1000...). These have been observed in several recent expriments: Bose Einstein Condensates, magnetized disks

#### **Key observation**

$$\begin{array}{l} \text{Vortex model: } \displaystyle \frac{dz_j}{dt} = i \sum_{k \neq j} \gamma_k \frac{z_j - z_k}{|z_j - z_k|^2}, \ j = 1 \dots N. \end{array} \tag{V} \\ \text{Relative equilibrium: } \displaystyle z_j(t) = e^{\omega i t} \xi_j \quad \Longleftrightarrow \quad 0 = \sum_{k \neq j} \gamma_k \frac{\xi_j - \xi_k}{|\xi_j - \xi_k|^2} - \omega \xi_j \\ \text{Aggregation model: } \displaystyle \frac{dx_j}{dt} = \sum_{k \neq j} \gamma_k \frac{x_j - x_k}{|x_j - x_k|^2} - \omega x_j. \end{aligned}$$

- One-to-one correspondence between the steady statates  $x_j(t) = \xi_j$  of (A) and the relative equilibrium  $z_j(t) = e^{\omega i t} \xi_j$  of (V).
- Spectral equivalence of (V) and (A): The equilibrium  $x_j(t) = \xi_j$  is asymptotically stable for the aggregation model (A) if and only if the relative equilibrium  $z_j(t) = e^{\omega i t} \xi_j$  is stable (neutrally, in the Hamiltonian sense) for the vortex model (V)!
- Aggregation model fully describes relative equilibria and their linear stability in the vortex model.
- Aggregation model is easier to study than the vortex model.

#### Vortices of equal strength $\gamma_k = \gamma$

Corresponding aggregation model:

$$\frac{dx_j}{dt} = \sum_{k \neq j} \gamma \frac{x_j - x_k}{\left|x_j - x_k\right|^2} - \omega x_j.$$
(23)

• Coarse-grain by defining the particle density to be

$$\rho(x) = \sum_{k=1\dots N} \delta(x - x_k).$$
(24)

Then (23) is equivalent to  $\dot{x}_j = v(x_j)$  where

$$v(x) \equiv -\omega x + \gamma \int_{\mathbb{R}^2} \frac{x - y}{\left|x - y\right|^2} \rho\left(y\right) dy,$$
(25)

and density is subject to conservation of mass

$$\rho_t + \nabla \cdot (\rho v) = 0. \tag{26}$$

• [Fetecau&Huang&Kolokolnikov2011]: In the limit  $N \to \infty$ , the steady state density of (A) is constant inside the ball of radius

$$R_0 = \sqrt{N\gamma/\omega}.$$



Fig. 1. Stable relative equilibria of N = 25,50 and 200 vortices of equal strength. The dashed line shows the analytical prediction  $R_0 = \sqrt{N\gamma/\omega}$  of the swarm radius in the  $N \to \infty$  limit (see (6)).



#### **Crystallization**

$$\begin{array}{l} \text{Vortex model: } \frac{dz_j}{dt} = i \sum_{k \neq j} \gamma_k \frac{z_j - z_k}{|z_j - z_k|^2}, \ \ j = 1 \dots N. \end{array} \tag{V} \\ \text{Reltive equiliria: } z_j(t) = e^{\omega i t} \xi_j \iff 0 = \sum_{k \neq j} \gamma_k \frac{\xi_j - \xi_k}{|\xi_j - \xi_k|^2} - \omega \xi_j \\ \text{Vortex with dissipation: } \frac{dz_j}{dt} = i \sum_{k \neq j} \gamma_k \frac{z_j - z_k}{|z_j - z_k|^2} + \mu \left( \sum_{k \neq j} \gamma_k \frac{z_j - z_k}{|z_j - z_k|^2} - \omega z_j \right) \end{array} \tag{D}$$

- In many physical experiments of BEC there is damping or dissipation involved.
- Spectral equivalence: Relative equilibria and their stability are the same for (V) and (D)
- Both the vortex model and the "aggregation model" model are limiting cases of (D).
- Taking  $\mu > 0$  *stabilizes vortex dynamics! chaos damped stable*
- This allows us to find stable relative equilibria numerically.

#### Vortex dynamics in BEC with trap

• For BEC, dynamics have extra term corresponding to pression around the trap:



• Large N limit:

$$\begin{split} v(x) &\equiv \left(f(r) - \omega\right) x + c \int_{\mathbb{R}^2} \frac{x - y}{\left|x - y\right|^2} \rho\left(y\right) dy. \\ &\int_{\mathbb{R}^2} \rho(x) dx = N, \end{split}$$

Non-uniform vortex lattice state:

$$\label{eq:rho} \begin{split} \rho \sim \frac{1}{\pi c} \left( \omega - \frac{a}{\left(1-r^2\right)^2} \right) \mbox{ if } r < R, \quad \rho = 0 \mbox{ otherwise,} \end{split}$$
 with  $\omega = \frac{a}{1-R^2} + \frac{cN}{R^2}$ 





Figure 2. Top row: stable equilibrium of Eq. (2.4) with f(r) as in Eq. (2.2), with N as shown in the title and with c = 0.5/N,  $\omega = 2.95139$ , a = 1. The dashed circle is the asymptotic boundary whose radius R = 0.6 is the smaller solution to Eq. (4.9). Bottom row: average of  $\rho(|x|)/\rho(0)$  as a function of r = |x|. Solid curve corresponds to the numerical computation. Dashed curve is the formula (4.10). Vertical line is the boundary r = R.

#### $\mathbf{Maximum}\;N$

$$\omega_{c} = \left(\sqrt{a} + \sqrt{cN}\right)^{2}; \quad R_{c}^{2} = \frac{\sqrt{cN}}{\sqrt{a} + \sqrt{cN}}$$

- No solutions if  $\omega < \omega_c$
- Two solutions  $R=R_{\pm}$  if  $\omega>\omega_c$ 
  - smaller is stable, larger has negative density (unphysical).
- $\bullet$  Corrollary: must have  $N < N_{\rm max}$  where

$$N_{\max} = \frac{\left(\sqrt{\omega} - \sqrt{a}\right)^2}{c}.$$
 (28)

## N+1 problem

• N vortices of equal strength and a single vortex of a much higher strength:

$$\frac{dx_j}{dt} = \frac{a}{N} \sum_{\substack{k=1...N\\k\neq j}} \frac{x_j - x_k}{|x_j - x_k|^2} + b \frac{x_j - \eta}{|x_j - \eta|^2} - x_j, \quad j = 1...N,$$
(29)  
$$\frac{d\eta}{dt} = \frac{a}{N} \sum_{\substack{k=1...N\\k=1...N}} \frac{\eta - x_k}{|\eta - x_k|^2} - \eta$$
(30)

• Mean-field limit  $N \to \infty$ :

$$\begin{cases} \rho_t + \nabla \cdot (\rho \nabla v) = 0; \\ v(x) = a \int_{\mathbb{R}^2} \rho(y) \frac{x - y}{|x - y|^2} dy + b \frac{x - \eta}{|x - \eta|^2} - x \\ \frac{d\eta}{dt} = a \int_{\mathbb{R}^2} \rho(y) \frac{\eta - y}{|\eta - y|^2} dy - \eta \end{cases}$$
(31)

• Main result: Define  $R_1 = \sqrt{b}$ ,  $R_0 = \sqrt{a+b}$  and suppose that  $\eta$  is any point such that  $B_{R_1}(\eta) \subset B_{R_0}(0)$ . Then the equilibrium solution for (31) is constant inside  $B_{R_0}(0) \setminus B_{R_1}(\eta)$  and is zero outside.



• Unlike the N+0 problem, the relative equilibrium for the N+1 problem is non-unique: any choice of  $\eta$  yields a steady state as long as  $|\eta| < R_0 - R_1$ .

#### **Degenerate case: big central vortex**



- Small vortices are constrained to a ring of radius  $R_0$ . with big vortex at the center.
- Non-uniform distribution of small particles!
- Question: Determine the size of the gap  $\Theta_{gap}$ .

#### • Main Result:

$$\Theta_{gap} \sim C N^{-1/3}.$$

where the constant C=8.244 satisfies

$$(8 - 6u + 2u^3) \ln(u - 1) = 3u(u^2 - 4); \quad C = 2\left(\frac{6\pi(2 - u)}{u(u^2 - 1)}\right)^{1/3}$$



#### **Sketch of proof**

• [Barry+Wayne, 2012]: Set  $x_j(t) \sim R_0 e^{i \theta_j(t)}$  then at leading order we get

$$\frac{d\theta_j}{dt} = \frac{1}{N} \sum_{k \neq j} \left( \frac{\sin\left(\theta_j - \theta_k\right)}{2 - 2\cos\left(\theta_j - \theta_k\right)} - \sin\left(\theta_j - \theta_k\right) \right).$$
(32)

• In the mean-field limit  $N \to \infty$ , the density distribution  $\rho(\theta)$  for the angles  $\theta_j$  satisfies

$$\begin{cases} \rho_t + (\rho v_\theta)_\theta = 0, \\ v(\theta) = PV \int_{-\pi}^{\pi} \rho\left(\phi\right) \left(\frac{\sin\left(\theta - \phi\right)}{2 - 2\cos\left(\theta - \phi\right)} - \sin\left(\theta - \phi\right)\right) d\phi, \end{cases} (33)$$

where PV denotes the principal value integral, and  $\int_{-\pi}^{\pi} \rho = 1$ .

• [Barry, PhD Thesis]: Up to rotations, the steady state density  $\rho(\theta)$  for which v=0 must be of the form

$$\rho(\theta) = \frac{1}{2\pi} \left( 1 + \alpha \cos \theta \right).$$
(34)

This follows from (33) and (formal) expansion

$$\frac{\sin t}{2 - 2\cos t} - \sin t = \sin(2t) + \sin(3t) + \sin(4t) + \dots$$

- $\alpha$  is free parameter in the continuum limit.
- For discrete N, particle positions satisfy



To estimate  $\Phi_{gap}$ , choose  $\theta_1$  so that  $v(\theta_1) \sim 0$ . See our paper for hairy details.

#### N + K problem



Main result: Let  $R_k = \sqrt{b_k}$ ,  $k = 1 \dots K$  and  $R_0 = \sqrt{a + b_1 + \dots + b_K}$ . Suppose  $\eta_1 \dots \eta_K$  are such  $B_{R_1}(\eta_1) \dots B_{R_K}(\eta_K)$  are all disjoint and are contained inside  $B_{R_0}(0)$ . The equilibrium density is constant inside  $B_{R_0}(0) \setminus \bigcup_{k=1}^K B_{R_k}(\eta_k)$  and is zero outside.

#### N+K problem, with very large K vortices



• The *blue ellipse* is described by the reduced system

$$\frac{d\xi_j}{dt} = \frac{1}{N} \sum_{\substack{k=1\dots N\\k\neq j}} \frac{1}{\overline{\xi_j - \xi_k}} + \frac{1}{2}\overline{\xi_k} - \xi_k$$

(35)

• From [K, Huang, Fetecau, 20011], its axis ratio is 3.