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DYNAMICS OF PARTICLES ON A CURVE WITH PAIRWISE HYPER-SINGULAR REPULSION

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Abstract. We investigate the large time behavior of N particles restricted to a smooth closed curve in $\mathbb{R}^d$ and subject to a gradient flow with respect to Euclidean hyper-singular repulsive Riesz s-energy with $s > 1$. We show that regardless of their initial positions, for all N and time t large, their normalized Riesz s-energy will be close to the N-point minimal possible energy. Furthermore, the distribution of such particles will be close to uniform with respect to arclength measure along the curve.

1. Introduction.

In this paper we consider the first-order N-particle model

$$\dot{z}_i = -N^{-s} \sum_{j \neq i} \nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i), \tag{1.1}$$

where the particles are interacting through the potential

$$W(\mathbf{x}) = W(|\mathbf{x}|) = \frac{|\mathbf{x}|^{-s}}{s}, \tag{1.2}$$

which is a power-law repulsion potential, assumed to be *hyper-singular*: $s > 1$. Here $\mathbf{x} : \mathbb{R} \to \mathbb{R}^d$ is a unit-length, smooth, closed, non-self-intersecting curve with 1-periodic arc-length parametrization; i.e., $|\mathbf{x}'(z)| = 1$ and $\mathbf{x}(z+1) = \mathbf{x}(z)$ for all $z \in \mathbb{R}$. The N-particle configuration $\{\mathbf{x}(z_i)\}_{i=1}^N$ is represented by the parameters

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$\mathbf{Z} = (z_1, z_2, \ldots, z_N)$, where $z_i = z_i(t)$ are real-valued functions of the time $t \in \mathbb{R}_{\geqslant 0}$ for $i = 1, 2, \ldots, N$. The system (1.1) can be rewritten as a gradient flow of the form

$$\dot{\mathbf{Z}} = -N\nabla E(\mathbf{Z}), \tag{1.3}$$

for the energy

$$E = E(\mathbf{Z}) := N^{-s-1} \sum_{1\leqslant i<j\leqslant N} W(\mathbf{x}(z_i) - \mathbf{x}(z_j)), \tag{1.4}$$

which satisfies the energy dissipation

$$\dot{E} = \nabla E(\mathbf{Z}) \cdot \dot{\mathbf{Z}} = -\frac{1}{N}\sum_i |\dot{z}_i|^2. \tag{1.5}$$

Without loss of generality, we assume that an N-point configuration parametrization $\mathbf{Z} = (z_1, z_2, \ldots, z_N)$ is ordered as

$$z_1 < \cdots < z_N < z_1 + 1, \tag{1.6}$$

and observe that if the initial data (at $t = 0$) satisfies (1.6), then (1.6) holds for all time due to the singularity of the interaction potential W at 0 and the fact that the total energy is non-increasing, by (1.5). As a consequence, the ODE system (1.1) is globally wellposed. Consistent with the periodicity of $\mathbf{x}$, we extend z_i to all $i \in \mathbb{Z}$ by setting $z_{i+N} = z_i + 1$ so that $\mathbf{x}(z_{i+N}) = \mathbf{x}(z_i)$.

The determination of optimal N-point configurations confined to a curve or more generally a manifold, whose pairwise interactions are governed by the Riesz s-potential W in (1.2) is sometimes referred to when the manifold is the unit sphere $S^d \subset \mathbb{R}^d$ and $s > 0$, as the "generalized Thomson problem." Determining the minimal energy positions for such points explicitly is a notoriously difficult problem for which only some very special cases are known, even for "small" values of N (see [3], [2]). One of these cases is that of the unit circle in $\mathbb{R}^2$, for which a simple convexity argument shows that N distinct equally spaced points (N-th roots of unity) are the unique (up to rotation) N-point configurations that minimize the energy for all $s > 0$ and all $N \geqslant 2$. There are, however, several well-known theorems that deal with the asymptotics as $N \to \infty$ for optimal configurations on manifolds in Euclidean space. For curves in $\mathbb{R}^d$ in the hyper-singular case $s > 1$, the following theorem was proved by Martinez-Finkelstein et. al. in [5].

Theorem 1.1. *If $s > 1$ and Γ is a rectifiable Jordan arc or closed curve embedded in $\mathbb{R}^d$ of length one with arc length parametrization $\mathbf{x}(s)$, then*

$$\lim_{N\to\infty} \min E(\mathbf{Z}) = \zeta(s)/s,$$

where the minimum is taken over all N-point configurations $\{\mathbf{x}(z_i)\}_{i=1}^N$ on Γ and $\zeta(s)$ is the classical Riemann zeta function. Moreover, N-point minimizing configurations $\{\mathbf{x}(z_i^*)\}_{i=1}^N$ are asymptotically uniformly distributed with respect to arc length and, with $d_i^* := z_{i+1}^* - z_i^*$, satisfy

$$\sum_{i=1}^N \left| d_i^* - \frac{1}{N} \right| \to 0 \ \ as \ \ N \to \infty. \tag{1.7}$$

This theorem together with its refinement [1], which is one of the main motivations for the present work, is a special case of the so-called *Poppy-seed bagel theorem* (see [2] and [4]) which applies to general d-rectifiable manifolds embedded in $\mathbb{R}^p$, $d \leqslant p$.

As stated in Theorem 1.1, any minimizer of the energy E defined in (1.4) has to be almost uniformly distributed. This paper studies the large time behavior of (1.1); namely, whether $\{z_i(t)\}_{i\in\mathbb{Z}}$ are "close to equally spaced" as $t \to \infty$.

2. Main results.

We will use the following quantities depending on s:

$$\zeta(s) := \sum_{i=1}^{\infty} i^{-s}, \quad \tilde{\zeta}(s) := \frac{\zeta(s)}{s}. \tag{2.1}$$

Every constant C or c appearing in this paper depends only on s and the curve $\mathbf{x}(z)$, if not stated otherwise.

2.1. Statement of main results.

Our first main result is the following.

Theorem 2.1. *Let $\mathbf{x}(z)$ be a non-self-intersecting C^4 closed curve, and let $s > 1$. For any $\epsilon > 0$, there exists N_0, depending on ϵ, s and the curve $\mathbf{x}(z)$, such that the following holds for $N > N_0$: for the solution to (1.1) with distinct initial data (see 1.6), there exists a positive constant C such that*

$$E(t) \leqslant \tilde{\zeta}(s)(1+\epsilon), \quad \forall t \geqslant \frac{C}{\epsilon}. \tag{2.2}$$

This theorem quantifies the convergence rate of the solution to (1.1) to an almost minimal energy state. In fact, since Lemma 4.3 shows that the global minimum of E is at least $\tilde{\zeta}(s)(1-\epsilon)$, Theorem 2.1 shows that, after time $\mathcal{O}(1/\epsilon)$, the energy will decay to the global minimum up to an error of $\mathcal{O}(\epsilon)$. This can be viewed as an energy decay rate of $\mathcal{O}(1/t)$ being *independent of* the number of particles N, as long as N is large enough.

Our second main result shows that upper bounds on the energy of N-point configurations such as provided by Theorem 2.1 impose geometrical constraints on the distribution of these configurations showing that they are near optimal configurations.

Theorem 2.2. *For given $\epsilon > 0$ and $s > 1$, there is some N_0 depending on s and ϵ such that if $N > N_0$ and $\mathbf{Z} = \{z_i\}_{i=1}^N$ satisfies*

$$E(\mathbf{Z}) \leqslant \tilde{\zeta}(s)(1+\epsilon), \tag{2.3}$$

then the mean absolute deviation of $d_i = z_{i+1} - z_i$, $i = 1, 2, \ldots, N$, satisfies

$$\frac{1}{N}\sum_{i=1}^{N} \left| d_i - \frac{1}{N} \right| \leqslant 2\left(\frac{2\tilde{\zeta}(s)}{s+1}\right)^{1/2} \frac{\epsilon^{1/2}}{N}, \tag{2.4}$$

and for all $a \in \mathbb{R}$ and $0 < L < 1$, we have

$$\left| \frac{\#\{i : [z_i, z_{i+1}) \subset [a, a+L)\}}{N} - L \right| \leqslant \Big[L(1-L)\tilde{\zeta}(s)\Big]^{1/2} (2\epsilon)^{1/2}. \tag{2.5}$$

Consequently, under the assumptions of Theorem 2.1, the conclusions (2.4) and (2.5) hold for N sufficiently large and $t \geqslant C/\epsilon$.

The proof of Theorem 2.1 is given in Sections 3-6. Below we discuss the motivation for the argument used in its proof. The proof of Theorem 2.2 is given in Section 7.

2.2. **Outline of the proof of Theorem 2.1.** It is known that the global minimizer of E defined in (1.4) converges to the uniform distribution as $N \to \infty$; therefore it is natural to expect that, for large N, the gradient flow (1.1) converges to some limiting configuration which is nearly equally distributed. However, we encounter the following difficulties:

- When the curve $\mathbf{x}(z)$ is not convex, the energy E is not necessarily a convex function of $\{z_i\}$.
- The global minimizer of E may not be unique, and there may be local minimizers and saddle points.

To handle these difficulties, we manage to extract some ideas from the mean field limit of (1.1). For a general recent treatment of integrable ($s < 1$ for curves) Riesz interactions through their interplay with the mean-field limit, we refer to [7]. In fact, it is proved in [6] that the analog of (1.1) on the real line has the porous medium equation

$$\partial_t \rho = \zeta(s)\partial_{zz}(\rho^{s+1}) \tag{2.6}$$

as its mean field limit, under certain assumptions on the initial data. This mean field limit can be understood intuitively as follows:

- Due to the fast decay of $W(\mathbf{x})$ for large $|\mathbf{x}|$, the particle interaction is *localized* when N is large, meaning that typically the interaction between particles with large distances can be neglected, at least for a fixed time interval $[0, T]$. The same holds for the curvature effect, i.e., the difference between (1.1) and its analog on the real line.
- Due to the strong localized repulsion, particles tend to distribute *locally* in a uniform way, similar to the local equilibrium in kinetic theory. This means, in a short interval I of length δ (which is still long enough to contain a large number of particles), the particles are approximately uniformly distributed. However, the particle density may still have variation on a macroscopic scale, according to some density profile $\rho(t, z)$.

  Since our current approach is based on the time evolution of the total energy which is a global quantity, we do not expect it to capture delicate local structure required for the mean field limit. A possible future direction to address this issue is to analyze the time evolution of the functions $E^k(\mathbf{Z})$ that takes into account only the distances between points whose indices differ by k , see Section 7.
- In a short interval I of length δ, if the particles inside are uniformly distributed with density ρ (i.e., the distance between adjacent particles is approximately $1/(N\rho)$, and the total number of particles inside is approximately $\delta N\rho$), then the total energy of the particles inside is approximately

$$N^{-s-1} \sum_{z_i \in I} \sum_{j \neq i} \frac{|z_i - z_j|^{-s}}{s} \approx N^{-s-1}(\delta N\rho) \cdot \sum_{j \in \mathbb{Z}, j \neq 0} \frac{|j/(N\rho)|^{-s}}{s} = 2\tilde{\zeta}(s)\rho^{s+1}\delta. \tag{2.7}$$

  Summing all the short intervals (and symmetrizing in i and j), this gives a Riemann sum which approximates

$$E(\mathbf{Z}) \approx \tilde{\zeta}(s) \int \rho^{s+1} \, \mathrm{d}z. \tag{2.8}$$

  Then notice that (1.1) is the gradient flow of E, while (2.6) is exactly the Wasserstein-2 gradient flow of the above right-hand side [RHS].

Although mean field limits are generally not true on the whole time axis $[0,\infty)$, we can indeed get some ideas from the energy structure of (2.6). To motivate the proof of Theorem 2.1, we start from the following two properties of the porous medium equation (2.6):

- Suppose at time t, there are two points z_M and z_S such that $\rho(t,z_M) > \rho(t,z_S)$ (assuming $z_M < z_S$ without loss of generality). Then

$$\int_{z_M}^{z_S} \Big(-\frac{s+1}{s}\zeta(s)\partial_z(\rho^s)\Big)\cdot \rho(t,z)\,\mathrm{d}z = \zeta(s)(\rho(t,z_M)^{s+1} - \rho(t,z_S)^{s+1}) > 0, \quad (2.9)$$

  where the term $-\frac{s+1}{s}\zeta(s)\partial_z(\rho^s)$ is the transport velocity of the porous medium equation, by writing $\partial_{zz}(\rho^{s+1}) = \frac{s+1}{s}\partial_z(\rho\partial_z(\rho^s))$. This means that we have a lower bound on the energy dissipation rate:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\int \rho^{s+1}\,\mathrm{d}z &= -\frac{s+1}{s}\zeta(s)\int |\partial_z(\rho^s)|^2\rho\,\mathrm{d}z \\ &\leqslant -\frac{s+1}{s}\zeta(s)\cdot\frac{\big(\int(-\partial_z(\rho^s))\rho\,\mathrm{d}z\big)^2}{\int\rho\,\mathrm{d}z}. \end{aligned} \quad (2.10)$$

  Since the total amount of energy is finite, $|\rho(t,z_M)-\rho(t,z_S)|$ will eventually get small after a long time. In particular, for some large T, $\sup_z \rho(T,z)$ will get close to the average density $\int\rho\,\mathrm{d}z/\int\,\mathrm{d}z$.
- The porous medium equation (2.6) obeys the maximum principle:

$$\sup_z \rho(t,z) \text{ is decreasing in } t. \quad (2.11)$$

  This means that, once $\sup_z \rho(T,z)$ gets close to the average density, it cannot become large again, which means $\rho(t,z)$ will be close to a uniform distribution for all $t \geqslant T$.

To prove Theorem 2.1, we aim to find the analogues of the above two properties for (1.1):

- In the case of a flat $\mathbb{T}$, we prove Lemma 3.1 as the counterpart of the first property. It says, once we have an interval in which the 'density' (number of particles divided by interval length) is small, then we can find a place to cut the interval, such that the total repulsion force between left and right is small. This concept of 'total repulsion force' is the counterpart of the term $\rho(t,z_S)^{s+1}$ in (2.9).
- We establish Lemma 5.2 as the counterpart of the second property. It says that the distance δ between the closest pair of particles basically cannot decrease (see (5.1), whose RHS is $o(1)$), in correspondence to the decreasing property. In fact, the quantity $\rho_M(t) := 1/(N\delta(t))$, as defined in (4.1), is a discrete analogue of $\rho(t,z_M)$. Furthermore, for reasonable situations, we have the lower bound (5.12) for the 'total repulsion force' at this closest pair of particles, serving as the counterpart of the term $\rho(t,z_M)^{s+1}$ in (2.9).

Finally, we have to deal with the finite-N effect and the curvature effect from $\mathbf{x}(z)$, which may produce errors to the above two properties. Therefore, we need to keep track of the N-dependence of error terms, as well as using the smoothness of curve $\mathbf{x}(z)$, to show that all such error terms are small enough.

3. **Lemmas on total repulsion cut.** For a given set of points $x_0 < \cdots < x_N \in \mathbb{R}$, we define the *total repulsion* of the *cut* at x_k, x_{k+1} by

$$P_k = P_k(x_0, \ldots, x_N) := \sum_{i,j:\, 0 \leqslant i \leqslant k < j \leqslant N} (x_j - x_i)^{-s-1} \tag{3.1}$$

The main purpose of this section is to prove the following lemma:

Lemma 3.1. *For any $0 < \epsilon \leqslant 0.01$, there exists $N_0 = N_0(\epsilon)$ such that if $N > N_0$, then for any $0 = x_0 < \cdots < x_N = 1$ there exists an index i_S such that $(x_{i_S}, x_{i_S+1}) \bigcap (\epsilon_1, 1-\epsilon_1) \neq \emptyset$ with $\epsilon_1 = \frac{\epsilon}{3(1+s)}$, and*

$$P_{i_S} \leqslant (1+\epsilon)\zeta(s) N^{s+1}. \tag{3.2}$$

Notice that the total repulsion between two infinite sets of equally distributed points $\{\frac{i}{N}\}_{i=0}^\infty$ and $\{-\frac{j}{N}\}_{j=1}^\infty$ is

$$\sum_{i=0}^\infty \sum_{j=1}^\infty \Big(\frac{i+j}{N}\Big)^{-s-1} = N^{s+1} \sum_{i=1}^\infty i \cdot i^{-s-1} = \zeta(s) N^{s+1}. \tag{3.3}$$

Therefore, Lemma 3.1 tells us that one can find an index i_S such that the total repulsion for $k = i_S$ there is at most slightly more than for equally distributed points.

The proof of this lemma follows a min-max type argument. Let $0 \leqslant i_L < i_R \leqslant N$ be two indices. Define

$$F_m(x_{i_L+1}, \ldots, x_{i_R-1}) := \min_{i_L \leqslant k \leqslant i_R-1} P_k, \tag{3.4}$$

viewing those x_i's with $i \leqslant i_L$ or $i \geqslant i_R$ as fixed. F_m is defined on

$$\begin{aligned} &\mathbb{R}_{\text{sort}}^{i_R-i_L-1}(x_{i_L}, x_{i_R}) \\ &\quad = \{(x_{i_L+1}, \ldots, x_{i_R-1}) \in \mathbb{R}^{i_R-i_L-1} : x_{i_L} < x_{i_L+1} < \cdots < x_{i_R-1} < x_{i_R}\}, \end{aligned} \tag{3.5}$$

which is a convex open set.

In the following lemma we describe the global maximum of F_m as a function of $x_{i_L+1}, \ldots, x_{i_R-1}$.

Lemma 3.2. *The global maximum of F_m on $\mathbb{R}_{\text{sort}}^{i_R-i_L-1}(x_{i_L}, x_{i_R})$ is achieved at the same point $X^* = (x^*_{i_L+1}, \ldots, x^*_{i_R-1})$, which is the only point satisfying*

$$P_{i_L} = \cdots = P_{i_R-1}. \tag{3.6}$$

Furthermore, X^* is the unique global minimizer of the energy functional

$$\mathcal{E}(x_{i_L+1}, \ldots, x_{i_R-1}) := \sum_{i,j:\, 0 \leqslant i < j \leqslant N} (x_j - x_i)^{-s}, \tag{3.7}$$

and

$$F_m(X^*) = \frac{1}{x_{i_R} - x_{i_L}} \sum_{0 \leqslant i < j \leqslant N,\, i < i_R,\, j > i_L} (x^*_{\min\{j, i_R\}} - x^*_{\max\{i, i_L\}})(x^*_j - x^*_i)^{-s-1}, \tag{3.8}$$

with $x^*_i := x_i$ for $0 \leqslant i \leqslant i_L$ or $i_R \leqslant i \leqslant N$.

Notice that the RHS of (3.8) is exactly $\mathcal{E}(X^*)$ if $i_L = 0$, $i_R = N$.

Proof. **Step 1**: Show that the global maximum of F_m is achieved inside $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$.

In fact, one can extend the definition of F_m to the closure of $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$ by interpreting $(x_j - x_i)^{-s-1}$ as infinity when $x_j = x_i$, and F_m remains continuous. We show that the (global) maximum of F_m on the closure of $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$ is not achieved at boundary. In fact, at any boundary point, one has either $x_{k_1-1} < x_{k_1} = x_{k_1+1} = \cdots = x_{k_2} < x_{k_2+1}$ for some $i_L < k_1 < k_2 < i_R - 1$, or $x_{i_L} = x_{i_L+1}$, or $x_{i_R} = x_{i_R-1}$. We show that maximum is not achieved in the first case, and the other cases can be handled similarly.

In the first case, by replacing x_{k_1} and x_{k_2} by $x_{k_1} - \delta$ and $x_{k_2} + \delta$ respectively, with $\delta > 0$ small enough, we claim that F_m is decreased. First of all, P_k with $k_1 \leqslant k < k_2$ is much larger than F_m if δ is small, and thus the minimum in (3.4) is achieved elsewhere. For any j with $k_2 < j \leqslant i_R$,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\delta}\Big|_{\delta=0}&[(x_j - (x_{k_1} - \delta))^{-s-1} + (x_j - (x_{k_2} + \delta))^{-s-1}]\\ &=(-s-1)[(x_j - (x_{k_1} - \delta))^{-s-2} - (x_j - (x_{k_2} + \delta))^{-s-2}]|_{\delta=0} > 0,\end{aligned} \tag{3.9}$$

since $-s-1 < 0$ and $x_j - x_{k_1} > x_j - x_{k_2}$. Similarly for any j with $i_L \leqslant j < k_1$,

$$\frac{\mathrm{d}}{\mathrm{d}\delta}\Big|_{\delta=0}[((x_{k_1} - \delta) - x_j)^{-s-1} + ((x_{k_2} + \delta) - x_j)^{-s-1}] > 0. \tag{3.10}$$

This shows that for any k with $k_2 \leqslant k \leqslant i_R - 1$ or $i_L \leqslant k < k_1$, P_k is increased if $\delta > 0$ is small. Thus F_m is increased. By doing this $[(k_2 - k_1)/2]$ times, one reaches the interior of $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$ while making F_m increased.

Step 2: Show (3.6) for X^m, the global maximum of F_m.

From STEP 1, the maximum of F_m is achieved in the interior of $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$, say at $X^m = (x^m_{i_L+1}, \ldots, x^m_{i_R-1})$. Suppose on the contrary that (3.6) is not true, then there exists k with $i_L \leqslant k \leqslant i_R - 1$ such that $P_k > F_m$. If $i_L < k < i_R - 1$, then by replacing x_k and x_{k+1} by $x_k - \delta$ and $x_{k+1} + \delta$ respectively, with $\delta > 0$ small enough, we can show similarly (see (3.9)) that P_k is slightly decreased, while still being larger than F_m, and all other $P_{k'}$, $k' \neq k$, are increased. Thus F_m is increased, which is a contradiction against the maximality. If $k = i_L$ or $k = i_R - 1$, then adjusting x_k or x_{k+1} respectively in a similar way will give the same conclusion.

Step 3: Show that (3.6) is exactly the characterizing condition of the unique global minimizer of $\mathcal{E}$.

Since $\mathcal{E}$ is convex and going to infinity near the boundary, the global minimizer of $\mathcal{E}$ on $\mathbb{R}^{i_R-i_L-1}_{\text{sort}}(x_{i_L}, x_{i_R})$ is clearly unique, calling it X^*, characterized by

$$\begin{aligned}\partial_k \mathcal{E} = -s \cdot \Big(&\sum_{i:\, 0 \leqslant i < k} (x_k - x_i)^{-s-1}\\ &- \sum_{i:\, k < i \leqslant N} (x_i - x_k)^{-s-1} \Big) = 0, \quad \forall i_L + 1 \leqslant k \leqslant i_R - 1.\end{aligned} \tag{3.11}$$

Notice that the quantity in the above parenthesis is exactly $P_k - P_{k-1}$. Therefore (3.11) is equivalent to (3.6). Since X^* is the unique point satisfying (3.11), and X^m satisfies (3.6), these two points coincide.

Step 4: Show (3.8).

Notice that

$$\begin{aligned}\sum_{k=i_L}^{i_R-1}(x_{k+1}-x_k)P_k &= \sum_{k=i_L}^{i_R-1}\sum_{i,j:\,0\leqslant i\leqslant k<j\leqslant N}(x_{k+1}-x_k)(x_j-x_i)^{-s-1} \\ &= \sum_{0\leqslant i<j\leqslant N}\sum_{k=\max\{i,i_L\}}^{\min\{j,i_R\}-1}(x_{k+1}-x_k)(x_j-x_i)^{-s-1} \\ &= \sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L}(x_{\min\{j,i_R\}}-x_{\max\{i,i_L\}})(x_j-x_i)^{-s-1}.\end{aligned}$$

At X^*, we have $F_m = P_k$, $i_L \leqslant k \leqslant i_R - 1$. Thus (3.8) follows. □

Proof of Lemma 3.1. We apply Lemma 3.2 with

$$i_L = \max\{i : x_i < \epsilon_1\}, \quad i_R = \min\{i : x_i > 1 - \epsilon_1\}. \tag{3.12}$$

Then we get

$$\begin{aligned}F_m(X) \leqslant\, & F_m(X^*) \\ &= \frac{1}{x_{i_R}-x_{i_L}}\sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L}(x^*_{\min\{j,i_R\}}-x^*_{\max\{i,i_L\}})(x^*_j-x^*_i)^{-s-1} \\ &\leqslant \frac{1}{x_{i_R}-x_{i_L}}\sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L}(x^*_j-x^*_i)^{-s} \\ &\leqslant \frac{1}{1-2\epsilon_1}\sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L}(x^*_j-x^*_i)^{-s}\end{aligned} \tag{3.13}$$

for $X = (x_{i_L+1}, \ldots, x_{i_R-1})$. Notice that

$$\begin{aligned}\sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L}(x_j-x_i)^{-s} &= \mathcal{E}(x_{i_L+1},\ldots,x_{i_R-1}) - C_0, \\ C_0 &:= \sum_{i_R\leqslant i<j\leqslant N \text{ or } 0\leqslant i<j\leqslant i_L}(x_j-x_i)^{-s}\end{aligned} \tag{3.14}$$

for any $X = (x_{i_L+1}, \ldots, x_{i_R-1})$, where C_0 is independent of X. Therefore

$$F_m(X) \leqslant \frac{1}{1-2\epsilon_1}(\mathcal{E}(X^*) - C_0). \tag{3.15}$$

To bound $\mathcal{E}(X^*)$ from above, we construct

$$\tilde{x}_i = \epsilon_1 + (1-2\epsilon_1)\frac{i}{N}, \quad i = 0, \ldots, N, \tag{3.16}$$

and denote

$$\tilde{\tilde{x}}_i = \begin{cases}\tilde{x}_i, & i_L + 1 \leqslant i \leqslant i_R - 1, \\ x_i, & \text{elsewhere}.\end{cases} \tag{3.17}$$

Then by the minimality of $\mathcal{E}(X^*)$,

$$\begin{aligned}\mathcal{E}(X^*) \leqslant& \mathcal{E}(\tilde{x}_{i_L+1},\dots,\tilde{x}_{i_R-1})\\ =& C_0 + \sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L} (\tilde{\tilde{x}}_j - \tilde{\tilde{x}}_i)^{-s}\\ \leqslant& C_0 + \sum_{0\leqslant i<j\leqslant N,\, i<i_R,\, j>i_L} (\tilde{x}_j - \tilde{x}_i)^{-s}\\ \leqslant& C_0 + (N+1)\sum_{i=1}^{\infty}\Big((1-2\epsilon_1)\frac{i}{N}\Big)^{-s}\\ =& C_0 + (1-2\epsilon_1)^{-s}\zeta(s)(N+1)N^s,\end{aligned} \tag{3.18}$$

where the second inequality is because when changing from $\tilde{\tilde{x}}$ to $\tilde{x}$, we have

$$\tilde{\tilde{x}}_j - \tilde{\tilde{x}}_i = \begin{cases} \tilde{x}_j - \tilde{x}_i, & i_L+1 \leqslant i < j \leqslant i_R - 1;\\ \tilde{x}_j - x_i \geqslant \tilde{x}_j - \epsilon_1 \geqslant \tilde{x}_j - \tilde{x}_i & i \leqslant i_L < j \leqslant i_R - 1;\\ x_j - \tilde{x}_i \geqslant (1-\epsilon_1) - \tilde{x}_i \geqslant \tilde{x}_j - \tilde{x}_i & i_L + 1 \leqslant i < i_R \leqslant j;\\ x_j - x_i \geqslant (1-\epsilon_1) - \epsilon_1 \geqslant \tilde{x}_j - \tilde{x}_i & i \leqslant i_L < i_R \leqslant j; \end{cases} \tag{3.19}$$

which includes all the cases appearing in the summation. Therefore we finish the proof by

$$\begin{aligned}F_m(X) &\leqslant (1+\frac{1}{N})(1-2\epsilon_1)^{-s-1}\zeta(s)N^{s+1}\\ &\leqslant (1+\frac{1}{N})(1+2.5(s+1)\epsilon_1)\zeta(s)N^{s+1} \leqslant (1+\epsilon)\zeta(s)N^{s+1}\end{aligned} \tag{3.20}$$

for $\epsilon_1 = \frac{\epsilon}{3(s+1)} \leqslant \frac{0.01}{3(s+1)}$ and N large enough, where the second inequality uses

$$(1-2\epsilon_1)^{-s-1} \leqslant (1+2.2\epsilon_1)^{s+1} \leqslant e^{2.2\epsilon_1(s+1)} \leqslant 1 + 2.5(s+1)\epsilon_1. \tag{3.21}$$

□

Remark 1. Under the same assumptions as in Lemma 3.1, one can show the existence of an index i_M such that $P_{i_M} \geqslant (1-\epsilon)\zeta(s)N^{s+1}$. We omit the details for this result because it will not be used in the proof of Theorem 2.1.

4. **Approximation by flat torus.** For given $z_1(t),\dots,z_N(t)$ satisfying (1.6), define the closest pairwise distance and the 'maximal density', respectively, by

$$\delta(t) := \min_{1\leqslant i\leqslant N}(z_{i+1}(t) - z_i(t)), \quad \rho_M(t) := \frac{1}{N\delta(t)} \tag{4.1}$$

with z_{N+1} understood as z_1. Furthermore, at a fixed time t, we set

$$i_M := \mathrm{argmin}_i(z_{i+1} - z_i) \tag{4.2}$$

as the index of the closest pair of particles. Finally, we define

$$d(y,z) := \min_{k\in\mathbb{Z}} |y - z + k| \tag{4.3}$$

as the distance between y and z on the flat torus. It is clear that $d(y,z) = |y-z|$ if $|y-z| \leqslant \frac{1}{2}$.

Lemma 4.1. *There exists $r_0 > 0$ such that*

$$|\mathbf{x}(y) - \mathbf{x}(z)| \geqslant \min\{\frac{1}{2}d(y,z), r_0\}, \quad \forall y,z. \tag{4.4}$$

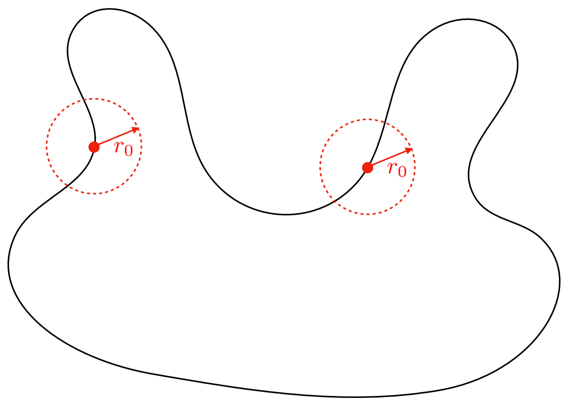

FIGURE 1. The number r_0 in Lemma 4.1 is the range for which $\mathbf{x}(z)$ can be approximated by a local Taylor expansion near $\mathbf{x}(y)$ for any fixed y.

See Figure 1 for an illustration of (4.4).

Proof. First, by the Taylor expansion

$$\mathbf{x}(y) - \mathbf{x}(z) = (y-z)\mathbf{x}'(y) + \mathcal{O}((y-z)^2) \tag{4.5}$$

we see that

$$\frac{1}{2}|y-z| \leqslant |\mathbf{x}(y) - \mathbf{x}(z)| \leqslant \frac{3}{2}|y-z| \tag{4.6}$$

if $|y-z| \leqslant r_1$ is small enough.

Consider the continuous function

$$F(y,z) = |\mathbf{x}(y) - \mathbf{x}(z)| \tag{4.7}$$

defined on $\{(y,z) \in \mathbb{T}^2 : d(y,z) \geqslant r_1\}$ which is compact. Since $\mathbf{x}(z)$ is non-self-intersecting, F is everywhere positive, and achieves its positive minimum on this set, calling it r_0.

To show (4.4), if $d(y,z) \geqslant r_1$, then the definition of r_0 gives

$$|\mathbf{x}(y) - \mathbf{x}(z)| \geqslant r_0. \tag{4.8}$$

If $d(y,z) = |y-z| < r_1$, then (4.6) gives

$$|\mathbf{x}(y) - \mathbf{x}(z)| \geqslant \frac{1}{2}|y-z| = \frac{1}{2}d(y,z). \tag{4.9}$$

$\square$

Lemma 4.2. *There exist $C_R > 0$ and $r_0 > 0$, depending on the curve $\mathbf{x}(z)$ and s, such that for any $y \neq z \in \mathbb{T}$ with $d(y,z) \leqslant r_0$, we have*

$$|\nabla W(\mathbf{x}(y) - \mathbf{x}(z)) \cdot \mathbf{x}'(y) - W'(y-z)(1 + \kappa(y)|y-z|^2)| \leqslant C_R|y-z|^{-s+2}, \tag{4.10}$$

where

$$\kappa(z) := \frac{s-2}{24}|\mathbf{x}''(z)|^2. \tag{4.11}$$

Furthermore,

$$\operatorname{sgn}(\nabla W(\mathbf{x}(y) - \mathbf{x}(z)) \cdot \mathbf{x}'(y)) = \operatorname{sgn}(W'(y-z)). \tag{4.12}$$

If y, z and $\tilde{y}$ additionally satisfy $\tilde{y}-1<z<y<\tilde{y}$, then

$$\begin{aligned}&\Big|\Big(\nabla W(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)-W'(y-z)(1+\kappa(y)|y-z|^2)\Big)\\&\quad-\Big(\nabla W(\mathbf{x}(\tilde{y})-\mathbf{x}(z))\cdot\mathbf{x}'(\tilde{y})-W'(\tilde{y}-z)(1+\kappa(y)|\tilde{y}-z|^2)\Big)\Big|\\&\leqslant C_R\min\{d(y,z),d(\tilde{y},z)\}^{-s+1}\cdot|y-\tilde{y}|\end{aligned}\tag{4.13}$$

and the same inequality holds if $\kappa(y)$ is replaced by $\kappa(\tilde{y})$.

Moreover, for any $r_1>0$, there exists $C_0(r_1)>0$ such that

$$|\nabla W(\mathbf{x}(y)-\mathbf{x}(z))|\leqslant C_0(r_1),\quad \forall d(y,z)>r_1.\tag{4.14}$$

Proof. We assume hereafter that r_0 is sufficiently small so that Lemma 4.1 applies.
Step 1: We first prove (4.10) and (4.12) with the assumption $d(y,z)=|y-z|\leqslant r_0$.

By Taylor expansion for $|y-z|$ small,

$$\mathbf{x}(y)-\mathbf{x}(z)=(y-z)\mathbf{x}'(y)-\frac{(y-z)^2}{2}\mathbf{x}''(y)+\frac{(y-z)^3}{6}\mathbf{x}'''(y)+\mathcal{O}((y-z)^4)\tag{4.15}$$

where the error term involves $\|\mathbf{x}^{(4)}\|_{L^\infty}$. Since the curve length parametrization satisfies $|\mathbf{x}'(z)|=1$, one obtains

$$\mathbf{x}''(z)\cdot\mathbf{x}'(z)=0,\quad \mathbf{x}'''(z)\cdot\mathbf{x}'(z)+|\mathbf{x}''(z)|^2=0\tag{4.16}$$

by differentiating with respect to z. Then we have

$$\begin{aligned}|\mathbf{x}(y)-\mathbf{x}(z)|^2=&(y-z)^2\Big[1+(y-z)^2\Big(\frac{1}{3}\mathbf{x}'(y)\cdot\mathbf{x}'''(y)+\frac{1}{4}|\mathbf{x}''(y)|^2\Big)\\&\qquad+\mathcal{O}((y-z)^3)\Big]\\=&(y-z)^2\left[1-(y-z)^2\frac{1}{12}|\mathbf{x}''(y)|^2+\mathcal{O}((y-z)^3)\right],\end{aligned}\tag{4.17}$$

and

$$\begin{aligned}(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)=&(y-z)\left[1+(y-z)^2\frac{1}{6}\mathbf{x}'(y)\cdot\mathbf{x}'''(y)+\mathcal{O}((y-z)^3)\right]\\=&(y-z)\left[1-(y-z)^2\frac{1}{6}|\mathbf{x}''(y)|^2+\mathcal{O}((y-z)^3)\right].\end{aligned}\tag{4.18}$$

Also, when r_0 is small, we have $O((y-z)^2)\leqslant 1/2$, and thus (4.17) implies

$$\begin{aligned}&|\mathbf{x}(y)-\mathbf{x}(z)|^{-s-2}\\&\quad=|y-z|^{-s-2}\left[1-(y-z)^2\frac{-s-2}{2}\cdot\frac{1}{12}|\mathbf{x}''(y)|^2+\mathcal{O}((y-z)^3)\right].\end{aligned}\tag{4.19}$$

Multiplying this with (4.18) gives

$$\begin{aligned}&\nabla W(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)\\&\qquad=|\mathbf{x}(y)-\mathbf{x}(z)|^{-s-2}(\mathbf{x}(y)-\mathbf{x}(z))\cdot\mathbf{x}'(y)\\&\qquad=|y-z|^{-s-2}(y-z)\left[1+(y-z)^2\frac{s-2}{24}|\mathbf{x}''(y)|^2+\mathcal{O}((y-z)^3)\right]\end{aligned}$$

and (4.10) with $|y-z|\leqslant r_0$ follows. Then (4.12) follows from the fact that $|W'(y-z)(1+\kappa(y)|y-z|^2)|\geqslant|y-z|^{-s-1}/2\geqslant C_R|y-z|^{-s+2}$ when $|y-z|$ is small enough.
Step 2: Here we prove (4.14).

If $|y-z|>r_1$, then by Lemma 4.1, there exists constant $r_1'=\min\{r_1/2,r_0/2\}>0$ such that

$$|\mathbf{x}(y)-\mathbf{x}(z)|\geqslant r_1'. \tag{4.20}$$

Then it follows that

$$|\nabla W(\mathbf{x}(y)-\mathbf{x}(z))| = |\mathbf{x}(y)-\mathbf{x}(z)|^{-s-1}\leqslant (r_1')^{-s-1}=: C_0(r_1). \tag{4.21}$$

This gives (4.14).
Step 3: Finally we prove (4.13).
We define a function[1]

$$\phi(z)=\nabla W(\mathbf{x}(z)-\mathbf{x}(z))\cdot\mathbf{x}'(z)-W'(z-z)(1+\kappa(y)|z-z|^2) \tag{4.22}$$

and then the LHS of (4.13) is $|\phi(y)-\phi(\tilde{y})|=|\phi'(\xi)|\cdot|\tilde{y}-y|$ for some $\xi\in(y,\tilde{y})$.
Write $\xi=y+\alpha(\tilde{y}-y)$, $0\leqslant\alpha\leqslant 1$. By assumption, $d(y,z)=y-z\leqslant r_0$ is small. Therefore

$$|\xi-z|=|y-z|+\alpha|\tilde{y}-y|\in[\,|y-z|,2r_0] \tag{4.23}$$

since both $y-z$ and $\tilde{y}-y$ are positive.
Then we compute

$$\begin{aligned}\phi'(\xi)=&\mathbf{x}'(\xi)^T\cdot\nabla^2W(\mathbf{x}(\xi)-\mathbf{x}(z))\cdot\mathbf{x}'(\xi)+\nabla W(\mathbf{x}(\xi)-\mathbf{x}(z))\cdot\mathbf{x}''(\xi)\\&-W''(\xi-z)(1+\kappa(y)|\xi-z|^2)-W'(\xi-z)\kappa(y)\cdot 2(\xi-z)\end{aligned} \tag{4.24}$$

where

$$\nabla^2 W(\bar{\mathbf{x}})=-|\bar{\mathbf{x}}|^{-s-2}I+(s+2)|\bar{\mathbf{x}}|^{-s-4}\bar{\mathbf{x}}\bar{\mathbf{x}}^T,\quad \bar{\mathbf{x}}:=\mathbf{x}(\xi)-\mathbf{x}(z). \tag{4.25}$$

Therefore, using $|\mathbf{x}'(\xi)|=1$,

$$\begin{aligned}\phi'(\xi)=&-|\bar{\mathbf{x}}|^{-s-2}+(s+2)|\bar{\mathbf{x}}|^{-s-4}(\mathbf{x}'(\xi)\cdot\bar{\mathbf{x}})^2-|\bar{\mathbf{x}}|^{-s-2}(\mathbf{x}''(\xi)\cdot\bar{\mathbf{x}})\\&-(s+1)|\xi-z|^{-s-2}(1+\kappa(y)|\xi-z|^2)\\&+|\xi-z|^{-s-2}(\xi-z)\kappa(y)\cdot 2(\xi-z)\\=&|\bar{\mathbf{x}}|^{-s-2}\Big[-1+(s+2)|\bar{\mathbf{x}}|^{-2}(\mathbf{x}'(\xi)\cdot\bar{\mathbf{x}})^2-(\mathbf{x}''(\xi)\cdot\bar{\mathbf{x}})\Big]\\&-(s+1)|\xi-z|^{-s-2}(1+\kappa(y)|\xi-z|^2)\\&+|\xi-z|^{-s-2}(\xi-z)\kappa(y)\cdot 2(\xi-z)\end{aligned} \tag{4.26}$$

[1]As auxiliary functions, ϕ may refer to different functions in different proofs.

(4.16), (4.18) and (4.19) with y replaced by ξ (which is allowed since $|z-\xi| \leqslant 2r_0$, by replacing r_0 with a smaller one if necessary), give

$$\begin{aligned}
&\phi'(\xi) \\
&\quad = |\xi - z|^{-s-2} \cdot \left[1 - (\xi - z)^2 \frac{-s-2}{2} \frac{1}{12} |\mathbf{x}''(\xi)|^2 + \mathcal{O}\right] \\
&\qquad \cdot \Big[-1 + (s+2)\left(1 + (\xi - z)^2 \frac{1}{12} |\mathbf{x}''(\xi)|^2 + \mathcal{O}\right) \cdot \left(1 - (\xi - z)^2 \frac{1}{6} |\mathbf{x}''(\xi)|^2 + \mathcal{O}\right)^2 \\
&\qquad\quad + (\xi - z)^2 \frac{1}{2} |\mathbf{x}''(\xi)|^2 + \mathcal{O}\Big] \\
&\qquad\quad - (s+1)|\xi - z|^{-s-2}(1 + \kappa(y)|\xi - z|^2) + |\xi - z|^{-s-2}(\xi - z)\kappa(y) \cdot 2(\xi - z) \\
&\quad = |\xi - z|^{-s-2} \cdot \Big[(s+1) \\
&\qquad\qquad + (\xi - z)^2 \cdot \left((s+1)\frac{s+2}{24} + \frac{s+2}{12} - \frac{s+2}{3} + \frac{1}{2}\right) |\mathbf{x}''(\xi)|^2 + \mathcal{O}\Big] \\
&\qquad - |\xi - z|^{-s-2}\Big[(s+1) + (\xi - z)^2 \cdot \Big((s+1)\kappa(y) - 2\kappa(y)\Big) + \mathcal{O}\Big] \\
&\quad = |\xi - z|^{-s-2} \cdot \Big[(\xi - z)^2 (s-1)\kappa(\xi) - (\xi - z)^2 (s-1)\kappa(y) + \mathcal{O}\Big] \\
&\quad = \mathcal{O}(|\xi - z|^{-s+1})
\end{aligned}$$

where $\mathcal{O}$ refers to $\mathcal{O}((\xi - z)^3)$, and in the last equality we used $|\kappa(y) - \kappa(\xi))| \leqslant \|\kappa'\|_{L^\infty} \cdot |y - \xi| \leqslant \|\kappa'\|_{L^\infty} \cdot |y - \tilde{y}|$. This gives (4.13).

When replacing $\kappa(y)$ by $\kappa(\tilde{y})$, the total change on the LHS of (4.13) is no more than $\mathcal{O}(|y - z|^{-s-1} \cdot |y - z|^2 \cdot |y - \tilde{y}|)$ since $|\kappa(y) - \kappa(\tilde{y})| \leqslant \|\kappa'\|_{L^\infty} \cdot |y - \tilde{y}|$, thus controled by the RHS. □

Lemma 4.3. *For any $\epsilon > 0$, there exists (large) N_0, depending on ϵ, s and the curve $\mathbf{x}(z)$, such that the following holds for $N > N_0$ and any positions of the particles $\mathbf{Z} = \{z_1, \ldots, z_N\}$:*

$$\tilde{\zeta}(s)(1 - \epsilon) \leqslant E(\mathbf{Z}) \leqslant \tilde{\zeta}(s)(1 + \epsilon)\rho_M^s \tag{4.27}$$

Proof. We first prove the right-hand inequality of (4.27). We rewrite (1.4)

$$2E(\mathbf{Z}) = N^{-s-1} \sum_i \sum_{j \neq i} W(\mathbf{x}(z_i) - \mathbf{x}(z_j)). \tag{4.28}$$

For each fixed i, let $i_L, \ldots, i_R$ be the indices j with $|z_i - z_j| \leqslant r_0$, where $r_0 > 0$ is a small constant to be chosen such that Lemma 4.1 applies. From Lemma 4.2 we can write

$$|\mathbf{x}(z_i) - \mathbf{x}(z_j)|^{-s} = |z_i - z_j|^{-s}(1 + \mathcal{O}((z_i - z_j)^2)), \tag{4.29}$$

for $j = i_L, \ldots, i_R$ with $j \neq i$. Since $z_{j+1} - z_j \geqslant \delta$ for all j, we have

$$|z_i - z_j| \geqslant |j - i|\delta. \tag{4.30}$$

For those j with $d(z_i, z_j) \geqslant r_0$, Lemma 4.1 gives $|\mathbf{x}(z_i) - \mathbf{x}(z_j)| \geqslant r_0/2$. Therefore

$$
\begin{aligned}
s\sum_{j\neq i} & W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \\
&\leqslant \sum_{i_L\leqslant j\leqslant i_R,\, j\neq i} |z_i - z_j|^{-s}(1 + \mathcal{O}((z_i - z_j)^2)) + CNr_0^{-s} \\
&\leqslant (1 + \mathcal{O}(r_0^2)) \sum_{i_L\leqslant j\leqslant i_R,\, j\neq i} (|j - i|\delta)^{-s} + CNr_0^{-s} \\
&\leqslant (1 + \mathcal{O}(r_0^2))2\zeta(s)\delta^{-s} + CNr_0^{-s}.
\end{aligned}
\tag{4.31}
$$

Summing over i, this gives

$$
\begin{aligned}
E(\mathbf{Z}) &\leqslant (1 + \mathcal{O}(r_0^2))\tilde{\zeta}(s)N^{-s}\delta^{-s} + CN^{1-s}r_0^{-s} \\
&= (1 + \mathcal{O}(r_0^2))\tilde{\zeta}(s)\rho_M^s + CN^{1-s}r_0^{-s},
\end{aligned}
\tag{4.32}
$$

where ρ_M is defined in (4.1). We first take r_0 small enough so that $r_0^2 \leqslant c\epsilon$, and then N large enough so that $CN^{1-s}r_0^{-s} \leqslant \epsilon$, and the conclusion is obtained (since $\rho_M \geqslant 1$).

Finally, inequalities (7.3) and (7.6) proved later in Section 7 imply that the left-hand inequality in (4.27) holds for N for sufficiently large. □

5. **Control on the closest pair.** In this section we analyze the evolution of the closest pairwise distance δ as defined in (4.1). We first give an unconditional lower bound of $\frac{\mathrm{d}}{\mathrm{d}t}\delta$.

Lemma 5.1. *There holds*

$$
\frac{\mathrm{d}}{\mathrm{d}t}\delta \geqslant -CN^{-s}N_*\delta^{-s+2}, \quad N_* := \begin{cases} 1, & s > 2; \\ \log N, & s = 2; \\ N^{-s+2}, & 1 < s < 2/ \end{cases}
\tag{5.1}
$$

Proof. We first compute the time derivative of δ:

$$
\begin{aligned}
N^s & \frac{\mathrm{d}}{\mathrm{d}t}(z_{i_M+1} - z_{i_M}) \\
&= -\sum_{j\neq i_M+1} \nabla W(\mathbf{x}(z_{i_M+1}) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_{i_M+1}) \\
&\quad + \sum_{j\neq i_M} \nabla W(\mathbf{x}(z_{i_M}) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_{i_M}) \\
&= \nabla W(\mathbf{x}(z_{i_M}) - \mathbf{x}(z_{i_M+1})) \cdot \mathbf{x}'(z_{i_M}) \\
&\quad + \nabla W(\mathbf{x}(z_{i_M}) - \mathbf{x}(z_{i_M+1})) \cdot \mathbf{x}'(z_{i_M+1}) \\
&\quad + \sum_{j\neq i_M, i_M+1} \Big(\nabla W(\mathbf{x}(z_{i_M}) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_{i_M}) \\
&\qquad\qquad - \nabla W(\mathbf{x}(z_{i_M+1}) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_{i_M+1})\Big).
\end{aligned}
\tag{5.2}
$$

See Figure 2 left as an illustration.

Now we estimate the summand in the last term of (5.2) for each j, see Figure 2 top for an illustration. First notice that if $d(z, z_{i_M}) \geqslant r_0$ and $d(z, z_{i_M+1}) \geqslant r_0$, then

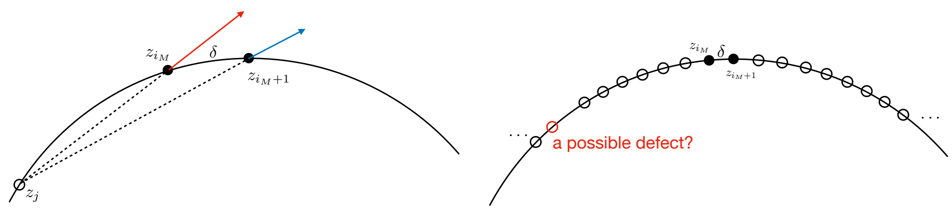

FIGURE 2. Lemmas 5.1 and 5.2. Left: the summand in the last term of (5.2). The two terms representing the forces from z_j acting on z_{i_M} (red) and z_{i_M+1} (blue), which decreases/increases δ respectively. Right: a local uniform distribution like $\{\tilde{z}_j\}$ makes $\frac{\mathrm{d}}{\mathrm{d}t}\delta \approx 0$ up to errors from curvature. A possible defect will release the total pushing force on δ, make $\frac{\mathrm{d}}{\mathrm{d}t}\delta$ positive, and thus violate (5.11).

Lemma 4.1 implies that $|\mathbf{x}(z) - \mathbf{x}(u)|$ is uniformly bounded below by some $r_1 > 0$ for any $z_{i_M} \leqslant u \leqslant z_{i_M+1}$. Then

$$\begin{aligned} &|\nabla W(\mathbf{x}(z_{i_M}) - \mathbf{x}(z)) \cdot \mathbf{x}'(z_{i_M}) - \nabla W(\mathbf{x}(z_{i_M+1}) - \mathbf{x}(z)) \cdot \mathbf{x}'(z_{i_M+1})| \\ &\qquad = \Big| \int_{z_{i_M}}^{z_{i_M+1}} \Big(\mathbf{x}'(u)^T \nabla^2 W(\mathbf{x}(u) - \mathbf{x}(z)) \mathbf{x}'(u) \\ &\qquad\qquad + \nabla W(\mathbf{x}(u) - \mathbf{x}(z)) \cdot \mathbf{x}''(u) \Big) \,\mathrm{d}u \Big| \\ &\qquad \leqslant C\delta, \qquad \forall z \text{ with } d(z, z_{i_M}) \geqslant r_0,\, d(z, z_{i_M+1}) \geqslant r_0. \end{aligned} \tag{5.3}$$

Then we deal with the case $z \in (z_{i_M} - r_0, z_{i_M})$. In view of (4.13), we need to estimate the following quantity:

$$\begin{aligned} -\phi(z) :=\, & W'(z_{i_M} - z)(1 + \kappa(z_{i_M})|z_{i_M} - z|^2) \\ & - W'(z_{i_M+1} - z)(1 + \kappa(z_{i_M})|z_{i_M+1} - z|^2) \\ =\, & \Big(|z_{i_M} - z|^{-s-1} + \kappa(z_{i_M})|z_{i_M} - z|^{-s+1} \Big) \\ & - \Big(|z_{i_M+1} - z|^{-s-1} + \kappa(z_{i_M})|z_{i_M+1} - z|^{-s+1} \Big) \end{aligned} \tag{5.4}$$

whose derivative can be expressed as

$$\begin{aligned} \phi'(z) &= \psi(z_{i_M+1}, z) - \psi(z_{i_M}, z), \\ \psi(y, z) &:= (-s-1)|y - z|^{-s-2} + \kappa(z_{i_M})(-s+1)|y - z|^{-s}. \end{aligned} \tag{5.5}$$

Notice that

$$\begin{aligned} \partial_y \psi(y, z) =& (s+1)(s+2)|y - z|^{-s-3} + \kappa(z_{i_M})(s-1)s|y - z|^{-s-1} \\ =& |y - z|^{-s-3} \Big((s+1)(s+2) - \kappa(z_{i_M})(s-1)s|y - z|^2 \Big) > 0 \end{aligned} \tag{5.6}$$

if $|y - z|$ is small. Thus $\phi'(z) > 0$ since $r_0 < z_{i_M} < z_{i_M+1}$ and all three points are within a distance of $r_0 + \delta \leqslant r_0 + \frac{1}{N}$ which is small.

Let $i_L, \ldots, i_R$ be the indices j with $|z_{i_M} - z_j| \leqslant r_0$. Define the uniform configuration with spacing δ:

$$\tilde{z}_j := z_{i_M} - (i_M - j)\delta, \quad i_L \leqslant j \leqslant i_M - 1$$

and notice that $z_j \leqslant \tilde{z}_j$ by definition of i_M. With $I_j := \int_{z_j}^{\tilde{z}_j} \phi'(z)\,\mathrm{d}z$, we have

$$
\begin{aligned}
&\sum_{j=i_L}^{i_M-1}\Big(W'(z_{i_M}-z_j)(1+\kappa(z_{i_M})|z_{i_M}-z_j|^2)\\
&\qquad - W'(z_{i_M+1}-z_j)(1+\kappa(z_{i_M})|z_{i_M+1}-z_j|^2)\Big)\\
&\quad=\sum_{j=i_L}^{i_M-1}\bigg(\Big(W'(z_{i_M}-\tilde{z}_j)(1+\kappa(z_{i_M})|z_{i_M}-\tilde{z}_j|^2)\\
&\qquad\quad -W'(z_{i_M+1}-\tilde{z}_j)(1+\kappa(z_{i_M})|z_{i_M+1}-\tilde{z}_j|^2)\Big)+I_j\bigg)\\
&\quad=\sum_{j=i_L}^{i_M-1}\bigg(\Big(W'((i_M-j)\delta)(1+\kappa(z_{i_M})|(i_M-j)\delta|^2)\\
&\qquad\quad -W'((i_M+1-j)\delta)(1+\kappa(z_{i_M})|(i_M+1-j)\delta|^2)\Big)+I_j\bigg)\\
&\quad=W'(\delta)(1+\kappa(z_{i_M})\delta^2)\\
&\qquad - W'((i_M+1-i_L)\delta)(1+\kappa(z_{i_M})|(i_M+1-i_L)\delta|^2)+\sum_{j=i_L}^{i_M-1}I_j\\
&\quad=-\,\delta^{-s-1}(1-|i_M+1-i_L|^{-s-1})\\
&\qquad -\delta^{-s+1}\kappa(z_{i_M})(1-|i_M+1-i_L|^{-s+1})+\sum_{j=i_L}^{i_M-1}I_j,
\end{aligned}
\tag{5.7}
$$

where the third equality follows from a telescoping summation. Now we have (5.3) (together with a similar equality for $i_M+2,\dots,i_R$) and (5.7) for the RHS of (5.2). Combining with (4.10) and (4.13), we get

$$
\begin{aligned}
N^s\frac{\mathrm{d}}{\mathrm{d}t}&(z_{i_M+1}-z_{i_M})\\
&=2\delta^{-s-1}(1+\kappa(z_{i_M})\delta^2)+\mathcal{O}(\delta^{-s+2})\\
&\quad+\sum_{\substack{i_L\leqslant j\leqslant i_R\\ j\neq i_M,\,i_M+1}}\Big[W'(z_{i_M}-z_j)(1+\kappa(z_{i_M})|z_{i_M}-z_j|^2)\\
&\quad- W'(z_{i_M+1}-z_j)(1+\kappa(z_{i_M})|z_{i_M+1}-z_j|^2)\\
&\quad+\mathcal{O}((z_{i_M+1}-z_{i_M})(|j-i_M|\delta)^{-s+1})\Big]+\mathcal{O}(N\delta)
\end{aligned}
$$

$$
\begin{aligned}
&= 2\delta^{-s-1}(1+\kappa(z_{i_M})\delta^2) + O(\delta^{-s+2}) \\
&\quad + \Big[-\delta^{-s-1}(1-|i_M+1-i_L|^{-s-1}) \\
&\qquad - \delta^{-s+1}\kappa(z_{i_M})(1-|i_M+1-i_L|^{-s+1}) + \sum_{j=i_L}^{i_M-1} I_j \Big] \\
&\quad + \Big[-\delta^{-s-1}(1-|i_R-i_M|^{-s-1}) \\
&\qquad - \delta^{-s+1}\kappa(z_{i_M})(1-|i_R-i_M|^{-s+1}) + \sum_{j=i_M+2}^{i_R} I_j \Big] \\
&\quad + \mathcal{O}\Big(\delta^{-s+2}\sum_{j=1}^{N} j^{-s+1}\Big) + O(N\delta) \\
&= \delta^{-s-1}(|i_M+1-i_L|^{-s-1} + |i_R-i_M|^{-s-1}) \\
&\quad + \delta^{-s+1}\kappa(z_{i_M})(|i_M+1-i_L|^{-s+1} + |i_R-i_M|^{-s+1}) \\
&\quad + \sum_{j=i_L}^{i_M-1} I_j + \sum_{j=i_M+2}^{i_R} I_j + \mathcal{O}(\delta^{-s+2}N_*) + \mathcal{O}(N\delta),
\end{aligned} \tag{5.8}
$$

where $N_* \sim \sum_{j=1}^{N} j^{-s+1}$ is defined in (5.1). In the last expression of (5.8), we can absorb the second term by the first term, using

$$\delta|i_M+1-i_L| \leqslant \delta\cdot\frac{r_0}{\delta} \leqslant r_0 \tag{5.9}$$

and the smallness of r_0. The two integrals of ϕ' are positive. Therefore

$$N^s\frac{\mathrm{d}}{\mathrm{d}t}(z_{i_M+1}-z_{i_M}) \geqslant -C(N_*\delta^{-s+2}+N\delta). \tag{5.10}$$

Then (5.1) follows directly by $N\delta \leqslant CN_*\delta^{-s+2}$ which can be easily checked in all three cases, using $N\delta \leqslant 1$. $\square$

Next we state the following lemma: either $\delta(t)$ is increasing very fast, or at i_M the total repulsion is as large as that of a uniform distribution of particles with spacing $\delta(t)$, which is approximately the RHS of (5.12).

Lemma 5.2. *Fix $\epsilon > 0$. For $N > N_0(\epsilon)$, if*

$$\frac{\mathrm{d}}{\mathrm{d}t}\delta \leqslant 1, \tag{5.11}$$

then

$$\sum_{i=i_L}^{i_M}\sum_{j=i_M+1}^{i_R}|z_i-z_j|^{-s-1} \geqslant \zeta(s)\delta^{-s-1}(1-\epsilon), \tag{5.12}$$

where $i_L,\dots,i_M-1$ are the indices of particles $z_i \in (z_{i_M}-r_0, z_{i_M})$, and $i_M+2,\dots,i_R$ are the indices of particles $z_i \in (z_{i_M+1}, z_{i_M+1}+r_0)$.

Proof. We will use the same notations as the previous proof. We claim that for any fixed J, there exists $N_0(\epsilon,J)$ such that, $N > N_0$ and $|i_M+2-j| \leqslant J$ imply

$$\tilde{z}_j - z_j \leqslant \epsilon\delta, \quad \forall j = i_L,\dots,i_M-1 \text{ with } |i_M+2-j| \leqslant J \tag{5.13}$$

under the condition (5.11), see Figure 2 right for an illustration.

Suppose on the contrary that $\tilde{z}_j - z_j > \epsilon\delta$ for some j in the range as in (5.13). Then by (5.5) and (5.6), for any $z \in [\tilde{z}_{j-1}, \tilde{z}_j]$,

$$\begin{aligned}
\phi'(z) = & \int_{z_{i_M}}^{z_{i_M+1}} \partial_y \psi(y,z)\,\mathrm{d}y \\
= & \int_{z_{i_M}}^{z_{i_M+1}} |y-z|^{-s-3}\Big((s+1)(s+2) - \kappa(z_{i_M})(s-1)s|y-z|^2\Big)\,\mathrm{d}y \\
\geqslant & \, c\int_{z_{i_M}}^{z_{i_M+1}} |y-\tilde{z}_j|^{-s-3}\,\mathrm{d}y \geqslant c\delta |z_{i_M+1} - z|^{-s-3} \\
\geqslant & \, c\delta^{-s-2}|i_M + 2 - j|^{-s-3},
\end{aligned} \tag{5.14}$$

where in the first inequality the second term in the integrand is absorbed by the first term using the smallness of $|y-z| \leqslant r_0$. Therefore

$$\begin{aligned}
\int_{z_j}^{\tilde{z}_j} \phi'(z)\,\mathrm{d}z \geqslant & \int_{\max\{z_j,\tilde{z}_{j-1}\}}^{\tilde{z}_j} \phi'(z)\,\mathrm{d}z \geqslant \min\{\delta, \tilde{z}_j - z_j\}\phi'(\tilde{z}_{j-1}) \\
& \geqslant \min\{\delta, \tilde{z}_j - z_j\}\delta^{-s-2}|i_M + 2 - j|^{-s-3}.
\end{aligned} \tag{5.15}$$

Therefore, if $\tilde{z}_j - z_j \geqslant \epsilon\delta$, then

$$\int_{z_j}^{\tilde{z}_j} \phi'(z)\,\mathrm{d}z \geqslant c\epsilon\delta^{-s-1}|i_M + 2 - j|^{-s-3} \tag{5.16}$$

which gives

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}(z_{i_M+1} - z_{i_M}) \geqslant & N^{-s}\Big(c\epsilon\delta^{-s-1}|i_M + 2 - j|^{-s-3} + \mathcal{O}(N_*\delta^{-s+2}) + O(N\delta)\Big) \\
= & c\epsilon(N\delta)^{-s-1}|i_M + 2 - j|^{-s-3}N + \mathcal{O}((N\delta)^{-s}N_*\delta^2) + \mathcal{O}(N^{-s}(N\delta))
\end{aligned} \tag{5.17}$$

in view of (5.8). Notice that $N\delta \leqslant 1$, $N_*\delta \leqslant 1$, and $|i_M + 2 - j|^{-s-3} \geqslant J^{-s-3}$. Therefore, by taking N large (in terms of ϵ and J), the first term can absorb the other two terms and gives

$$\frac{\mathrm{d}}{\mathrm{d}t}(z_{i_M+1} - z_{i_M}) \geqslant c\epsilon(N\delta)^{-s-1}J^{-s-3}N \geqslant 2 \tag{5.18}$$

which contradicts (5.11) if N is large enough. Therefore we proved (5.13).

Similarly one can show that $z_j - \tilde{z}_j \leqslant \epsilon\delta$ for $j = i_M+2, \ldots, i_R$ with $|j+1-i_M| \leqslant J$, and also $i_M - i_L \geqslant J$, $i_R - 1 - i_M \geqslant J$.

Now we aim to show (5.12). In fact, (5.13) gives

$$
\begin{aligned}
&\sum_{i=i_L}^{i_M}\sum_{j=i_M+1}^{i_R}|z_i-z_j|^{-s-1}\\
&\qquad\geqslant \sum_{i=i_M-J+1}^{i_M}\sum_{j=i_M+1}^{i_M+J}|(\tilde{z}_j+\epsilon\delta)-(\tilde{z}_i-\epsilon\delta)|^{-s-1}\\
&\qquad= \delta^{-s-1}\sum_{i=i_M-J+1}^{i_M}\sum_{j=i_M+1}^{i_M+J}|j-i+2\epsilon|^{-s-1}\\
&\qquad\geqslant \delta^{-s-1}\sum_{i=i_M-J+1}^{i_M}\sum_{j=i_M+1}^{i_M+J}(|j-i|^{-s-1}-(s+1)|j-i|^{-s-2}2\epsilon)\\
&\qquad\geqslant \delta^{-s-1}\left(\sum_{i=i_M-J+1}^{i_M}\sum_{j=i_M+1}^{i_M+J}|j-i|^{-s-1}-C\epsilon\right)
\end{aligned}
\tag{5.19}
$$

where in the second inequality we used the convexity of the function $x\mapsto|x|^{-s-1}$, and in the third inequality we used the convergence of the series $\sum_{i=-\infty}^{i_M}\sum_{j=i_M+1}^{\infty}|j-i|^{-s-2}$. Since $\sum_{i=-\infty}^{i_M}\sum_{j=i_M+1}^{\infty}|j-i|^{-s-1}=\zeta(s)$, one can take $J=J(\epsilon)$ large enough so that

$$\sum_{i=i_M-J+1}^{i_M}\sum_{j=i_M+1}^{i_M+J}|j-i|^{-s-1}\geqslant\zeta(s)-\epsilon,$$

and then (5.12) follows. □

6. **Proof of Theorem 2.1.**

Proof of Theorem 2.1. **Step 1**: We aim to give a *positive* lower bound

$$\sum_{i_M+1\leqslant i\leqslant i_S}\dot{z}_i\geqslant\lambda(\rho_M)N \tag{6.1}$$

(where ρ_M is defined in (4.1)) under the assumption (5.11), where

$$\lambda(\rho_M)=\begin{cases}c(\rho_M-1-\epsilon), & \rho_M\leqslant 2\\ c\rho_M^{s+1}\end{cases} \tag{6.2}$$

for some indices i_M and i_S. Notice that the assumption (5.11) is equivalent to

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_M\geqslant -N^{-1}\delta^{-2}=-N\rho_M^2 \tag{6.3}$$

since $\rho_M=\frac{1}{N\delta}$, see Figure 3 for an illustration.

Using the same notation as in the proof of Lemma 5.2 (with the same choice of J), we have (5.13) from (5.11). We take $i_1=i_M-J$ and $i_2=i_M+J$. Then we have

$$\sum_{i_1\leqslant i\leqslant i_M<j\leqslant i_2}(z_j-z_i)^{-s-1}\geqslant\zeta(s)\delta^{-s-1}(1-\frac{\epsilon}{100})=\zeta(s)(1-\frac{\epsilon}{100})(N\rho_M)^{s+1}. \tag{6.4}$$

Then we take $i_1'=i_2+1$ and $i_2'=i_1+N-1$, which satisfy

$$i_2'-i_1'\geqslant N-2J-2\geqslant\frac{N}{2} \tag{6.5}$$

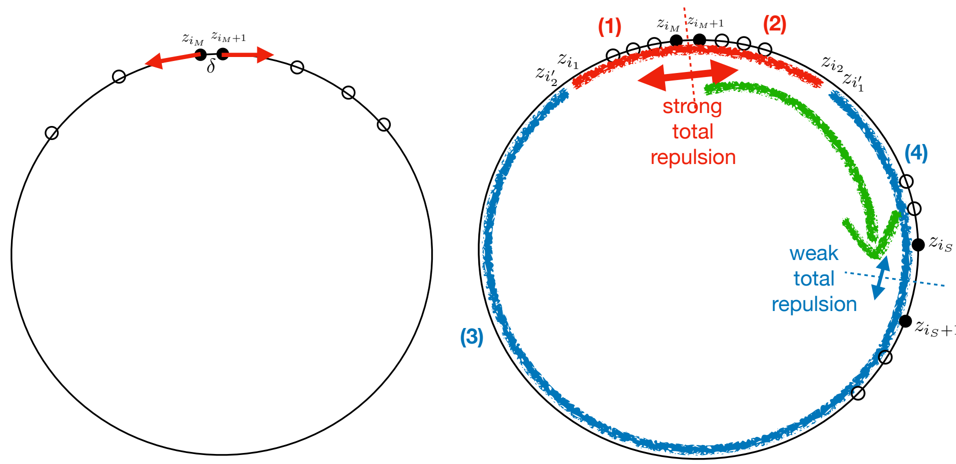

FIGURE 3. Proof of Theorem 2.1. Left: when (5.11) does not hold, δ is increasing very fast (i.e., ρ_M is decreasing very fast). Right: when (5.11) holds, there is almost uniform distribution near z_{i_M} (red parts) with average density near ρ_M, and the total repulsion at z_{i_M} is strong (see (5.12)). The rest part has average density at most $1+\epsilon$, and Lemma 3.1 applies to give a weak total repulsion cut. The strong/weak total repulsion ((1)-(2) good contribution, I_1, and (3)-(4) bad contribution, I_2, see (6.9)) forces the green part to rotate. The parameter r_1 is to guarantee that (3) or (4) cannot be too short, so that the possible bad contribution from (1)-(4) or (2)-(3) (the term I_3) can be neglected.

if N is large. Also, by (5.13) we have $z_{i_1'} - z_{i_M} \leqslant (J+1+\epsilon)\delta \leqslant \frac{J+1+\epsilon}{N}$ and $z_{i_M} - (z_{i_2'} - 1) \leqslant \frac{J+1+\epsilon}{N}$, which implies

$$z_{i_2'} - z_{i_1'} \geqslant 1 - \frac{2(J+1+\epsilon)}{N} \geqslant 1 - \frac{\epsilon}{100} \tag{6.6}$$

if N is large.

Then Lemma 3.1 (with suitable rescaling) applied to $i_1', \dots, i_2'$ gives: there exists an index i_S such that

$$\sum_{i_1' \leqslant i \leqslant i_S < j \leqslant i_2'} (z_j - z_i)^{-s-1} \leqslant (1 + \frac{\epsilon}{100})\zeta(s) N^{s+1} \tag{6.7}$$

and

$$(z_{i_S}, z_{i_S+1}) \cap (z_{i_1'} + r_1, z_{i_2'} - r_1) \neq \emptyset, \quad r_1 = \frac{\epsilon}{600(s+1)}. \tag{6.8}$$

Now we prove (6.1).

$$\begin{aligned}\sum_{i_M+1 \leqslant i \leqslant i_S} \dot{z}_i =& - N^{-s} \sum_{i_M+1 \leqslant i \leqslant i_S} \sum_{i_S+1 \leqslant j \leqslant i_M+N} \nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i) \\ =& - N^{-s} \Big(\sum_{i_1 \leqslant j \leqslant i_M < i \leqslant i_2} + \sum_{i_1' \leqslant i \leqslant i_S < j \leqslant i_2'} + \sum_{\text{others}} \Big) \\ =&: N^{-s}(I_1 + I_2 + I_3).\end{aligned} \tag{6.9}$$

Every term in I_1 satisfies $0 < z_i - z_j \leqslant 2J\delta \leqslant \frac{2J}{N}$ which is small. Thus by applying (4.10),

$$I_1 \geqslant \sum_{i_1 \leqslant j \leqslant i_M < i \leqslant i_2} ((z_i - z_j)^{-s-1} + R_{1,ij}) \tag{6.10}$$

with $|R_{1,ij}| \leqslant C_R(z_i - z_j)^{-s+1}$.

For the terms in I_2, if $z_j - z_i > \frac{1}{2}$ and $d(z_i, z_j) < r_0$, then $d(z_i, z_j) = d(z_i, z_j - 1) = z_i - (z_j - 1)$, and then by (4.12) applied to z_i and $(z_j - 1)$, we have $\nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i) < 0$ which makes its contribution in (6.9) positive. If $|z_j - z_i| > r_0$ then $|\nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i)| \leqslant C$ by (4.14). Combined with a similar argument as above for the case $d(z_i, z_j) = z_j - z_i < r_0$, we get

$$I_2 \geqslant - \sum_{i'_1 \leqslant i \leqslant i_S < j \leqslant i'_2} ((z_j - z_i)^{-s-1} + R_{2,ij}) - CN^2 \tag{6.11}$$

with $|R_{2,ij}| \leqslant C_R(z_j - z_i)^{-s+1}$.

We first bound I_1 from below. In fact, there exists $C = C(\epsilon)$ such that

$$|R_{1,ij}| \leqslant C_R(z_i - z_j)^{-s+1} \leqslant \frac{\epsilon}{100}(z_i - z_j)^{-s-1} + C(\epsilon). \tag{6.12}$$

Combining with (6.4) we get

$$I_1 \geqslant \sum_{i_1 \leqslant j \leqslant i_M < i \leqslant i_2} (1 - \frac{\epsilon}{100})(z_i - z_j)^{-s-1} - C(\epsilon)N^2 \geqslant (1 - \frac{\epsilon}{100})^2 \zeta(s)(N\rho_M)^{s+1} - C(\epsilon)N^2.$$

Similarly

$$I_2 \geqslant -(1 + \frac{\epsilon}{100})^2 \zeta(s)(N(1+\epsilon))^{s+1} - C(\epsilon)N^2.$$

To bound I_3, we recall the definition of r_1 in (6.8). We notice that for $i \in [i_M+1, i_S]$ and $j \in [i_S+1, i_M+N]$, if $d(z_i, z_j) \leqslant r_1$ and $\nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i) > 0$, then by (4.13) one necessarily has $z_j \in [z_i, z_i + r_1]$. The only possibility for this to happen is when $z_i \in [z_{i_S+1} - r_1, z_{i_S+1}]$ and $z_j \in [z_{i_S}, z_{i_S} + r_1]$. But by (6.8), $[z_{i_S+1} - r_1, z_{i_S+1}] \subset [z_{i_2}, z_{i_S+1}]$ and $[z_{i_S}, z_{i_S} + r_1] \subset [z_{i_S}, z_{i'_1}]$, and thus the term in (6.9) with indices (i, j) is already included in I_2. Therefore, every term in I_3 has either $d(z_i, z_j) > r_1$ or $\nabla W(\mathbf{x}(z_i) - \mathbf{x}(z_j)) \cdot \mathbf{x}'(z_i) \leqslant 0$, and thus

$$I_3 \geqslant -C(\epsilon)N^2$$

by (4.14) (where the ϵ-dependence comes from that of r_1).

In conclusion, we get

$$\sum_{i_M+1 \leqslant i \leqslant i_S} \dot{z}_i \geqslant \left((1 - \frac{\epsilon}{100})^2 \rho_M^{s+1} - (1 + \frac{\epsilon}{100})^2 (1+\epsilon)^{s+1} \right) \zeta(s)N - C(\epsilon)N^{-s+2}.$$

Now we show that the quantity in the big parenthesis above is bounded below. In fact, using $\epsilon < 1$,

$$\begin{aligned}
(1 - \frac{\epsilon}{100})^2 \rho_M^{s+1} &- (1 + \frac{\epsilon}{100})^2 (1+\epsilon)^{s+1} \\
&\geqslant \frac{1}{2}(\rho_M - 1 - 2\epsilon) + (1 - \frac{\epsilon}{100})^2 (1 + 2\epsilon)^{s+1} - (1 + \frac{\epsilon}{100})^2 (1+\epsilon)^{s+1} \\
&\geqslant \frac{1}{2}(\rho_M - 1 - 2\epsilon) + (1+\epsilon)^{s+1}((1 - \frac{\epsilon}{100})^2(1 + \frac{\epsilon}{2}) - (1 + \frac{\epsilon}{100})^2) \\
&\geqslant \frac{1}{2}(\rho_M - 1 - 2\epsilon).
\end{aligned}$$

Therefore, we get

$$\sum_{i_M+1\leqslant i\leqslant i_S} \dot{z}_i \geqslant \frac{1}{2}(\rho_M - 1 - 2\epsilon)\zeta(s)N - C(\epsilon)N^{-s+2} \geqslant \frac{1}{4}(\rho_M - 1 - 3\epsilon)\zeta(s)N$$

if N is large. Also, if $\rho_M \geqslant 2$, then

$$\begin{aligned}(1-\frac{\epsilon}{100})^2\rho_M^{s+1} &- (1+\frac{\epsilon}{100})^2(1+\epsilon)^{s+1} \\ &\geqslant \frac{1}{4}\rho_M^{s+1} + 2^s(1-\frac{\epsilon}{100})^2 - (1+\frac{\epsilon}{100})^2(1+\epsilon)^{s+1} \geqslant \frac{1}{4}\rho_M^{s+1}\end{aligned}$$

and we get

$$\sum_{i_M+1\leqslant i\leqslant i_S} \dot{z}_i \geqslant c\rho_M^{s+1}N \tag{6.13}$$

if N is large.

Step 2: We use (6.1) (under the condition (6.3)) to give energy dissipation rate, and use it to define a Lyapunov-like functional.

If $\rho_M - 1 - \epsilon \geqslant 0$, then Cauchy-Schwarz gives

$$c^2(\rho_M - 1 - \epsilon)^2 N^2 \leqslant \Big(\sum_{i_M+1\leqslant i\leqslant i_S} \dot{z}_i\Big)^2 \leqslant (i_S - i_M)\sum_{i_M+1\leqslant i\leqslant i_S} |\dot{z}_i|^2 \leqslant N\sum_i |\dot{z}_i|^2.$$

Recalling the energy dissipation law (1.5), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) \leqslant -c^2((\rho_M - 1 - \epsilon)_{\geqslant 0})^2, \quad \text{if } \frac{\mathrm{d}}{\mathrm{d}t}\rho_M \geqslant -N\rho_M^2 \tag{6.14}$$

and similarly

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) \leqslant -c^2\rho_M^{2(s+1)}, \quad \text{if } \frac{\mathrm{d}}{\mathrm{d}t}\rho_M \geqslant -N\rho_M^2, \quad \rho_M \geqslant 2. \tag{6.15}$$

Since $\rho_M = \frac{1}{N\delta}$, Lemma 5.1 gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_M = -\frac{1}{N\delta^2}\cdot\frac{\mathrm{d}}{\mathrm{d}t}\delta \leqslant CN^{-1}\delta^{-2}\cdot N^{-s}N_*\delta^{-s+2} = \frac{CN_*}{N}\rho_M^s. \tag{6.16}$$

Define a Lyapunov-like functional

$$F(t) = E(t) + \rho_M(t)^s. \tag{6.17}$$

Then at any time t with $\rho_M(t) \geqslant 1 + 2\epsilon$, at least one of the following three options must hold:

- When $\frac{\mathrm{d}}{\mathrm{d}t}\rho_M < -N\rho_M^2$, using $\frac{\mathrm{d}}{\mathrm{d}t}E \leqslant 0$,
$$\frac{\mathrm{d}}{\mathrm{d}t}F \leqslant -sN\rho_M^{s+1}. \tag{6.18}$$
- When $\frac{\mathrm{d}}{\mathrm{d}t}\rho_M \geqslant -N\rho_M^2$ and $\rho_M \geqslant 2$, (6.15) and (6.16) give
$$\frac{\mathrm{d}}{\mathrm{d}t}F \leqslant -c\rho_M^{2s+2} + \frac{CN_*}{N}\rho_M^{2s-1} \leqslant -c\rho_M^{2s+2} \tag{6.19}$$
by taking N large, since $\rho_M \geqslant 1$ always holds and $\lim_{N\to\infty}\frac{N_*}{N} = 0$.
- When $\frac{\mathrm{d}}{\mathrm{d}t}\rho_M \geqslant -N\rho_M^2$ and $1+2\epsilon \leqslant \rho_M < A$ (with $A > 2$ an absolute constant to be determined), (6.14) and (6.16) give
$$\frac{\mathrm{d}}{\mathrm{d}t}F \leqslant -c(\rho_M - 1 - \epsilon)^2 + \frac{CN_*}{N}\rho_M^{2s-1} \leqslant -c(\rho_M - 1 - 2\epsilon)^2 \tag{6.20}$$
by taking N large (which may depend on A).

Step 3: We use the functional F to give convergence rate of ρ_M to 1 up to an error of $\mathcal{O}(\epsilon)$.

Let T_1 be the first time such that $\rho_M \leqslant 2$, and we aim to estimate T_1. For $0 \leqslant t \leqslant T_1$, either (6.18) or (6.19) happens. Recall that $E \leqslant C\rho_M^s$ from Lemma 4.3, and therefore we have

$$\frac{\mathrm{d}}{\mathrm{d}t}F \leqslant -cF^{\frac{s+1}{s}}. \tag{6.21}$$

Since $\frac{s+1}{s} > 1$, there exists an absolute constant $C_{T,1}$ (independent of $F(0)$) such that $F(C_{T,1}) \leqslant 1/2$ if the above ODE holds for $0 \leqslant t \leqslant C_{T,1}$, which contradicts the fact that $F \geqslant 1$. Therefore there must hold

$$T_1 \leqslant C_{T,1}. \tag{6.22}$$

Then we have the estimate

$$F(T_1) \leqslant C\rho_M(T_1)^s \leqslant C2^s =: A^s \tag{6.23}$$

where A is the constant appeared in the condition of (6.20).

Let T_2 be the first time such that $\rho_M \leqslant 1 + B\epsilon$, where $B > 2$ is a positive constant to be determined. For $T_1 \leqslant t \leqslant T_2$, if $\rho_M(t) \leqslant A$, then either (6.18) or (6.20) happens, and we have

$$\frac{\mathrm{d}}{\mathrm{d}t}F \leqslant -c(\rho_M - 1 - 2\epsilon)^2. \tag{6.24}$$

This in particular implies $F(t) \leqslant A^s$ for $T_1 \leqslant t \leqslant T_2$, which in turn implies the assumption $\rho_M(t) \leqslant A$. Then

$$\begin{aligned}\rho_M - 1 - 2\epsilon &\geqslant c\Big((1+\epsilon)\tilde{\zeta}(s) + 1\Big)\Big(\rho_M^s - (1+2\epsilon)^s\Big) \\ &\geqslant c\Big[\Big((1+\epsilon)\tilde{\zeta}(s) + 1\Big)\Big(\rho_M^s - (1+2\epsilon)^s\Big) \\ &\quad + \Big(E - (1+\epsilon)\tilde{\zeta}(s)\rho_M^s\Big)\Big] \\ &= c[F - ((1+\epsilon)\tilde{\zeta}(s) + 1)(1+2\epsilon)^s]\end{aligned} \tag{6.25}$$

where the second inequality uses Lemma 4.3. Therefore $\tilde{F} := F - ((1+\epsilon)\tilde{\zeta}(s) + 1)(1+2\epsilon)^s$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{F} \leqslant -c\tilde{F}^2, \quad T_1 \leqslant t \leqslant T_2 \tag{6.26}$$

which implies

$$\tilde{F}(t) \leqslant \frac{1}{c(t-T_1) + \frac{1}{\tilde{F}(T_1)}} \leqslant \frac{1}{c(t-T_1) + A^{-s}}. \tag{6.27}$$

Therefore if $t - T_1 \geqslant \frac{C}{\epsilon}$ with $T_1 \leqslant t \leqslant T_2$, then $\tilde{F}(t) \leqslant \epsilon$, which implies

$$F(t) \leqslant ((1+\epsilon)\tilde{\zeta}(s) + 1)(1+2\epsilon)^s + \epsilon. \tag{6.28}$$

On the other hand $\rho_M(t) \leqslant 1 + B\epsilon$. This together with Lemma 4.3 implies

$$F(t) \geqslant (1-\epsilon)\tilde{\zeta}(s) + (1+B\epsilon)^s \tag{6.29}$$

which is a contradiction against (6.28) if B is large enough (only depending on s). Therefore we get

$$T_2 \leqslant \frac{C}{\epsilon} \tag{6.30}$$

and then Lemma 4.3 gives

$$E(T_2) \leqslant (1+\epsilon)\tilde{\zeta}(s)\rho_M(T_2)^s \leqslant (1+\epsilon)\tilde{\zeta}(s)(1+B\epsilon)^s \leqslant (1+C\epsilon)\tilde{\zeta}(s). \tag{6.31}$$

$E(t)$ also satisfies the last inequality if $t \geqslant T_2$, since $E(t)$ is non-increasing. □

7. Energy and distribution.

Recall that the energy of a configuration paramatrized by $\mathbf{Z}$ is

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

and observe that

$$\begin{aligned} E(\mathbf{Z}) &= \frac{1}{2sN^{s+1}} \sum_{i=1}^{N} \sum_{j=i+1}^{i+N-1} |\mathbf{x}(z_j) - \mathbf{x}(z_i)|^{-s} = \frac{1}{2sN^{s+1}} \sum_{i=1}^{N} \sum_{k=1}^{N-1} |\mathbf{x}(z_{i+k}) - \mathbf{x}(z_i)|^{-s} \\ &= \frac{1}{2} \sum_{k=1}^{N-1} E^k(\mathbf{Z}), \end{aligned}$$

where

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

One may easily verify that $E^k(\mathbf{Z}) = E^{N-k}(\mathbf{Z})$ for $1 \leqslant k < N$ and thus

$$E(\mathbf{Z}) = \begin{cases} \sum_{k=1}^{\frac{N-1}{2}} E^k(\mathbf{Z}), & \text{for } N \text{ odd}, \\ \sum_{k=1}^{\frac{N}{2}-1} E^k(\mathbf{Z}) + (1/2)E^{N/2}(\mathbf{Z}), & \text{for } N \text{ even}. \end{cases} \tag{7.1}$$

For $1 \leqslant k \leqslant N-1$, we define

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

and

$$\tilde{E}(\mathbf{Z}) = \begin{cases} \sum_{k=1}^{\frac{N-1}{2}} \tilde{E}^k(\mathbf{Z}), & \text{for } N \text{ odd}, \\ \sum_{k=1}^{\frac{N}{2}-1} \tilde{E}^k(\mathbf{Z}) + (1/2)\tilde{E}^{N/2}(\mathbf{Z}), & \text{for } N \text{ even}. \end{cases} \tag{7.2}$$

Since $\mathbf{x}(z)$ is an arc-length parametrization, we have $|\mathbf{x}(z) - \mathbf{x}(z')| \leqslant |z - z'|$ for all $z, z' \in \mathbb{R}$ and thus

$$\tilde{E}(\mathbf{Z}) \leqslant E(\mathbf{Z}), \tag{7.3}$$

for any $\mathbf{Z}$. Let

$$\zeta(s; N) := \sum_{k=1}^{\lfloor \frac{N-1}{2} \rfloor} k^{-s}. \tag{7.4}$$

Lemma 7.1. *For $k, N \in \mathbb{N}$ and $s > 0$,*

$$s^{-1}k^{-s} \leqslant \tilde{E}^k(\mathbf{Z}) \leqslant k^{-s}\tilde{E}^1(\mathbf{Z}), \tag{7.5}$$

and

$$s^{-1}\zeta(s; N) \leqslant \tilde{E}^1(\mathbf{Z}) + s^{-1}(\zeta(s; N) - 1) \leqslant \tilde{E}(\mathbf{Z}). \tag{7.6}$$

Proof. By Jensen's inequality,

$$\begin{aligned} sN^{s+1}\tilde{E}^1(\mathbf{Z}) &= \sum_{i=1}^{N} (z_{i+1} - z_i)^{-s} = \frac{1}{k} \sum_{j=0}^{k-1} \sum_{i=1}^{N} (z_{i+j+1} - z_{i+j})^{-s} \\ &= \sum_{i=1}^{N} \frac{1}{k} \sum_{j=0}^{k-1} (z_{i+j+1} - z_{i+j})^{-s} \geqslant sN^{s+1}k^s\tilde{E}^k(\mathbf{Z}), \end{aligned}$$

and

$$\tilde{E}^k(\mathbf{Z}) = s^{-1}N^{-s}\sum_{i=1}^{N}(z_{i+k}-z_i)^{-s}\frac{1}{N} \geqslant s^{-1}\left(\sum_{i=1}^{N}(z_{i+k}-z_i)\right)^{-s} = s^{-1}k^{-s},$$

proving (7.5). From (7.2), it follows that $\tilde{E}(\mathbf{Z}) \geqslant \sum_{k=1}^{\lfloor\frac{N-1}{2}\rfloor}\tilde{E}^k(\mathbf{Z})$ which together with (7.5) establishes (7.6). □

In the next lemma we show that the mean absolute deviation of the neighbor arclength distances $d_i := z_{i+1}-z_i$ is small on the microscopic scale. As a consequence we derive a macroscopic result showing that the density of points is nearly uniform when N is sufficiently large and the energy is sufficiently close to its minimal value.

Lemma 7.2. *Let $\epsilon > 0$, $s > 1$, $N \geqslant 2$, and define*

$$\Delta := 2\left(\frac{2\zeta(s)}{s(s+1)}\right)^{1/2}. \tag{7.7}$$

If $\mathbf{Z} = (z_1, z_2, \ldots, z_N)$ satisfies

$$\tilde{E}(\mathbf{Z}) \leqslant s^{-1}\zeta(s;N)(1+\epsilon), \tag{7.8}$$

then the mean absolute deviation of $d_i := z_{i+1}-z_i$, $i = 1, 2, \ldots, N$, satisfies

$$\frac{1}{N}\sum_{i=1}^{N}\left|d_i - \frac{1}{N}\right| \leqslant \frac{\Delta\epsilon^{1/2}}{N}. \tag{7.9}$$

Proof. Inequalities (7.6) and (7.8) imply

$$s\tilde{E}^1(\mathbf{Z}) \leqslant 1 + \zeta(s;N)\epsilon. \tag{7.10}$$

We write $\tilde{E}^1(\mathbf{Z})$ as

$$\tilde{E}^1(\mathbf{Z}) = \frac{1}{N^{s+1}}\sum_i W(d_i), \quad W(x) := \frac{x^{-s}}{s}. \tag{7.11}$$

The Taylor expansion of W at $\frac{1}{N}$ gives

$$W(d_i) = W(\frac{1}{N}) + W'(\frac{1}{N})(d_i - \frac{1}{N}) + \frac{1}{2}W''(\xi_i)(d_i - \frac{1}{N})^2, \tag{7.12}$$

where ξ_i is between d_i and $\frac{1}{N}$. Substituting into the previous equation gives

$$\begin{aligned} s\tilde{E}^1(\mathbf{Z}) =& \frac{s}{N^{s+1}}\sum_i\left(W(\frac{1}{N}) + W'(\frac{1}{N})(d_i-\frac{1}{N}) + \frac{1}{2}W''(\xi_i)(d_i-\frac{1}{N})^2\right) \\ =& \frac{s}{N^{s+1}}\sum_i W(\frac{1}{N}) + W'(\frac{1}{N})\frac{s}{N^{s+1}}\sum_i(d_i - \frac{1}{N}) \\ &+ \frac{s}{2N^{s+1}}\sum_i W''(\xi_i)(d_i-\frac{1}{N})^2 \\ =& 1 + \frac{1}{2}\cdot\frac{s}{N^{s+1}}\sum_i W''(\xi_i)(d_i-\frac{1}{N})^2, \end{aligned} \tag{7.13}$$

using $\sum_i d_i = 1 = \sum_i \frac{1}{N}$. Combined with (7.10), we get

$$\frac{1}{2}\cdot\frac{s}{N^{s+1}}\sum_i W''(\xi_i)(d_i-\frac{1}{N})^2 \leqslant \zeta(s;N)\epsilon. \tag{7.14}$$

Notice that for every i with $d_i < 1/N$, we have $\xi_i \in (d_i, \frac{1}{N})$, and thus

$$W''(\xi_i) = (s+1)\xi_i^{-s-2} \geqslant (s+1)N^{s+2}. \tag{7.15}$$

Therefore,

$$\begin{aligned}
\frac{1}{N}\sum_{i:\, d_i<1/N}\left|d_i - \frac{1}{N}\right| &\leqslant \left(\frac{1}{N}\sum_{i:\, d_i<1/N}\left|d_i - \frac{1}{N}\right|^2\right)^{1/2} \\
&\leqslant \left(\frac{1}{(s+1)N^{s+3}}\sum_{i:\, d_i<1/N} W''(\xi_i)\left|d_i - \frac{1}{N}\right|^2\right)^{1/2} \\
&\leqslant \left(\frac{1}{(s+1)N^{s+3}}\cdot\frac{2N^{s+1}}{s}\zeta(s;N)\epsilon\right)^{1/2} \\
&= \left(\frac{2\zeta(s;N)}{s(s+1)}\right)^{1/2}\frac{\epsilon^{1/2}}{N}.
\end{aligned} \tag{7.16}$$

Combined with the fact that

$$\frac{1}{N}\sum_i\left|d_i - \frac{1}{N}\right| = 2\cdot\frac{1}{N}\sum_{i:\, d_i<1/N}\left|d_i - \frac{1}{N}\right|, \tag{7.17}$$

we obtain the conclusion. □

We next show that the macroscopic density must be nearly uniform when the energy is nearly optimal.

Lemma 7.3. *Let* $0 < \epsilon < 1$, $s > 1$, *and* $N \geqslant 2^{-s+1}(s+1)\epsilon^{-1}$. *If* $\mathbf{Z} = (z_1, z_2, \ldots, z_N)$ *satisfies*

$$\tilde{E}(\mathbf{Z}) \leqslant s^{-1}\zeta(s;N)(1+\epsilon), \tag{7.18}$$

then for all $a \in \mathbb{R}$ *and* $0 < L < 1$,

$$\left|\frac{\#\{i:\ [z_i, z_{i+1}) \subset [a, a+L)\}}{N} - L\right| \leqslant \left[L(1-L)\tilde{\zeta}(s)\right]^{1/2}(2\epsilon)^{1/2}. \tag{7.19}$$

Proof. First, we may assume $L \leqslant 1/2$, since one can reduce the case $L > 1/2$ to $L \leqslant 1/2$ by replacing $[a, a+L)$ by $[a+L, a+1)$.

Let $M := \#\{i:\ z_i \in [a,b]\}$, $J_1 := \{i \in \mathbb{Z} : a \leqslant z_i < z_{i+1} < b\}$, $J_2 := \{i \in \mathbb{Z} : b \leqslant z_i < z_{i+1} < a+1)\}$, $N_1 := \#J_1$, $N_2 := \#J_2$, and $\alpha = N_1/N$. If $0 < M < N$, then $N_1 = M-1$ and $N_2 = N-M-1$ so that $N_1 + N_2 = N-2$. If $M = 0$ or $M = N$, then $N_1 + N_2 = N-1$. Thus, $N - N_1 - 2 \leqslant N_2 \leqslant N - N_1 - 1$. Using the conditions $\epsilon < 1$ and $L \leqslant 1/2$, it is straightforward to show that N_2 is always positive for sufficiently large N. We also observe that $\sum_{i\in J_1} d_i \leqslant L$ and $\sum_{i\in J_2} d_i \leqslant 1-L$.

Therefore, by Jensen's inequality, when $N_1 > 0$,

$$\begin{aligned} s\tilde{E}^1(\mathbf{Z}) \geqslant& \frac{1}{N^{s+1}} \sum_{i\in J_1} d_i^{-s} + \frac{1}{N^{s+1}} \sum_{i\in J_2} d_i^{-s} \\ \geqslant& \frac{N_1}{N^{s+1}} \left(\frac{1}{N_1} \sum_{i\in J_1} d_i \right)^{-s} + \frac{N_2}{N^{s+1}} \left(\frac{1}{N_2} \sum_{i\in J_2} d_i \right)^{-s} \\ \geqslant& \frac{N_1}{N^{s+1}} \left(\frac{L}{N_1} \right)^{-s} + \frac{N_2}{N^{s+1}} \left(\frac{1-L}{N_2} \right)^{-s} \\ =& \alpha^{s+1} L^{-s} + (1 - \frac{2}{N} - \alpha)^{s+1} (1-L)^{-s} \\ \geqslant& \alpha^{s+1} L^{-s} + (1-\alpha)^{s+1} (1-L)^{-s} - \frac{2(s+1)\cdot 2^{-s}}{N} \end{aligned}$$

and it is clear that the last inequality is also true when $N_1 = 0$. Using now the convexity of $x \to x^s$, we have

$$\begin{aligned} s\tilde{E}^1(\mathbf{Z}) &+ \frac{2(s+1)\cdot 2^{-s}}{N} \\ &\geqslant \alpha(\alpha/L)^s + (1-\alpha)((1-\alpha)/(1-L))^s \geqslant \left(\frac{\alpha^2}{L} + \frac{(1-\alpha)^2}{1-L} \right)^s \qquad (7.20) \\ &= \left(1 + \frac{(\alpha - L)^2}{L(1-L)} \right)^s \geqslant 1 + \frac{s}{L(1-L)} (\alpha - L)^2. \end{aligned}$$

As in the proof of Lemma 7.2, inequalities (7.6) and (7.18) imply that (7.10) holds. By assumption, $\frac{2(s+1)\cdot 2^{-s}}{N} \leqslant \epsilon \leqslant \zeta(s;N)\epsilon$. So, in light of (7.20), we obtain

$$(\alpha - L)^2 \leqslant 2\epsilon\zeta(s;N)L(1-L)/s \leqslant \tilde{\zeta}(s)L(1-L)\cdot 2\epsilon,$$

which, gives (7.19). □

Theorem 2.2 follows directly from Lemmas 7.2 and 7.3.

Proof of Theorem 2.2. Let N_0 be large enough so that $(1+\epsilon)\zeta(s)/\zeta(s;N_0) \leqslant (1 + 2\epsilon)$. From (7.3), we have

$$\tilde{E}(\mathbf{Z}) \leqslant E(\mathbf{Z}) \leqslant \tilde{\zeta}(s)(1+\epsilon) \leqslant s^{-1}\zeta(s;N)(1+2\epsilon).$$

Then Lemma 7.2 implies (2.4) while Lemma 7.3 shows that (2.5) holds. □

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