Dynamics of particles on a curve with pairwise hyper-singular repulsion

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The particle dynamics

- Given a smooth, closed, non-self-intersecting curve

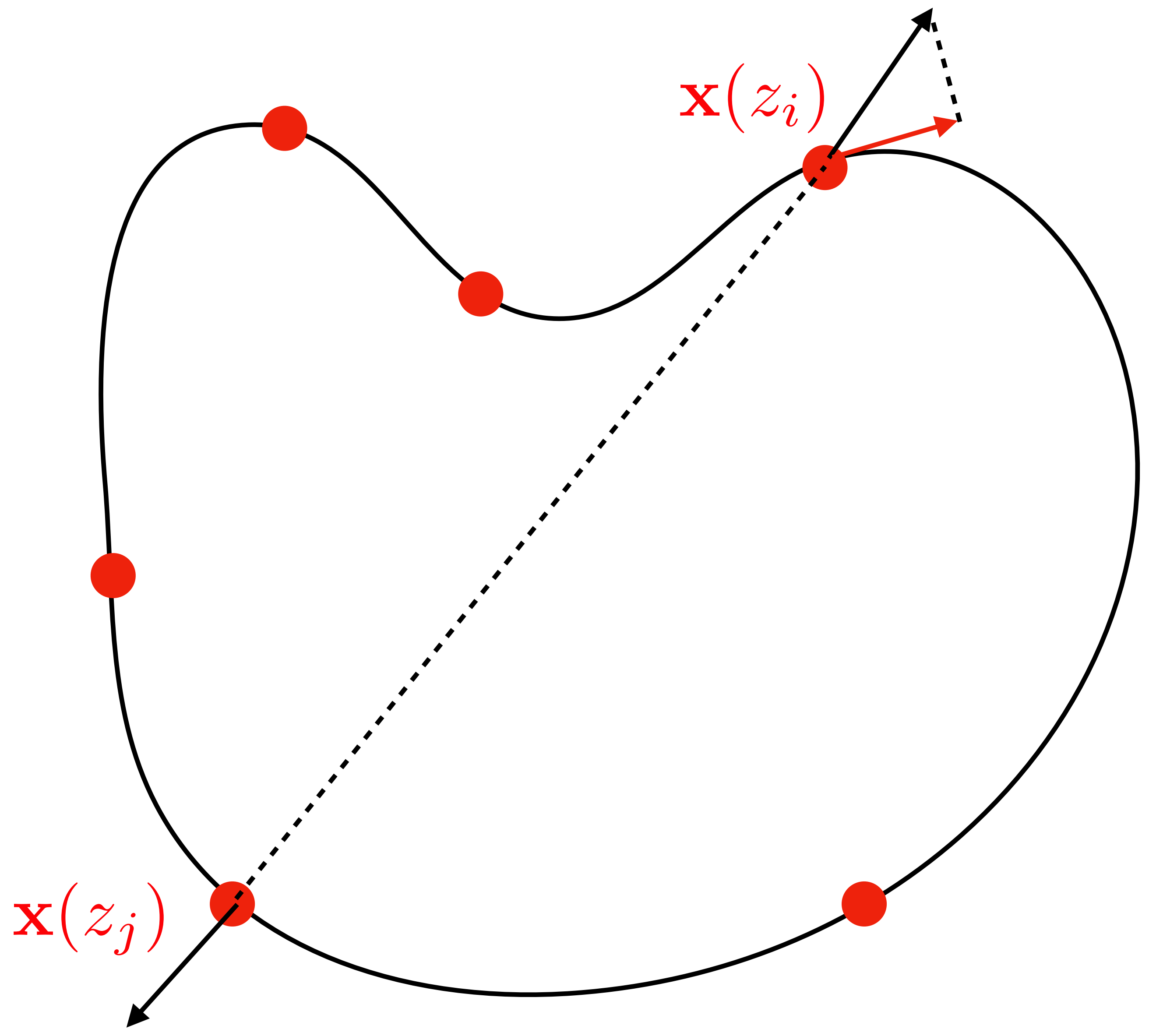
  $$\mathbf{x}(z) : \mathbb{R} \to \mathbb{R}^d \qquad \mathbf{x}(z+1) = \mathbf{x}(z) \qquad |\mathbf{x}'(z)| = 1$$

- $\{\mathbf{x}(z_i)\}_{i=1}^N \quad z_i = z_i(t)$: N moving particles on the curve

- The particle dynamics

  $$\dot{z}_i = -N^{-s} \sum_{j \neq i} \nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i)$$

- Repulsion potential (Riesz type) $W(\mathbf{x}) = W(|\mathbf{x}|) = \frac{|\mathbf{x}|^{-s}}{s}$



$s > 1$ hyper-singular

The total energy

- The total energy $$E = E(\mathbf{Z}) := N^{-s-1} \sum_{1 \leqslant i < j \leqslant N} W(\mathbf{x}(z_i) - \mathbf{x}(z_j))$$
- Gradient flow structure $$\dot{\mathbf{Z}} = -N \nabla E(\mathbf{Z})$$ $$\mathbf{Z} = (z_1, z_2, \ldots, z_N)$$
- Energy dissipation law $$\dot{E} = \nabla E(\mathbf{Z}) \cdot \dot{\mathbf{Z}} = -\frac{1}{N} \sum_i |\dot{z}_i|^2$$
- Expected large time behavior: convergence to a local energy minimizer

The total energy

$$E = E(\mathbf{Z}) := N^{-s-1} \sum_{1 \leqslant i < j \leqslant N} W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \qquad W(\mathbf{x}) = W(|\mathbf{x}|) = \frac{|\mathbf{x}|^{-s}}{s}$$

integrable — 1 — hyper-singular → s

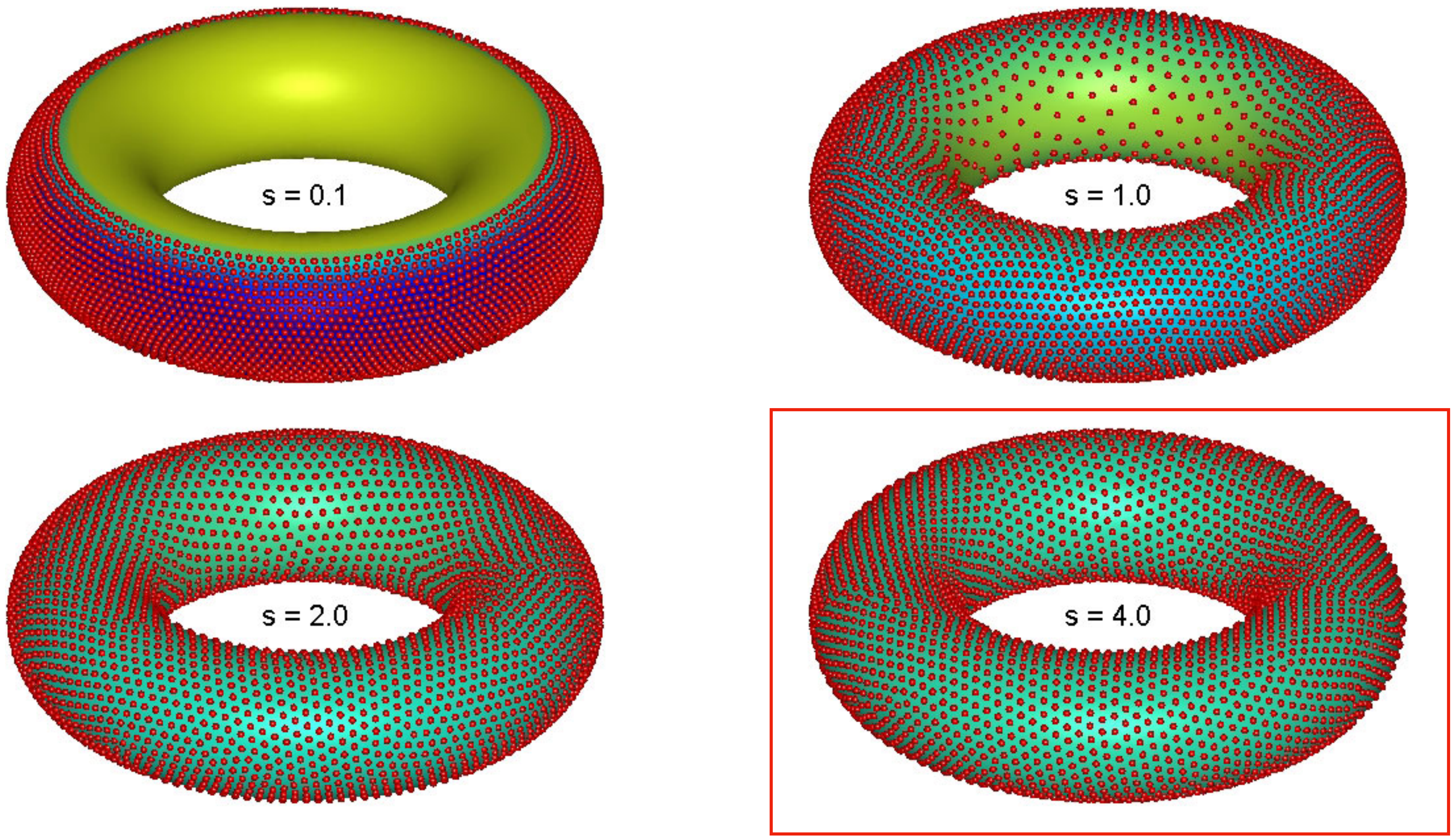
has a formal continuum limit:

$$E[\rho] = \int_{\mathbb{T}} \int_{\mathbb{T}} W(\mathbf{x}(z) - \mathbf{x}(y))\rho(y)\mathrm{d}y\rho(z)\mathrm{d}z$$

What should be expected for large N?

Previous results: energy minimizers

- The “Poppy-seed Bagel Theorem” (Hardin-Saff 05’, Borodachov 12’): For hyper-singular Riesz energy of an m-dimensional rectifiable set, the global energy minimizer is almost a uniform distribution, when N is large.



manifold dimension m = 2

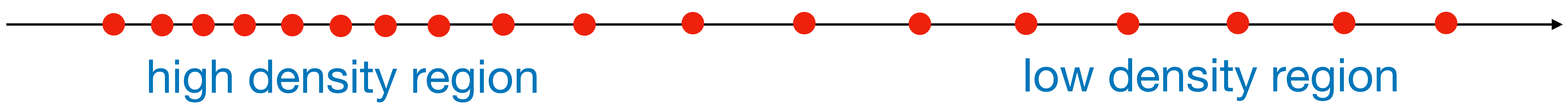
hyper-singular $s > m$

Previous results: mean-field limit

$$\dot{z}_i = -N^{-s} \sum_{j \neq i} \nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i) \qquad W(\mathbf{x}) = W(|\mathbf{x}|) = \frac{|\mathbf{x}|^{-s}}{s}$$

- In the hyper-singular case, the interaction becomes essentially local when N is large
- As $N \to \infty$, one can describe the particles by a particle density function $\rho(t, z)$
- The mean-field limit (Oelschlager 90'): on the real line, $\rho(t, z)$ solves the porous medium equation

$$\partial_t \rho = \zeta(s) \partial_{zz}(\rho^{s+1})$$



- When N is large, the strong local repulsion enforces the particles to be locally uniformly distributed, according to some macroscopic density $\rho(z)$

- For an interval I with length δ

$$N^{-s-1}\sum_{z_i\in I}\sum_{j\neq i}\frac{|z_i-z_j|^{-s}}{s}\approx N^{-s-1}(\delta N\rho)\cdot\sum_{j\in\mathbb{Z},j\neq 0}\frac{|j/(N\rho)|^{-s}}{s}=2\tilde{\zeta}(s)\rho^{s+1}\delta.$$

- Therefore $E(\mathbf{Z})\approx\tilde{\zeta}(s)\int\rho^{s+1}\,\mathrm{d}z.$

$$\zeta(s):=\sum_{i=1}^{\infty}i^{-s},\quad \tilde{\zeta}(s):=\frac{\zeta(s)}{s}$$

- As the gradient flow of this energy, one gets the porous medium equation

Our result

$$\zeta(s) := \sum_{i=1}^{\infty} i^{-s}, \quad \tilde{\zeta}(s) := \frac{\zeta(s)}{s}$$

$$\dot{z}_i = -N^{-s} \sum_{j \neq i} \nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i)$$

- **Theorem** (Hardin-Saff-S.-Tadmor 20'): For any $\epsilon > 0$, there exists N_0 depending on ϵ, s and the curve, such that the following holds for $N > N_0$:

Energy almost converges to the minimal energy

$$E(t) \leqslant \tilde{\zeta}(s)(1+\epsilon), \quad \forall t \geqslant \frac{C}{\epsilon}$$

gives a convergence rate like O(1/t) independent of N!

- Also, for $a \in \mathbb{R}$ and $0 < L < 1$

Particles almost converge to the uniform distribution

$$\left| \frac{\#\{i : [z_i, z_{i+1}) \subset [a, a+L)\}}{N} - L \right| \leqslant \left[L(1-L)\tilde{\zeta}(s) \right]^{1/2} (2\epsilon)^{1/2}$$

Main difficulties

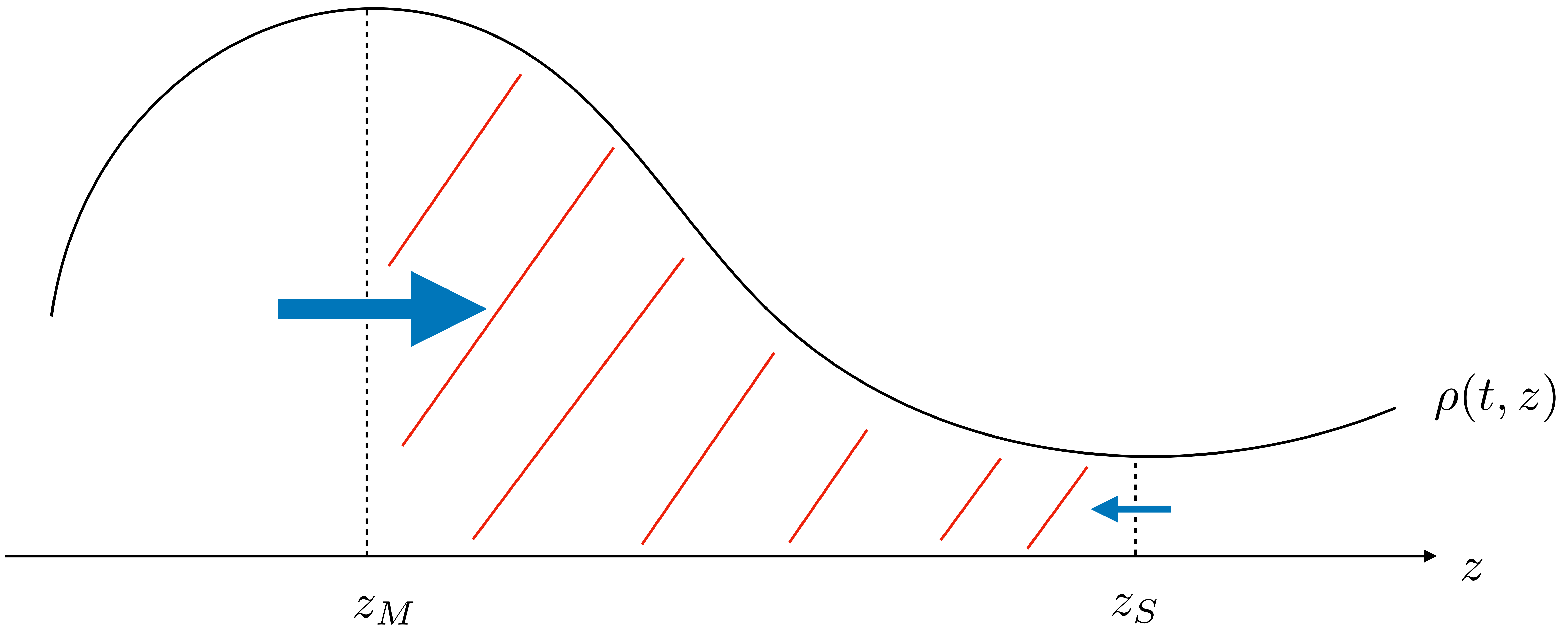
- The gradient flow could be trapped into local energy minimizers / saddles
- Mean-field limits cannot be applied because they are finite-time results: the error often grows exponentially in time
- When the curve is complicated, W restricted on the curve may lose convexity

Strategy of proof

- The interaction should be essentially local. Control the error from the “curvature effects”.
- Find intuitions from the mean-field limit, and seek for analogues for particles
    - The total momentum of an interval of mass
    - Maximum principle

$$\partial_t \rho = \zeta(s)\partial_{zz}(\rho^{s+1}) \qquad \partial_{zz}(\rho^{s+1}) = \frac{s+1}{s}\partial_z(\rho \underline{\partial_z(\rho^s)})$$

transport velocity



total momentum = $\displaystyle\int_{z_M}^{z_S} \left(-\frac{s+1}{s}\zeta(s)\partial_z(\rho^s)\right)\cdot \rho(t,z)\,\mathrm{d}z = \zeta(s)\left(\underline{\rho(t,z_M)^{s+1}} - \underline{\rho(t,z_S)^{s+1}}\right) > 0$

lead to energy dissipation

$$\int_{z_M}^{z_S} \left(-\frac{s+1}{s}\zeta(s)\partial_z(\rho^s)\right)\cdot\rho(t,z)\,\mathrm{d}z = \zeta(s)(\rho(t,z_M)^{s+1} - \rho(t,z_S)^{s+1}) > 0$$

- Lower bound on energy dissipation rate:

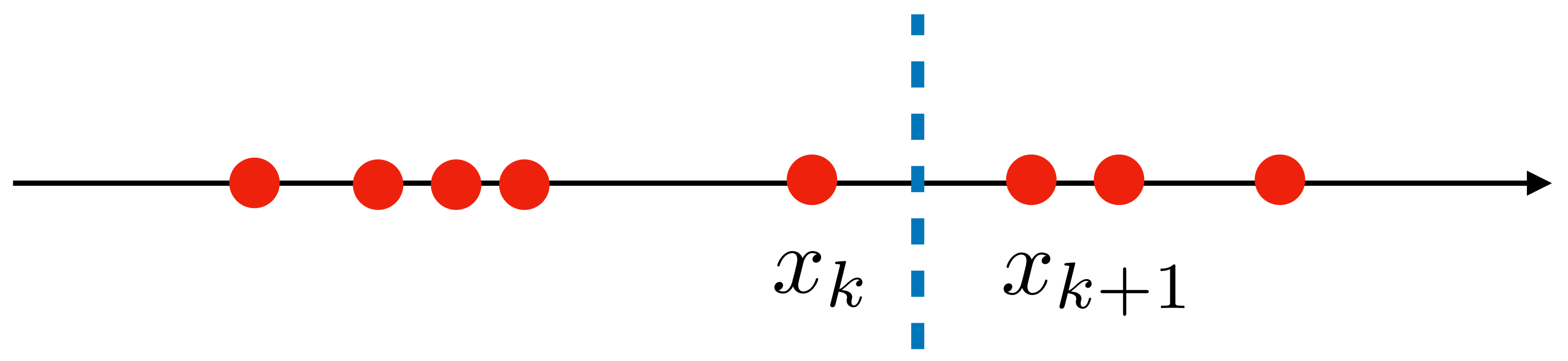
$$\frac{\mathrm{d}}{\mathrm{d}t}\int \rho^{s+1}\,\mathrm{d}z = -\frac{s+1}{s}\zeta(s)\int |\partial_z(\rho^s)|^2\rho\,\mathrm{d}z \quad \leqslant -\frac{s+1}{s}\zeta(s)\cdot\frac{\left(\int(-\partial_z(\rho^s))\rho\,\mathrm{d}z\right)^2}{\int\rho\,\mathrm{d}z}.$$

- Then $\rho(t,z_M)$ cannot be large for all time

- Maximum principle: once $\rho(t,z_M)$ gets small, it cannot become large again

Part 1: “total repulsion cut”

- Consider points $x_0 < \cdots < x_N \in \mathbb{R}$



- The total repulsion at the cut x_k, x_{k+1}

$$P_k = P_k(x_0, \ldots, x_N) := \sum_{i,j:\, 0 \leqslant i \leqslant k < j \leqslant N} (x_j - x_i)^{-s-1}$$

- **Lemma**: For any $\epsilon > 0$, if N is large, then for any $0 = x_0 < \cdots < x_N = 1$ there exists an index i_S such that $(x_{i_S}, x_{i_S+1}) \bigcap (\epsilon_1, 1 - \epsilon_1) \neq \emptyset$

$$P_{i_S} \leqslant (1+\epsilon)\underline{\zeta(s)N^{s+1}}$$

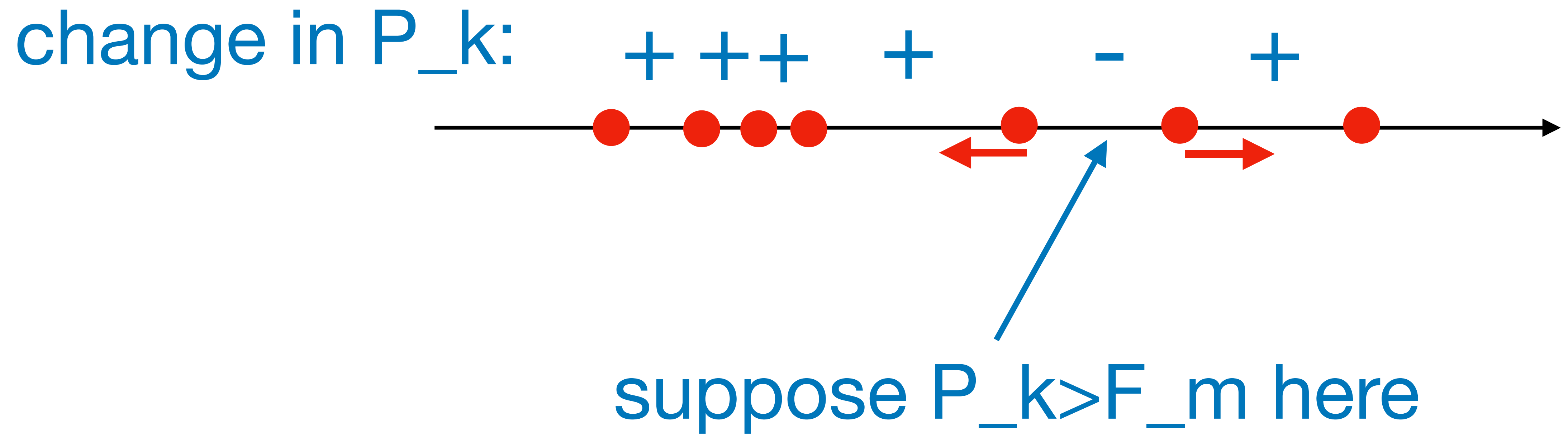
exactly the total repulsion
for uniformly distributed particles

A min-max argument

$$F_m(x_{i_L+1}, \ldots, x_{i_R-1}) := \min_{i_L \leqslant k \leqslant i_R-1} P_k \qquad \mathcal{E}(x_{i_L+1}, \ldots, x_{i_R-1}) := \sum_{i,j:\, 0 \leqslant i < j \leqslant N} (x_j - x_i)^{-s}$$

- The unique maximum of F_m is achieved at the same point as the unique minimum of $\mathcal{E}$, characterized by

$$P_{i_L} = \cdots = P_{i_R-1}$$



$\mathcal{E}$ is convex

-> unique minimum at $\nabla \mathcal{E} = 0$

Part 2: analogue of maximum principle

$$\delta(t) := \min_{1\leqslant i\leqslant N}(z_{i+1}(t) - z_i(t)), \quad \rho_M(t) := \frac{1}{N\delta(t)}$$

- Closest pairwise distance: an analogue of the maximal density

- **Lemma**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\delta \geqslant -C\underline{N^{-s}N_*\delta^{-s+2}}, \quad N_* := \begin{cases} 1, & s > 2; \\ \log N, & s = 2; \\ N^{-s+2}, & 1 < s < 2 \end{cases}$$

very small quantity

- This almost says that the “maximal density” never increases

- **Lemma**: when N is large, if $\frac{\mathrm{d}}{\mathrm{d}t}\delta \leqslant 1$ then

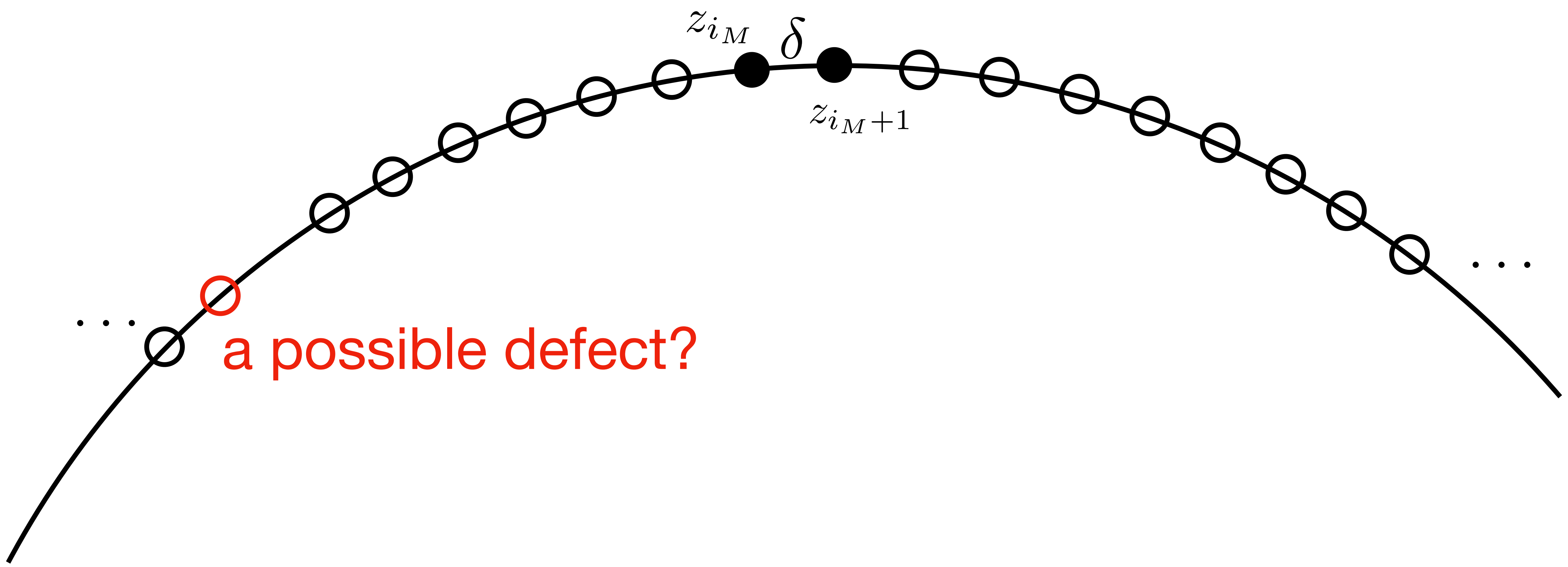
$$\sum_{i=i_L}^{i_M} \sum_{j=i_M+1}^{i_R} |z_i - z_j|^{-s-1} \geqslant \zeta(s)\delta^{-s-1}(1-\epsilon) \qquad i_M := \mathrm{argmin}_i(z_{i+1} - z_i)$$

- If "maximal density" is not decreasing very fast, then Lemma says that the "total repulsion" at the maximal density point is as large as the continuum case.

- If "maximal density" is decreasing very fast, then it helps us: it cannot go back to large values.

Proof of the lemmas

- The best possible way of keeping δ not increasing is to pack particles near i_M as dense as possible
- In this case, one recovers the continuum case, and one can compute the "total repulsion" like a uniform distribution
- Otherwise, if there is a defect, then delta has to decrease very fast



Handling the “curvature effect”

- **Lemma**: For y, z being close enough,

$$|\underbrace{\nabla W(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)}_{\text{forcing from z to y}}-\underbrace{W'(y-z)}_{\text{as the real line}}(1+\underbrace{\kappa(y)|y-z|^2}_{\text{with curvature effect}})|\leqslant C_R|y-z|^{-s+2}$$

$$\kappa(z):=\frac{s-2}{24}|\mathbf{x}''(z)|^2$$

$$\Big|\Big(\nabla W(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)-W'(y-z)(1+\kappa(y)|y-z|^2)\Big)$$
$$-\Big(\nabla W(\mathbf{x}(\tilde{y})-\mathbf{x}(z))\cdot\mathbf{x}'(\tilde{y})-W'(\tilde{y}-z)(1+\kappa(y)|\tilde{y}-z|^2)\Big)\Big|$$
$$\leqslant C_R\min\{d(y,z),d(\tilde{y},z)\}^{-s+1}\cdot|y-\tilde{y}|$$

- Proof by Taylor expansions…

Proof of main result

- When the "maximal density" is not decreasing too fast, we have

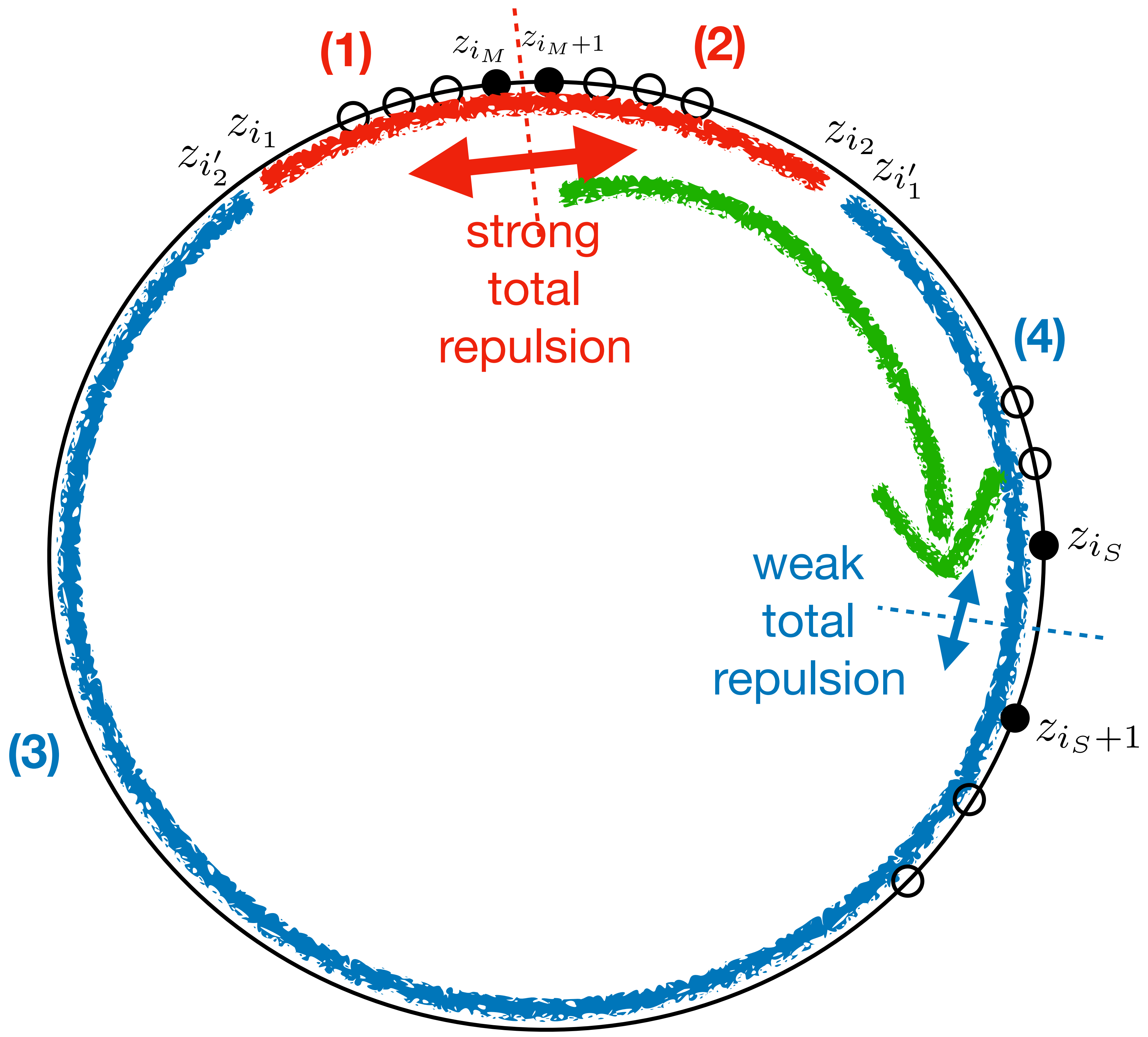
$$\sum_{i_M+1\le i\le i_S} \dot{z}_i \ge c(\rho_M - 1 - \epsilon)_{\ge 0} \cdot N$$

- This provides energy dissipation

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) \leqslant -c^2((\rho_M - 1 - \epsilon)_{\geqslant 0})^2$$

- Use Lemma: $E(\mathbf{Z}) \leqslant \tilde{\zeta}(s)(1+\epsilon)\rho_M^s$ to close the estimate

- Construct Lyapunov functional for exceptional cases (maximal density decrease fast)



Energy convergence implies uniform distribution

- **Theorem:** $E(\mathbf{Z}) \leqslant \tilde{\zeta}(s)(1+\epsilon)$ implies

$$\left| \frac{\#\{i : [z_i, z_{i+1}) \subset [a, a+L)\}}{N} - L \right| \leqslant \left[L(1-L)\tilde{\zeta}(s) \right]^{1/2} (2\epsilon)^{1/2}$$

- Introduce $E^k(\mathbf{Z}) := \frac{1}{sN^{s+1}} \sum_{i=1}^{N} |\mathbf{x}(z_{i+k}) - \mathbf{x}(z_i)|^{-s}$

$$E = E(\mathbf{Z}) := \frac{1}{sN^{s+1}} \sum_{1 \leqslant i < j \leqslant N}^{N} |\mathbf{x}(z_j) - \mathbf{x}(z_i)|^{-s} = \frac{1}{2} \sum_{k=1}^{N-1} E^k(\mathbf{Z})$$

$$\tilde{E}^k(\mathbf{Z}) := \frac{1}{sN^{s+1}} \sum_{i=1}^{N} (z_{i+k} - z_i)^{-s} \qquad \tilde{E}(\mathbf{Z}) \leqslant E(\mathbf{Z})$$

- **Lemma:** $s^{-1}k^{-s} \leqslant \tilde{E}^k(\mathbf{Z})$ $\quad\quad$ $\tilde{E}^1(\mathbf{Z}) + s^{-1}(\zeta(s;N) - 1) \leqslant \tilde{E}(\mathbf{Z})$
- Therefore $s\tilde{E}^1(\mathbf{Z}) \leqslant 1 + \boxed{\zeta(s;N)\epsilon}.$
- Write $\tilde{E}^1(\mathbf{Z}) = \frac{1}{N^{s+1}} \sum_i W(d_i), \quad W(x) := \frac{x^{-s}}{s}.$ $\quad\quad$ $d_i = z_{i+1} - z_i$
- Taylor expansion of W at 1/N:

$$s\tilde{E}^1(\mathbf{Z}) = 1 + \boxed{\frac{1}{2} \cdot \frac{s}{N^{s+1}} \sum_i W''(\xi_i)(d_i - \frac{1}{N})^2}$$

- Use convexity of W to obtain smallness of $d_i - \frac{1}{N}$

Future work

- Exponential convergence rate?
- Uniform-in-time mean field limit?
- Convergence to local equilibrium (local uniform distribution) in very short time?
- Extension to multi-dimensions?