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# ENERGY SCALING AND ASYMPTOTIC PROPERTIES OF STEP BUNCHING IN EPITAXIAL GROWTH WITH ELASTICITY EFFECTS*

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**Abstract.** In epitaxial growth on vicinal surfaces, elasticity effects give rise to step bunching instability and some self-organization phenomena, which are widely believed to be important in the fabrication of nanostructures. It is challenging to model and analyze these phenomena due to the nonlocal effects and interactions between different length scales. In this paper, we study a discrete model for epitaxial growth with elasticity. We rigorously identify the minimum energy scaling law and prove the formation and appearance of one bunch structure. We also provide sharp bounds for the bunch size and the slope of the optimal step bunch profile. Both periodic and Neumann boundary conditions are considered.

**Key words.** epitaxial growth, elasticity, step bunching, asymptotic analysis, energy scaling law

**AMS subject classifications.** 74G65, 74G45, 74A50, 49K99

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## 1. Introduction.

In epitaxial film growth, elastic effects often lead to surface morphological instabilities. These elastic effects can be caused by surface defects such as steps as well as the mismatch between the lattice constants of the substrate and the film. In this paper, we concentrate on the step bunching phenomena on vicinal surfaces [15, 18, 7]. Below the roughening transition temperature, a vicinal surface consists of a succession of terraces and atomic height steps, while the angle between this surface and the crystallographic plane is small, say, a few tenths of a degree. Due to elastic interactions, the steps are attracted to each other and coalesce into step bunches. The sizes of these step bunches increase gradually as further coalescence of small step bunches in the evolution. As a self-organization phenomenon, step bunching instability attracts considerable research interest in the materials science community because of its potential to facilitate the fabrication of nanostructures on the epitaxial surfaces. However, the understanding of this phenomenon is still incomplete. For instance, the length scale and coarsening rate of the step bunching dynamics have not been well-studied yet.

The elastic interactions between steps that lead to such step bunching instability include the force dipole interaction arising from the surface stress and the force monopole interaction coming from misfit stress in the bulk due to the mismatch between the lattice constants of the substrate and the film in heterogeneous epitaxy. The force dipole interaction between steps is repulsive, stabilizing the uniform step train, while the force monopole interaction between steps is attractive, destabilizing the uniform step train [15, 18, 6, 7, 17]. Figure 1 is an illustration of the mechanisms of these interactions.

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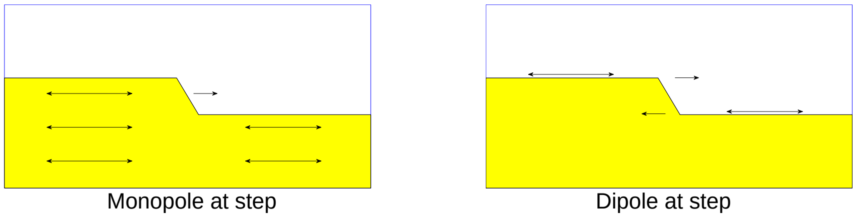


FIG. 1. *Monopole and dipole effects of a step on the epitaxial surface,* [17]. *The double arrows represent the compressive stress, which is in the bulk of the film in the left image and on the film surface in the right image.*

Based on the Burton, Cabrera, and Frank (BCF) theory [3], which assumes the diffusion of adatoms on the terraces until their attachment to the steps, Tersoff and others [18, 13] proposed a discrete model for the dynamics of steps incorporating the two elasticity effects. In their model, the motion of the steps is given by

$$\frac{1}{a^2}\frac{\mathrm{d}x_i}{\mathrm{d}t} = F_{\mathrm{ad}}\frac{l_i + l_{i+1}}{2} + \frac{\rho_0 D}{k_B T}\left(\frac{f_{i+1} - f_i}{l_i} - \frac{f_i - f_{i-1}}{l_{i-1}}\right),\ i \in \mathbb{Z}. \tag{1}$$

In the above, $x_i$ is the position of the $i$th step, $l_i = x_{i+1} - x_i$ is the length of the $i$th terrace, $a$ is the lattice constant, $F_{\mathrm{ad}}$ is adatom flux, and $\rho_0$, $D$, $k_B$, and $T$ are the equilibrium adatom density on a step in the absence of elastic interactions, the diffusion constant on the terrace, Boltzmann constant and temperature, respectively. The elastic force per unit length on the $i$th step is given by

$$f_i = -\sum_{j \neq i}\left(\frac{\alpha_1}{x_j - x_i} - \frac{\alpha_2}{(x_j - x_i)^3}\right), \tag{2}$$

where the attractive interaction $-\sum_{j\neq i}\frac{\alpha_1}{x_j - x_i}$ is due to the force monopole effect of steps, and the repulsive interaction $\sum_{j\neq i}\frac{\alpha_2}{(x_j-x_i)^3}$ is due to the force dipole effects of steps. The coefficients $\alpha_1, \alpha_2$ are assumed to be positive constants. In their work, Tersoff and others analyzed linear instability for equispaced steps under small perturbation and then studied the size and spacing of the bunches as well as the coarsening rate by numerical simulation. Duport and others [6, 7] also studied the step bunching phenomenon. Besides force monopole and dipole, they considered two more effects: the elastic interaction between the adatoms and steps and the Schweobel barrier. Depending on the sign of the misfit, the former can stabilize or destabilize the uniform step train, while the latter is always stabilizing.

The previously introduced models are discrete in the sense that they capture all step positions. Continuum models of larger length scales have also been developed. However, the traditional surface morphological model [2, 10, 16] which demonstrates the long wave length instability of a planar surface of a stressed solid is not applicable here due to the fact that the temperature is lower than the roughening transition point so that discrete effects remain important. To incorporate the atomic structure of the crystal, Xiang [19] derived a continuum model by taking the continuum limit from the discrete models of [18, 13, 6, 7]. Xu and Xiang [21] extended this to 2+1 dimensions. Margetis and Kohn [14] also rigorously derived a 2+1 dimensional continuum model from the BCF model. Their model includes the force dipole effect but does not include the force monopole effect in the heterogeneous epitaxial films. Considering step line tension and force dipole interaction between adjacent steps together with the Schweobel barriers, Fok, Rosales, and Margetis [8] derived a continuum model for concentric circular steps. They unified the step bunching phenomena under these effects by pointing out that the line tension and the other physical effects, such as desorption, deposition, or drift, all contribute to a destabilizing, backward diffusion term in the resulting PDEs. Kukta and Bhattacharya [11] proposed a three-dimensional continuum model, coupling stress with diffusion.

Xiang and E [20] performed linear stability analysis and numerical simulations to validate their continuum model for step bunching under elastic interactions. The continuum model is able to predict linear instability of a uniform step train and evolution of a stepped surface in the nonlinear regime, which are in agreement with the results of the discrete model. Zhu, Xu, and Xiang [22] performed linear instability analysis and numerical simulations using the 2+1 dimensional continuum model. Dal Maso, Fonseca, and Leoni [5] and Fonseca, Leoni, and Lu [9] proved the existence and regularity of weak solutions of Xiang and E's 1+1 dimensional continuum model [19, 20]. There are also several analytical results for the dynamics of epitaxial growth without elasticity. Al Hajj Shehadeh, Kohn, and Weare [1] considered both discrete and continuum models in the attachment-detachment-limited regime. Their model only included the force dipole interaction between nearest steps, and hence there is no step bunching phenomenon. Li and Liu [12] studied well-posedness, perturbation analysis, as well as numerical simulation of epitaxial growth with or without slope selection.

As linear stability analysis is valid only for step profiles close to a uniform step train, it cannot provide complete information about step bunching which is a highly nonlinear phenomena. This is similar to the Cahn–Hilliard theory [4] of phase transition which also involves multiple stage phenomena: the initial spinodal decomposition and the later coarsening process. To the best of our knowledge, there is not yet a complete rigorous analysis on the step bunching phenomenon in epitaxial growth with elasticity.

In this paper, we study the Tersoff's discrete model (equations (1) and (2)) in the periodic setting, concentrating on the structures of the surface profiles when the number of steps is large. This is to mimic the behavior of such a surface under long-range elastic interactions. Specifically, from numerical simulation, with a large number of initial steps, it appears that many step bunches will form as the first stage. They are roughly equidistant from each other. Hence the periodic boundary condition can capture the essential picture, even quantitatively. In the second stage, these step bunches will coarsen. We believe our results can lead to better understanding of the pattern formation and self-organization phenomenon. After reformulating our model as a gradient flow of an underlying elastic energy functional, we will investigate the properties of the energy minimizer. Roughly speaking, we have the following questions and answers:

1. Q: Is there a solution for the minimization and dynamical problems?
   A: Existence of minimizer and gradient structure of the dynamics.
2. Q: What is the energy of the minimizer?
   A: Energy scaling law.
3. Q: Does the minimizer have only one step bunch?
   A: All steps concentrate in a narrow band.
4. Q: What is the structure of this bunch?
   A: Size of the bunch and slope of the bunch profile.

The above questions are very subtle and yet we are able to provide quite satisfactory answers. The main difficulty is due to the long-range interaction leading to nonlocal effects. Estimating the energy of individual pairs of steps is far from enough in controlling the total energy. To obtain sharp energy bounds for our model, we have to take the interrelation of step positions into account. Furthermore, due to the periodic setting, the distance between the steps is measured on a circle. This destroys the monotonicity property of the pairwise potential and hence leads to some difficulties in the analysis.

**2. Main results and outline of proofs.** We will study the step bunching instability based on energy consideration. The no-flux condition $F_{\text{ad}} = 0$ will be assumed. In [18], Tersoff et al. reported the existence of step bunching without the adatom flux by simulations. Their model with one attraction term and one repulsion term in (1) and (2) seems to be the simplest formulation to capture the essential effects. In practice, the vicinal surface is very large, and we shall use the periodic boundary condition. But our results can be extended to the Neumann boundary condition and even more general pairwise interactions (see section 12).

We first introduce the notation for the periodic setting. Let the physical length of one period be $L$. Then all the step locations $\{x_i\}_{i=-\infty}^{\infty}$ can be completely described by some $N$ steps:

$$X = (x_1, x_2, \dots, x_N)^T \quad \text{with} \quad 0 \le x_1 < x_2 < \cdots < x_N < L. \tag{3}$$

The periodicity is enforced by the condition $x_{i+N} - x_i = L$ for all $i \in \mathbb{Z}$. Hence $X$ lives inside the $N$-dimensional torus $\mathbb{T}^N = [0, L)^N$. We also introduce $l$ to be the average length of the terrace in one period. Then we have $L = Nl$. Our main analysis concerns asymptotic properties of solutions for $N \gg 1$ or $N \to \infty$ (with $l$ fixed).

With the above periodic boundary condition, the step motion (1) is turned into

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \frac{a^2\rho_0 D}{k_B T}\left(\frac{f_{i+1} - f_i}{l_i} - \frac{f_i - f_{i-1}}{l_{i-1}}\right), \; i = 1, 2, \dots, N. \tag{4}$$

We denote the initial data as

$$x_i(0) = x_i^0, \; i = 1, 2, \dots, N. \tag{5}$$

The elastic force $f_i$ now can be explicitly written as

$$f_i = -\sum_{1\le j\le N, j\ne i}\left[\frac{\alpha_1\pi}{Nl}\cot\frac{\pi(x_j - x_i)}{Nl} - \frac{\alpha_2\pi^3}{N^3l^3}\cot\frac{\pi(x_j - x_i)}{Nl}\left(\sin\frac{\pi(x_j - x_i)}{Nl}\right)^{-2}\right] \tag{6}$$

for $i = 1, 2, \dots, N$. This form has the advantage that we only need to calculate the long-range summation over the finite $N$ steps within one period while the original form in (2) requires the summation over all steps including the steps in each period and all their periodic images.

We relate the $f_i$'s to some underlying elastic energy $E(X) = E(x_1, x_2, \dots, x_N)$ as follows:

$$f_i = \frac{\partial E}{\partial x_i}, \tag{7}$$

where

$$E(X) = \sum_{1\le i<j\le N}\left[\frac{\alpha_1}{2}\log\sin^2\frac{\pi(x_j - x_i)}{Nl} + \frac{\alpha_2\pi^2}{2N^2l^2}\left(\sin\frac{\pi(x_j - x_i)}{Nl}\right)^{-2}\right] - E_N^0(l), \tag{8}$$

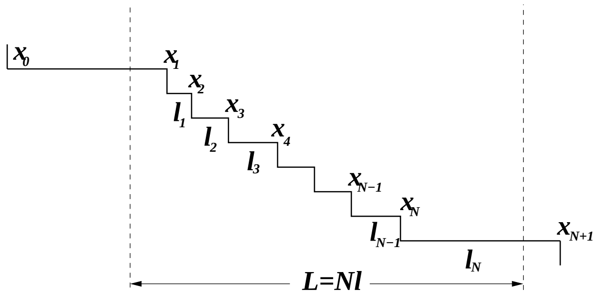


FIG. 2. *An example of step configuration. Recall the definition* $l_i = x_{i+1} - x_i$ *for* $i = 1, 2, \dots N$ *and* $l^{(1)} \leq l^{(2)} \leq \cdots \leq l^{(N)} = l_N$. *By the periodicity assumption, we have* $x_{i+N} = x_i + L$.

and $E_N^0(l)$ (often simply denoted by $E_N^0$) is some renormalization constant chosen to ensure that the uniform step train (with average terrace length $l$) has zero energy. The derivations of (6)–(8) are given in the appendix. Using $F = (f_1, f_2, \dots f_N)^T$, (7) can be written as

$$F = \mathrm{D}_X E. \tag{9}$$

Note that there is no negative sign because we are not applying Newton's second law. Indeed, $E$ is the total elastic energy and $f_i$ is the corresponding chemical potential for the dynamics in (4).

For the readers' convenience, we summarize our physical setting and notation.

**Physical constants**. We assume that the interaction coefficients $\alpha_1$, $\alpha_2$ in (2), the lattice constants $a$, and the average slope $A$ of the surface are all constants. Consequently, the average terrace length $l = \frac{a}{A}$ is also fixed. We further use $r$ to denote the constant

$$r := \frac{\alpha_2 \pi^2}{\alpha_1 l^2}, \tag{10}$$

which indicates the relative importance between the force monopole and dipole interactions.

**Geometric setting**. Recall that in the periodic setting, we have $x_{i+N} - x_i = Nl$ for all $i \in \mathbb{Z}$. The terrace length is defined as $l_i = x_{i+1} - x_i$ for all $i \in \mathbb{Z}$. A *step profile* $X$ is defined as $X = (x_1, x_2, \dots, x_N)^T$ with $0 \leq x_1 < x_2 < \cdots < x_N < L$, i.e., $x \in \mathbb{T}^N = [0, L)^N$. We rearrange the terrace lengths $\{l_i\}_{i=1}^N$ as $l^{(1)} \leq l^{(2)} \leq \cdots \leq l^{(N)}$. Without loss of generality, we set $l_N = l^{(N)} = \max_{1 \leq j \leq N} l_j$. See Figure 2.

The distance between any two steps $x_i$ and $x_j$ is defined as

$$\operatorname{dist}(x_i, x_j) := \min\{|x_i - x_j|, Nl - |x_i - x_j|\} \tag{11}$$

for $0 \leq x_i, x_j < Nl$.

Let $S = \{x_1, x_2, \dots, x_N\}$ be the set of all steps and $S_1, S_2$ be subsets of $S$. The distance between two step sets $S_1$ and $S_2$ is defined as

$$\operatorname{dist}(S_1, S_2) := \min_{x_i \in S_1, x_j \in S_2} \operatorname{dist}(x_i, x_j). \tag{12}$$

A *step chain* is any subset $T \subseteq S$ consisting of *consecutive steps* $x_i, x_{i+1}, \dots, x_j$. Note that $x_N$ and $x_1$ are regarded as two consecutive steps. We say that a step chain

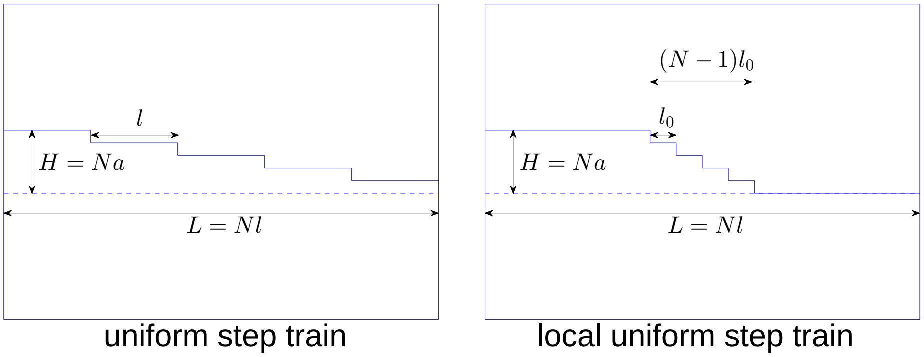


FIG. 3. *Uniform step train and local uniform step train. The latter is used to construct suitable ansatz to compute the mimimum energy.*

$T$ is *well isolated* from all the other steps if

$$\text{dist}(T, S\backslash T) > l_{**} = \frac{Nl}{\pi} \arcsin \sqrt{\frac{3r}{N^2 + 2r}}. \tag{13}$$

See (20) for the definition of $l_{**}$.

A *uniform step train* is any profile $X$ with $l_1 = l_2 = \cdots = l_N = l$, while a *local uniform step train* is any profile $X$ with $l_1 = l_2 = \cdots = l_{N-1}$. Note that $l_1$ may be less than $l$ in the latter one. See Figure 3.

**Interaction potential**. The total elastic energy can be written as

$$E(X) = E(x_1, \ldots, x_N) = \sum_{1 \le i < j \le N} e(x_j - x_i) - E_N^0, \tag{14}$$

where the pairwise energy density $e(\cdot)$ and the reference energy $E_N^0 = E_N^0(l)$ are defined as

$$e(x) := \frac{\alpha_1}{2} \left[ \log \sin^2 \frac{\pi x}{Nl} + \frac{r}{N^2} \left( \sin \frac{\pi x}{Nl} \right)^{-2} \right], \tag{15}$$

$$E_N^0 := \sum_{1 \le i < j \le N} e((j-i)l). \tag{16}$$

The first and second derivatives of $e(\cdot)$ are given by

$$e'(x) = \frac{\alpha_1 \pi}{Nl} \left( 1 - \frac{r}{N^2} \left( \sin \frac{\pi x}{Nl} \right)^{-2} \right) \cot \frac{\pi x}{Nl}, \tag{17}$$

$$e''(x) = \frac{\alpha_1 \pi^2}{N^2 l^2} \left[ \frac{3r}{N^2} - \left( 1 + \frac{2r}{N^2} \right) \sin^2 \frac{\pi x}{Nl} \right] \left( \sin \frac{\pi x}{Nl} \right)^{-4}. \tag{18}$$

By the periodicity assumption, we have

$$e(x) = e(Nl - x), \ \ e'(x) = -e'(Nl - x), \ \ e''(x) = e''(Nl - x). \tag{19}$$

The graphs of $e(\cdot), e'(\cdot)$ and $e''(\cdot)$ are given in Figure 4.

The following two properties of $e(\cdot)$ and $e'(\cdot)$ will be used often in our proofs.

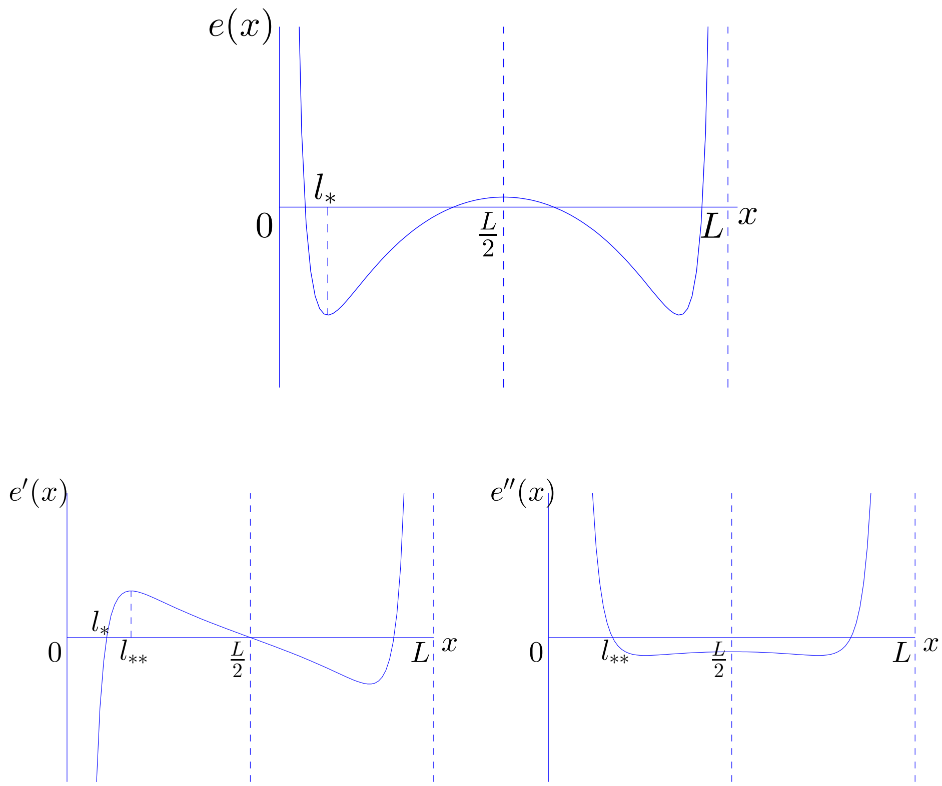


FIG. 4. *Plots of energy density and its derivatives* $e(\cdot)$, $e'(\cdot)$, *and* $e''(\cdot)$. *See* (15), (17), *and* (18).

1. For $N^2 > r$, there exist a unique $l_*$ and a unique $l_{**}$ satisfying

$$l_* := \arg \min_{0 \le x < \frac{Nl}{2}} e(x), \quad l_{**} := \arg \max_{0 \le x < \frac{Nl}{2}} e'(x). \tag{20}$$

Note that $e'(l_*) = 0$, $e''(l_{**}) = 0$ and $0 < l_* < l_{**} < \frac{Nl}{2}$. See Figure 4. In fact, for $N \gg 1$, we have

$$l_* = \frac{Nl}{\pi} \arcsin \frac{\sqrt{r}}{N} = \frac{\sqrt{r}l}{\pi} + O(N^{-2}), \tag{21}$$

$$l_{**} = \frac{Nl}{\pi} \arcsin \sqrt{\frac{3r}{N^2 + 2r}} = \frac{\sqrt{3r}l}{\pi} + O(N^{-2}). \tag{22}$$

2. The function $e(\cdot)$ is decreasing on $(0, l_*)$ and $(Nl/2, Nl - l_*)$ while increasing on $(l_*, Nl/2)$ and $(Nl - l_*, Nl)$. The function $e'(\cdot)$ is increasing on $(0, l_{**})$ and $(Nl - l_{**}, Nl)$ while decreasing on $(l_{**}, Nl - l_{**})$.

**Notation used in the proofs**. We use $C$ to denote positive constants which may depend on the physical constants $\alpha_1$, $\alpha_2$, $a$, and $A$ but not on $N$. We also use $C_\beta$ to indicate the possible dependence on some parameter $\beta$ other than the physical constants. The value of such $C$ may change from line to line. Next, we use $N \gg 1$ to indicate that $N$ is sufficiently large. Finally, we use $\#S$ to denote the cardinality of a finite set $S$.

As mentioned above, we will be mainly interested in the asymptotic behaviors of minimizers as $N \to +\infty$. These include the well-posedness issue as well as the structure and stability of the step profile in our model. Our main results are summarized below.

THEOREM 1 (existence).
(a) (Initial value problem) *For all $N$, the initial value problem* (4)–(5) *has a global in time solution. In other words, there is no finite time blow-up.*
(b) (Minimization problem) *For all $N$, there exists a global minimizer for the energy $E$ in* (14).
(c) (Equivalence) *For all $N$, the stable stationary states of* (4) *are the same as the local minimizers of $E$.*

THEOREM 2 (energy scaling law). *For any $\delta > 0$, there exist constants $c_\delta$ and $C$ such that*

$$-\left(\frac{\alpha_1}{4} + \delta\right) N^2 \log N - c_\delta N^2 \le \inf_{X \in \mathbb{T}^N} E(X) \le -\frac{\alpha_1}{4} N^2 \log N + CN^2 \tag{23}$$

*for all $N$. Consequently,* $\lim_{N\to+\infty} \frac{\inf E(X)}{N^2 \log N} = -\frac{\alpha_1}{4}$.

THEOREM 3 (one bunch structure).
(a) (Closeness of steps) *For all $N$, any step profile with a well-isolated step chain is not a stable stationary state. In other words, any local minimizer of $E$ has the property that*

$$\operatorname{dist}(T, S\backslash T) \le l_{**} \text{ for all } T \subset S. \tag{24}$$

*In particular, $l^{(i)} \le l_{**}$ for all $i = 1, 2, \dots, N-1$.*
(b) (Bunch size less than half period) *For any global minimizer of $E$ with $N \gg 1$, we have*

$$l_1 + \cdots + l_{N-1} \le \frac{Nl}{2} \quad \text{and} \quad l_N \ge \frac{Nl}{2}. \tag{25}$$

(c) (Asymptotically narrow bunch size) *For any global minimizer of $E$, we have*

$$\lim_{N\to+\infty} \frac{l_1 + \cdots + l_{N-1}}{l_N} = 0. \tag{26}$$

THEOREM 4 (size of the bunch). *For any global minimizer of $E$ and for all $N$, we have the following:*
(a) (Lower bound) *There exists $C$ such that*

$$CN^{1/2} (\log N)^{-1/2} \le l_1 + \cdots + l_{N-1}. \tag{27}$$

(b) (Upper bound) *For any $\delta > 0$ and any $0 < s < 1$, there exists $C_{\delta,s}$ such that*

$$\min_i \left\{ l_i + \cdots + l_{i+[sN]} \right\} \le C_{\delta,s} N^{1/2+\delta}. \tag{28}$$

THEOREM 5 (slope of the bunch profile). *For any global minimizer of $E$, we have the following:*
(a) (Estimates on the minimal terrace length $l^{(1)}$) *For any $\delta > 0$, there exist constants $c_\delta$ and $C_\delta$ such that*

$$c_\delta N^{-1/2-\delta} \le l^{(1)} \le C_\delta N^{-1/2+\delta} \tag{29}$$

*for all $N$.*

(b) (Estimates on the next-maximal terrace length $l^{(N-1)}$) *For any* $\delta > 0$, *there exist constants* $c_\delta$ *and* $C$ *such that*

$$c_\delta N^{-1/6-\delta} \le l^{(N-1)} \le C \tag{30}$$

*for all* $N$. *Furthermore,* $l^{(N-1)} \le l_*$ *for* $N \gg 1$.

The main strategy of proofs is to investigate the energy $E$. There are three key considerations:

1. Construction of good approximate ansatz to give good energy upper and lower bounds.
2. Analysis of the vanishing condition of the first variation of $E$, $D_X E = 0$, which is equivalent to the force balance $F = 0$. The results obtained in fact hold for any critical point of the energy functional. In terms of $x_i$'s, the condition reads

$$\frac{\partial E}{\partial x_i} = 0, \text{ i.e., } \sum_{1 \le j < i} e'(x_i - x_j) - \sum_{i < k \le N} e'(x_k - x_i) = 0, \text{ for } i = 1, \ldots, N. \tag{31}$$

   This is equivalent to, in terms of $l_i$'s,

$$\frac{\partial E}{\partial l_i} = 0, \text{ i.e., } \sum_{1 \le j \le i \le k \le N-1} e'(l_j + \cdots + l_i + \cdots + l_k) = 0, \text{ for } i = 1, \ldots, N-1. \tag{32}$$

3. Analysis of the second variation of $E$, $D_X^2 E$. For minimizer (or stable local minimizer), it must hold that

$$D_X^2 E \ge 0. \tag{33}$$

The remainder of this paper is organized as follows. In section 3, we reformulate the system into a gradient flow dynamics and then prove the existence of minimizers (Theorem 1). In section 4, using a suitable ansatz, we obtain a weak version of Theorem 2 for the minimum energy scaling law. The whole theorem (the strong version) is proved in section 9. By analyzing the Hessian matrix of a critical point, section 5 proves that an isolated bunch is unstable (Theorem 3(a)). In section 6, we first find a lower bound for the minimal terrace length $l^{(1)}$ by controlling the first variation of the energy. This gives the lower bounds in Theorem 5(a) and (b). Then an iteration scheme is applied to improve this bound. The main idea in the iteration scheme is to group the $O(N^2)$ interacting pairs into $N$ step chains and then estimate the contribution of each chain. Section 7 shows that all the steps of an energy minimizer concentrate in half period (Theorem 3(b)). This is crucial to the proofs for the remaining results. Indeed, the distance $\text{dist}(x_i, x_j)$ equals $|x_i - x_j|$, provided they are in the same half period. In section 8, we study the distribution of the terrace lengths, and then the lower bound for the bunch size is obtained (Theorem 4(a)). In section 9, we complete the strong version of the minimum energy scaling law (Theorem 2). In section 10, we use the energy estimates on each step chain to prove the upper bound for the bunch size (Theorem 4(b)). In section 11, we combine all the previous results to prove the upper bound for terrace lengths (upper bounds in Theorem 5(a) and (b)) and the one bunch structure property (Theorem 3(c)). Finally, section 12 provides an extension to Neumann boundary condition.

**3. Gradient flow structure and existence of minimizers.** Mathematical foundation and preliminary results are established in this section, including the gradient flow structure and global in time solution of the initial value problem (4)–(5) and the existence of a minimizer for the energy functional $E$ in (14). These are essentially the statements of Theorem 1. We start with an observation of the energy dissipation law.

PROPOSITION 1 (energy dissipation law). *For the initial value problem* (4)–(5) *with* $N \geq 2$*, we have the energy dissipation law*

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\frac{a^2\rho_0 D}{k_B T}\sum_{i=1}^{N}\frac{1}{l_i}(f_{i+1}-f_i)^2. \tag{34}$$

*Therefore, the energy* $E$ *decreases in time.*

*Proof.* By using (4) and (7), this follows from a direct computation:

$$\begin{aligned}\frac{\mathrm{d}E}{\mathrm{d}t} = \sum_{i=1}^{N}\frac{\partial E}{\partial x_i}\dot{x}_i &= \frac{a^2\rho_0 D}{k_B T}\sum_{i=1}^{N} f_i\left(\frac{f_{i+1}-f_i}{l_i} - \frac{f_i - f_{i-1}}{l_{i-1}}\right)\\ &= -\frac{a^2\rho_0 D}{k_B T}\sum_{i=1}^{N}\frac{1}{l_i}(f_{i+1}-f_i)^2.\end{aligned}$$

∎

Because of the above statement, one may expect (4) to be some kind of gradient flow. In fact, we can construct an abstract gradient flow structure for this system. Notice that for our step dynamics, the center of mass of the step positions defined as $\frac{x_1+\cdots+x_N}{N}$ remains a constant, which without loss of generality is assumed to be $\frac{L}{2}$. Therefore, our dynamics lives on $\mathcal{M}^{N-1} := \left\{X \in \mathbb{T}^N : x_1+\cdots+x_N = \frac{L}{2}\right\}$. In the next proposition, we will equip the manifold $\mathcal{M}^{N-1}$ with a Riemannian metric $g$ so that the system is a gradient flow with respect to $g$.

PROPOSITION 2 (gradient flow structure). *For any* $N \geq 2$*, there exists a Riemannian metric* $g$*, which can be regarded as an* $(N-1)\times(N-1)$ *positive definite matrix, such that* (4) *has the gradient flow structure*

$$\dot{X}|_{N-1} = -grad_g E, \tag{35}$$

*where* $X|_{N-1} = (x_1, x_2, \ldots, x_{N-1})^T$ *with* $x_1+x_2+\cdots+x_{N-1}+x_N = \text{constant}$*. Under this metric, the dissipation law reads as* $\dot{E} = -g_{X(t)}(\dot{X}|_{N-1}, \dot{X}|_{N-1})$.

*Remark* 1. The precise meaning of $\dot{X}|_{N-1} = -\mathrm{grad}_g E$ is that for all $t > 0$ and $Y \in T_{X(t)}\mathcal{M}^{N-1}$, we have

$$g_{X(t)}(\dot{X}|_{N-1}(t), Y) + \langle \mathrm{diff} E_{X(t)}, Y\rangle = 0, \tag{36}$$

where $T_{X(t)}\mathcal{M}^{N-1}$ is the tangent space of $\mathcal{M}^{N-1}$ at $X(t)$ and $\langle\cdot,\cdot\rangle$ is the inner product on $\mathcal{M}^{N-1}$ endowed from $\mathbb{R}^N$.

*Proof.* Let $A = (A_1, A_2, \ldots, A_{N-1})^T$ with $A_i = \frac{f_{i+1}-f_i}{x_{i+1}-x_i}$ for $i = 1, 2, \ldots, N-1$. Denote $A_N = \frac{f_1 - f_N}{Nl + x_1 - x_N}$. Note that $\sum_{i=1}^{N} l_i A_i = 0$ and hence $A_N = -\frac{\sum_{i=1}^{N-1} l_i A_i}{l_N}$. Using this notation, we have

$$\dot{x}_1 = \frac{a^2\rho_0 D}{k_B T}(A_1 - A_N), \quad \dot{x}_i = \frac{a^2\rho_0 D}{k_B T}(A_i - A_{i-1}), \quad i = 2, 3, \ldots, N-1, N.$$

We put the above into a matrix form $\dot{X}|_{N-1} = \frac{a^2\rho_0 D}{k_B T} JA$, where $J$ is an $(N-1)\times(N-1)$ matrix defined as follows:

$$J = \begin{pmatrix} 1+\frac{l_1}{l_N} & \frac{l_2}{l_N} & \cdots & \frac{l_{N-1}}{l_N} \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}.$$

Let $\Lambda$ be the $(N-1)\times(N-1)$ diagonal matrix $\Lambda = \mathrm{diag}\{l_1, \ldots, l_{N-1}\}$ and $\tilde{\Lambda}$ with $\tilde{\Lambda}_{ij} = \Lambda_{ij} + \frac{l_i l_j}{l_N}$ for $i, j = 1, 2, \ldots, N-1$. Then (34) can be written as

$$\begin{aligned} \dot{E} = -\frac{a^2\rho_0 D}{k_B T}\sum_{i=1}^{N} l_i A_i^2 &= -\frac{a^2\rho_0 D}{k_B T}\left[\sum_{i,j=1}^{N-1} A_i \Lambda_{ij} A_j + \frac{\left(\sum_{i=1}^{N-1} l_i A_i\right)^2}{l_N}\right] \\ &= -\frac{a^2\rho_0 D}{k_B T}\left[\sum_{i,j=1}^{N-1} A_i \tilde{\Lambda}_{ij} A_j\right]. \end{aligned}$$

It is easy to check that $\det(J) = \frac{Nl}{l_N} \neq 0$ and $\tilde{\Lambda}$ is positive definite. Hence $J$ and $\tilde{\Lambda}$ are both invertible. Therefore, we can define the positive definite metric

$$g = \left(\frac{a^2\rho_0 D}{k_B T}\right)^{-1} (J^{-1})^T \tilde{\Lambda} J^{-1}. \tag{37}$$

Now, the energy dissipation law (34) can be written as

$$\begin{aligned} \dot{E} = -\frac{a^2\rho_0 D}{k_B T} A^T \tilde{\Lambda} A &= -\left(\frac{a^2\rho_0 D}{k_B T} A^T J^T\right) g \left(\frac{a^2\rho_0 D}{k_B T} JA\right) \\ &= -\left(\dot{X}|_{N-1}\right)^T g \dot{X}|_{N-1} = -g_{X(t)}(\dot{X}|_{N-1}, \dot{X}|_{N-1}), \end{aligned}$$

which is the desired statement. ∎

It is important to remark that our manifold $\mathcal{M}^{N-1}$ is open in the sense that $x_i < x_{i+1}$ for $i = 1, 2, \ldots, N-1$. The Cauchy–Lipschitz theory, in general, only guarantees the local in time existence of the initial value problem (4)–(5). Next we provide a positive lower bound for $x_{i+1} - x_i$ which is used to prove that there will be no finite time blow-up for the solution.

PROPOSITION 3 (minimal terrace length). *For any $N \geq 2$ and any solution of (4) with initial data (5) and initial energy $E(X(0))$, at any time $t$ at which the solution exists, we have the following lower bound for the terrace lengths:*

$$l_{\min}(t) \geq \min\left\{\frac{\alpha_2 A}{2\alpha_1 a} N^{-1}, \left[\frac{4}{\alpha_2} E(X(0)) + \frac{4C}{\alpha_2} N^2 \log N\right]^{-\frac{1}{2}}\right\}, \tag{38}$$

*where $l_{\min}(t) = \min_{1\leq i\leq N} l_i(t)$ and $C$ is independent of $N$ and initial value. Note that $l_N(t) = Nl + x_1(t) - x_N(t)$.*

*Proof.* Notice that $\min_{s\in\mathbb{R}^+}\left\{\log s + \frac{r}{N^2 s}\right\} = \log\frac{r}{N^2} + 1$. By definition (15), we have

$$e(x) \geq \frac{\alpha_1}{2}\left(\log\frac{r}{N^2} + 1\right) \quad \text{for all} \quad x > 0. \tag{39}$$

By energy dissipation law (34), we deduce that

$$E(X(0)) \geq E(X(t)) \geq \left[\frac{\alpha_1}{2}\log\sin^2\frac{\pi l_{\min}(t)}{Nl} + \frac{\alpha_2\pi^2}{2N^2l^2}\left(\sin\frac{\pi l_{\min}(t)}{Nl}\right)^{-2}\right] + \left[\frac{N(N-1)}{2}-1\right]\frac{\alpha_1}{2}\left(\log\frac{r}{N^2}+1\right) - E_N^0.$$

Note that $\frac{2l_{\min}}{Nl} \leq 1$ leading to $\log\frac{2l_{\min}}{Nl} \geq -\left(\frac{2l_{\min}}{Nl}\right)^{-1}$. If $l_{\min}(t) \leq \frac{\alpha_2}{2\alpha_1 Nl} = \frac{\alpha_2 A}{2\alpha_1 a}N^{-1}$, then

$$\frac{\alpha_1}{2}\log\sin^2\frac{\pi l_{\min}(t)}{Nl} \geq \alpha_1\log\frac{2l_{\min}}{Nl} \geq -\alpha_1\left(\frac{2l_{\min}}{Nl}\right)^{-1} \geq -\frac{\alpha_2\pi^2}{4N^2l^2}\left(\frac{\pi l_{\min}}{Nl}\right)^{-2} \geq -\frac{\alpha_2\pi^2}{4N^2l^2}\left(\sin\frac{\pi l_{\min}}{Nl}\right)^{-2}. \tag{40}$$

Hence

$$E(X(0)) \geq \frac{\alpha_2}{4}\left(l_{\min}(t)\right)^{-2} + \frac{\alpha_1}{2}\left[\frac{N(N-1)}{2}-1\right]\left(\log\frac{r}{N^2}+1\right) - E_N^0.$$

By Lemma 1 (in section 4), $E_N^0 \leq -\frac{\alpha_1}{2}N^2\log\frac{2e}{\pi} + O(N\log N)$, there exists a constant $C$ such that

$$E(X(0)) \geq \frac{\alpha_2}{4}\left(l_{\min}(t)\right)^{-2} - CN^2\log N.$$

We then obtain the lower bound for the minimal terrace length

$$l_{\min}(t) \geq \min\left\{\frac{\alpha_2 A}{2\alpha_1 a}N^{-1}, \left[\frac{4}{\alpha_2}E(X(0)) + \frac{4C}{\alpha_2}N^2\log N\right]^{-1/2}\right\}$$

for all $t \in [0,T]$, where the initial value problem of ODE system has a solution. ∎

*Proof of Theorem* 1(a). We have the local in time existence by means of the local Lipschitz property of the right-hand side of (4). This, combined with Proposition 3, guarantees that the solution can be extended to all time. ∎

The next result shows that the velocities of the steps decay to zero as time goes to infinity.

PROPOSITION 4 (long time behavior of initial value problem). *For any $N \geq 2$ and for any initial data* (5)*, the velocity of all steps go to zero, i.e.,* $\lim_{t\to+\infty}\dot{X}(t) = 0$.

*Proof.* We prove the proposition by contradiction. Suppose there exist some $\delta > 0$ and a sequence $0 < t_1 < t_2 < \cdots < t_k < \cdots$ with $\lim_{k\to+\infty} t_k = +\infty$ such that $|\dot{X}(t_k)| > \delta$ for all $k$.

We rewrite (4) into $\dot{X}(t) = G(X(t))$, where

$$G_i(X(t)) = \frac{a^2\rho_0 D}{k_B T}\left(\frac{f_{i+1}-f_i}{l_i} - \frac{f_i - f_{i-1}}{l_{i-1}}\right) \quad \text{for } i = 1,2,\ldots,N. \tag{41}$$

Notice that $G(\cdot)$ is a smooth map from $\mathcal{M}^{N-1}$ to $\mathbb{R}^N$. Given initial data $X(0)$, by Proposition 3, $X(t)$ always lives on a compact submanifold $\overline{\mathcal{N}}$ of $\mathcal{M}^{N-1}$. Let

$M = \max_{X\in\overline{\mathcal{N}}}\{|G(X)|, |\mathrm{D}_X G(X)|\} < +\infty$ and $m = \min_{X\in\overline{\mathcal{N}}} \|g(X)\|_{l^2} > 0$, where the metric $g$ is given by (37).

Since $|G(X(t_n))| = |\dot{X}(t_n)| > \delta$ for $t \in [t_n, t_n + \frac{\delta}{2M^2}]$, the Taylor theorem gives

$$\begin{aligned}|\dot{X}(t)| = |G(X(t))| &\geq |G(X(t_n))| - |\mathrm{D}_X G(\xi)|\,|X(t) - X(t_n)| \\ &\geq |G(X(t_n))| - \max_{\xi\in\overline{\mathcal{N}}} |\mathrm{D}_X G(\xi)| \left|\int_{t_n}^{t} G(X(\tau))\mathrm{d}\tau\right| \\ &\geq \delta - M\cdot\frac{\delta}{2M^2}\cdot M \geq \frac{\delta}{2}.\end{aligned}$$

By Proposition 2, we have $\dot{E}(t) = -(\dot{X}|_{N-1})^T g \dot{X}|_{N-1} \leq -\frac{m\delta^2}{4}$ for $t \in \left[t_n, t_n + \frac{\delta}{2M^2}\right]$ and $n = 1, 2, \ldots$. Hence, on the one hand, we have

$$\lim_{T\to+\infty} E(X(T)) - E(X(0)) = -\infty. \tag{42}$$

On the other hand, $E_N^0$ is a fixed finite number (see Lemma 1). Hence for any $T > 0$, $E(X(T)) - E(X(0)) \geq \frac{\alpha_1 N(N-1)}{4}\left(\log\frac{r}{N^2} + 1\right) - E_N^0 - E(X(0))$ is finite and independent of $T$. This contradicts (42). Therefore $\lim_{t\to+\infty}\dot{X}(t) = 0$. ∎

It is reasonable to believe that for most initial data, the system will tend to certain stable stationary state $X(\infty)$. We will show the equivalence between the stable stationary states of (4) and the local minimizers of $E$, that is, Theorem 1(c). Then we prove the existence of the minimum energy states Theorem 1(b) and hence the existence of the stable stationary state of (4).

*Proof of Theorem* 1(c). Let $G(X)$ be the one defined in (41). Indeed we are going to prove the equivalence between the following two stability conditions:

$$(1)\ G(X) = 0,\ \mathrm{D}_X G(X) \leq 0; \quad (2)\ \mathrm{D}_X E = 0,\ \mathrm{D}_X^2 E \geq 0.$$

1. *Critical points are the same.* On the one hand, if $\frac{\partial E}{\partial x_i} = 0$ for $i = 1, 2, \ldots, N$, then $f_i = 0$ for $i = 1, 2, \ldots, N$. This immediately implies $G_i = 0$ for $i = 1, 2, \ldots, N$.

On the other hand, if $G_i = 0$ for $i = 1, 2, \ldots, N$, then $\frac{f_1 - f_N}{Nl - (l_1 + \cdots + l_{N-1})} = \frac{f_2 - f_1}{l_1} = \cdots = \frac{f_N - f_{N-1}}{l_{N-1}}$. We denote this number as $C$. Thus, $0 = (f_1 - f_N) + (f_2 - f_1) + \cdots + (f_N - f_{N-1}) = NlC$. Hence $C = 0$ and $f_1 = f_2 = \cdots = f_N$. Note that $f_1 + f_2 + \cdots + f_N = 0$. Therefore $f_1 = f_2 = \cdots = f_N = 0$ and $\frac{\partial E}{\partial x_i} = 0$ for $i = 1, 2, \ldots, N$.

2. *Stability of local minimizer:* $\mathrm{D}_X^2 E \geq 0$. Denote Hessian matrix of $E$ as $H = (H_{ij})_{N\times N} := (\frac{\partial^2 E}{\partial x_i \partial x_j})_{N\times N}$. Direct computation shows that

$$H_{ij} = \begin{cases} -e''(x_j - x_i), & i \neq j, \\ \sum\limits_{1\leq k\leq N, k\neq i} e''(x_k - x_i), & i = j. \end{cases}$$

For local minimizer $X = (x_1, x_2, \ldots, x_N)^T$, the stability condition is $H \geq 0$.

3. *Stability at critical point of ODE system:* $D_X G \leq 0$. Linearize the equation at any critical point. Note that $f_1 = f_2 = \cdots = f_N$ at this critical point. Using $f_i = \frac{\partial E}{\partial x_i}$, we have

$$-\left(\frac{a^2\rho_0 D}{k_B T}\right)^{-1}\frac{\partial G_i}{\partial x_j} = -\frac{1}{l_i}\frac{\partial f_{i+1}}{\partial x_j} + \left(\frac{1}{l_i} + \frac{1}{l_{i-1}}\right)\frac{\partial f_i}{\partial x_j} - \frac{1}{l_{i-1}}\frac{\partial f_i}{\partial x_j}$$

$$
\begin{aligned}
&+\frac{f_{i+1}-f_i}{l_i^2}\frac{\partial l_i}{\partial x_j}-\frac{f_i-f_{i-1}}{l_{i-1}^2}\frac{\partial l_{i-1}}{\partial x_j}\\
&=-\frac{1}{l_i}\frac{\partial f_{i+1}}{\partial x_j}+\left(\frac{1}{l_i}+\frac{1}{l_{i-1}}\right)\frac{\partial f_i}{\partial x_j}-\frac{1}{l_{i-1}}\frac{\partial f_i}{\partial x_j}\\
&=-\frac{1}{l_i}H_{(i+1)j}+\left(\frac{1}{l_{i-1}}+\frac{1}{l_i}\right)H_{ij}-\frac{1}{l_{i-1}}H_{(i-1)j}\\
&=A_{ik}H_{kj},
\end{aligned}
$$

where $H_{0j} := H_{Nj}$, $H_{(N+1)j} := H_{1j}$ for $j = 1, 2, \ldots, N$ and $A$ is defined as the $N \times N$ symmetric matrix

$$
A := \begin{pmatrix}
\frac{1}{l_1}+\frac{1}{l_N} & -\frac{1}{l_1} & 0 & \cdots & 0 & -\frac{1}{l_N}\\
-\frac{1}{l_1} & \frac{1}{l_1}+\frac{1}{l_2} & -\frac{1}{l_2} & 0 & \cdots & 0\\
0 & -\frac{1}{l_2} & \frac{1}{l_2}+\frac{1}{l_3} & -\frac{1}{l_3} & \cdots & 0\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\
0 & \cdots & 0 & -\frac{1}{l_{N-2}} & \frac{1}{l_{N-2}}+\frac{1}{l_{N-1}} & -\frac{1}{l_{N-1}}\\
-\frac{1}{l_N} & 0 & \cdots & 0 & -\frac{1}{l_{N-1}} & \frac{1}{l_{N-1}}+\frac{1}{l_N}
\end{pmatrix}.
$$

For critical point $X = (x_1, x_2, \ldots, x_N)^T$, the stability condition is $AH \geq 0$.

4. *Equivalence between the two stability conditions.* Note that $H = H^T, A = A^T$, and $AH = HA$. Thus $A$ and $H$ can be simultaneously diagonalized. Moreover, $A$ is a rank $(N-1)$ positive semidefinite matrix. Therefore, there exists an invertible matrix $P$ such that $P^{-1}AP = \Lambda_1 = \mathrm{diag}(0, \lambda_2, \lambda_3, \ldots, \lambda_N)$ and $P^{-1}HP = \Lambda_2 = \mathrm{diag}(0, \mu_2, \mu_3, \ldots, \mu_N)$ with $0 < \lambda_2 \leq \lambda_3 \cdots \leq \lambda_N$. Note that $P^{-1}AHP = \Lambda_1\Lambda_2 = \mathrm{diag}(0, \lambda_2\mu_2, \lambda_3\mu_3, \ldots, \lambda_N\mu_N)$. Obviously, $\mu_i \geq 0$ for $i = 2, 3, \ldots, N$ if and only if $\lambda_i\mu_i \geq 0$ for $i = 2, 3, \ldots, N$. This shows the equivalence between the two stability conditions. ∎

The proof of the existence of minimum energy solution mainly relies on the observation that whenever two adjacent steps approach each other, the energy blows up to positive infinity. This is reminiscent of the similar lower bound (38) for the initial value problem (4)–(5).

*Proof of Theorem* 1(b). Note that the energy is a continuous function of the multivariables $X = (x_1, x_2, \ldots, x_N)^T$. The conclusion follows from the following two statements.

1. *Energy bounded from below.* By (39), we obtain a uniform lower bound for the energy $E(X) \geq \frac{\alpha_1 N(N-1)}{4}\left(\log \frac{r}{N^2} + 1\right) - E_N^0$.

2. *Coercivity of the energy.* Recall that $l^{(1)}$ is the minimal terrace length $l^{(1)} = \min_{1\leq i\leq N} l_i$. Similar to (40), if $l^{(1)} \leq \frac{\alpha_2}{2\alpha_1 Nl} = \frac{\alpha_2 A}{2\alpha_1 a}N^{-1}$, then $\frac{\alpha_1}{2}\log\sin^2\frac{\pi l^{(1)}}{Nl} \geq -\frac{\alpha_2\pi^2}{4N^2l^2}(\sin\frac{\pi l^{(1)}}{Nl})^{-2}$. Hence we have

$$
\begin{aligned}
E(X) &\geq \frac{\alpha_2\pi^2}{4N^2l^2}\left(\sin\frac{\pi l^{(1)}}{Nl}\right)^{-2} + \frac{\alpha_1}{2}\left[\frac{N(N-1)}{2} - 1\right]\left(\log\frac{r}{N^2} + 1\right) - E_N^0\\
&\geq \frac{\alpha_2}{4}(l^{(1)})^{-2} + \frac{\alpha_1}{2}\left[\frac{N(N-1)}{2} - 1\right]\left(\log\frac{r}{N^2} + 1\right) - E_N^0.
\end{aligned}
$$

Therefore $\lim_{l^{(1)}\to 0} E(X) = +\infty$. ∎

Next we turn to the main focus of this paper: energy scaling law and spatial structure of minimizers in the asymptotic regime $N \gg 1$ or $N \to +\infty$.

**4. Energy scaling law: Weak version.** In this section, we analyze the energy scaling law of global minimizer as $N$ goes to infinity. Recall the physical setting in section 2. We have fixed $\alpha_1$, $\alpha_2$, $a$, $A$, and hence $l = \frac{a}{A}$, $r = \frac{\alpha_2 \pi^2}{\alpha_1 l^2}$. We further have $L = Nl \to +\infty$. Although the exact minimum energy value is too complicated to be obtained explicitly, we can find both its lower and upper bounds within the order $O(N^2 \log N)$.

PROPOSITION 5 (energy scaling law, weak version). *There exist constants $c, C > 0$ such that, for all $N$, we have*

$$-\frac{\alpha_1}{2} N^2 \log N - cN^2 \leq \inf_{X \in \mathbb{T}^N} E(X) \leq -\frac{\alpha_1}{4} N^2 \log N + CN^2. \tag{43}$$

*Remark* 2. This proposition is a weak version of Theorem 2 in the sense that the leading coefficient of the lower bound is not sharp. In section 9, we will provide a sharp lower bound which is indispensible in the analysis of the optimal profile.

Inspired by numerical simulations, we construct a simple approximate solution which has almost the minimum energy. This ansatz is a local uniform step train (see Figure 3) with the optimal terrace width to be determined later. The energy of this approximate solution provides the upper bound for minimum energy. Then we prove that the lower bound is of the same order. Before going into the details, we introduce the following lemma giving that the energy of the uniform step train is of order $O(N^2)$.

LEMMA 1 (energy of a uniform step train). *There exist $c$ and $C$ such that $-cN^2 \leq E_N^0 \leq CN^2$ for all $N$. More precisely, there exist $\tilde{c}$ and $\tilde{C}$ such that*

$$-\frac{\alpha_1}{2} N^2 - \tilde{c} N \log N \leq E_N^0 \leq -\frac{\alpha_1}{2} \left(1 - \log \frac{\pi}{2}\right) N^2 + \tilde{C} N \log N \tag{44}$$

*for all $N$.*

*Remark* 3. The dependence of $E_N^0 = E_N^0(l)$ on the average terrace length $l$ is in lower order terms.

*Proof.* For the uniform step train, $x_i = (i-1)l$ for $i = 1, 2, \ldots, N$, we have

$$\begin{aligned}
E_N^0 &= \frac{\alpha_1}{2} \sum_{1 \leq i < j \leq N} \left[ \log \sin^2 \frac{(j-i)\pi}{N} + \frac{r}{N^2} \left( \sin \frac{(j-i)\pi}{N} \right)^{-2} \right] \\
&= \frac{\alpha_1}{2} \sum_{k=1}^{N-1} (N-k) \left[ 2 \log \left| \sin \frac{k\pi}{N} \right| + \frac{r}{N^2} \left( \sin \frac{k\pi}{N} \right)^{-2} \right] \\
&= \begin{cases} \frac{\alpha_1}{2} \sum\limits_{k=1}^{(N-1)/2} N \left[ 2 \log |\sin \frac{k\pi}{N}| + \frac{r}{N^2} \left( \sin \frac{k\pi}{N} \right)^{-2} \right] & \text{for } N \text{ odd,} \\ \frac{\alpha_1}{2} \left\{ \sum\limits_{k=1}^{N/2} N \left[ 2 \log |\sin \frac{k\pi}{N}| + \frac{r}{N^2} \left( \sin \frac{k\pi}{N} \right)^{-2} \right] - \frac{r}{2N} \right\} & \text{for } N \text{ even.} \end{cases}
\end{aligned}$$

Since $\frac{\alpha_1}{2} \cdot \frac{r}{2N} = O(N^{-1})$, it is sufficient to prove the result for even $N$. Note that $\frac{2}{\pi} x \leq \sin x \leq x$ for $0 \leq x = \frac{k\pi}{N} \leq \frac{\pi}{2}$ is due to $k \leq \frac{N}{2}$. On the one hand,

$$E_N^0 \leq \frac{\alpha_1 N}{2} \sum_{k=1}^{N/2} \left[ 2 \log \frac{k\pi}{N} + \frac{r}{N^2} \left( \frac{2k}{N} \right)^{-2} \right] + O(N^{-1})$$

$$
\begin{aligned}
&= \frac{\alpha_1 N}{2}\left[N\log\frac{\pi}{N} + 2\log{(N/2)!} + \sum_{k=1}^{N/2}\frac{r}{4k^2}\right] + O(N^{-1})\\
&\le \frac{\alpha_1 N}{2}\left[N\log\frac{\pi}{N} + N\log\frac{N}{2} - N + O(\log N) + \frac{r\pi^2}{24}\right] + O(N^{-1})\\
&= -\frac{\alpha_1}{2}\left(1-\log\frac{\pi}{2}\right)N^2 + \tilde{C}N\log N,
\end{aligned}
$$

where we have used the Stirling formula $\log n! = n\log n - n + O(\log n)$ with $n=\frac{N}{2}$ and the fact that $\sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6}$. On the other hand,

$$
\begin{aligned}
E_N^0 &\ge \frac{\alpha_1 N}{2}\sum_{k=1}^{N/2}\left[2\log\frac{2k}{N} + \frac{r}{N^2}\left(\frac{k\pi}{N}\right)^{-2}\right] + O(N^{-1})\\
&\ge \frac{\alpha_1 N}{2}\left[N\log\frac{2}{N} + 2\log{(N/2)!}\right] + O(N^{-1})\\
&\ge \frac{\alpha_1 N}{2}\left[N\log\frac{2}{N} + N\log\frac{N}{2} - N + O(\log N)\right] + O(N^{-1})\\
&= -\frac{\alpha_1}{2}N^2 - \tilde{c}N\log N. \qquad \square
\end{aligned}
$$

*Proof of Proposition* 5. 1. *Construction of approximate solution.* We first construct a good enough approximate solution $X^0 = (x_1^0, x_2^0, \ldots, x_N^0)^T$ to a global minimizer $X$. Take $x_i^0 = (i-1)l_0$ for $i = 1, 2, \ldots, N$ for some $l_0 > 0$ to be determined later. Here, we assume $l_0 = o(1)$ as $N \to \infty$ and hence $\frac{x_j - x_i}{Nl} = o(1)$ as $N \to +\infty$. This will be checked after we choose such an $l_0$. Utilizing Lemma 1, we have

$$
\begin{aligned}
E(X^0) &= \frac{\alpha_1}{2}\sum_{1\le i<j\le N}\left[\log\sin^2\frac{\pi(x_j^0 - x_i^0)}{Nl} + \frac{r}{N^2}\left(\sin\frac{\pi(x_j^0 - x_i^0)}{Nl}\right)^{-2}\right] - E_N^0\\
&= \frac{\alpha_1}{2}\sum_{1\le i<j\le N}\left(2\log\frac{|j-i|l_0\pi}{Nl} + \frac{rl^2}{(j-i)^2 l_0^2\pi^2}\right) + O(N^2)\\
&= \frac{\alpha_1}{2}\sum_{k=1}^{N-1}\left[2(N-k)\log\frac{kl_0\pi}{Nl} + \frac{rl^2}{\pi^2 l_0^2}\cdot\frac{N-k}{k^2}\right] + O(N^2)\\
&= \frac{\alpha_1}{2}\left[N^2\log\frac{l_0\pi}{Nl} + 2\sum_{k=1}^{N-1}(N-k)\log k + \frac{rl^2}{\pi^2 l_0^2}\cdot\frac{\pi^2}{6}N\right] + O(N^2 + l_0^{-2}\log N).
\end{aligned}
$$

The last step is due to

$$
\sum_{k=1}^{N-1}\frac{N-k}{k^2} = \frac{\pi^2}{6}N + O(\log N). \tag{45}
$$

Next, we have used the following estimate:

$$
\sum_{k=1}^{N-1}(N-k)\log k = N^2\sum_{k=1}^{N-1}\frac{1}{N}\left(1-\frac{k}{N}\right)\log\frac{k}{N} + \sum_{k=1}^{N-1}(N-k)\log N
$$

$$= N^2 \int_{1/N}^{1} (1-x)\log x \mathrm{d}x + \frac{N(N-1)}{2}\log N + O(N^2)$$

$$= \frac{1}{2}N^2 \log N + O(N^2). \tag{46}$$

Therefore,

$$E(X^0) = \frac{\alpha_1}{2}\left[N^2 \log l_0 + \frac{rl^2}{6l_0^2}N\right] + O(N^2 + l_0^{-2}\log N).$$

2. *Determination of the bunch size.* To choose the optimal $l_0$, we take $\frac{\partial E}{\partial l_0} = 0$ and keep the leading order. This gives $\frac{N^2}{l_0} - \frac{2rl^2}{6l_0^3}N = 0$. Thus

$$l_0 = \sqrt{\frac{r}{3}}lN^{-1/2}.$$

This is the optimal $l_0$ to minimize $E$ under the ansatz $x_i^0 = (i-1)l_0$ for all $i$'s. Note that our assumption $l_0 = o(1)$, as $N \to +\infty$, is satisfied.

3. *Upper bound for minimum energy.* Let $l_0 = \sqrt{\frac{r}{3}}lN^{-1/2}$ and $x_i^0 = (i-1)l_0$ for $i = 1, 2, \ldots, N$. We have the energy upper bound of this approximate solution

$$E(X^0) \le \frac{\alpha_1}{2}\sum_{1\le i<j\le N}\left[2\log\frac{|j-i|l_0\pi}{Nl} + \frac{rl^2}{4(j-i)^2 l_0^2}\right] + O(N^2)$$

$$= \frac{\alpha_1}{2}\sum_{k=1}^{N-1}(N-k)\left[2\log\frac{k\sqrt{r/3}\pi}{N^{3/2}} + \frac{3N}{4k^2}\right] + O(N^2).$$

By the same estimates used above (equations (45) and (46)), we obtain

$$\inf_{X\in\mathbb{T}^N} E(X) \le E(X^0) \le -\frac{\alpha_1}{4}N^2\log N + CN^2.$$

4. *Lower bound for minimum energy.* Utilizing (39) and (44), we have

$$\inf_{X\in\mathbb{T}^N} E(X) \ge \frac{\alpha_1 N(N-1)}{4}\left(\log\frac{r}{N^2} + 1\right) - \frac{\alpha_1 N^2}{2}\log\frac{\pi}{2e} + O(N\log N)$$

$$\ge -\frac{\alpha_1}{2}N^2\log N - cN^2.$$

□

**5. Instability of an isolated step bunch.** We now proceed to investigate the structure of any (local) minimizer. From the ansatz in the proof of Proposition 5, it seems that the minimizer consists of only one step bunch. This is consistent with the results from numerical simulations. As a first result toward the one bunch structure, we show the instability of any step configuration which has a well-isolated step bunch (Theorem 3(a)). Consequently, there will not be a step bunch too far away from any other bunches or steps. In other words, any local minimizer essentially contains one bunch. The key idea is to exploit the fact that the second variation of $E$ at a local minimizer must be positive semidefinite. We will make use of the following lemma, which gives a sufficient condition for instability.

LEMMA 2. *Let $H$ be the $(n+m)\times(n+m)$ matrix $\left(\begin{smallmatrix} A & B \\ B^T & C\end{smallmatrix}\right)$, where $A = A^T$, $C = C^T$, $B$ are $n\times n$, $m\times m$, $n\times m$ matrices, respectively. Assume that each row of $H$ sums up to 0. If $\sum_{i,j} B_{ij} > 0$, then $H$ is not positive semidefinite.*

*Proof.* Choose $x = (1, 1, \ldots, 1, 0, 0, \ldots, 0)^T$ (first $n$ components are 1's). Then we have

$$x^T H x = \sum_{i,j=1}^{n} A_{ij} = \sum_{i=1}^{n} \left( 0 - \sum_{k=1}^{m} B_{ik} \right) < 0$$

giving the desired result. ∎

*Proof of Theorem* 3(a). We prove the statement by contradiction. Without loss of generality, we assume $T = \{x_1, \ldots, x_n\}$ and $\text{dist}(T, S \backslash T) > l_{**}$. Recall that

$$H_{ij} = \frac{\partial^2 E}{\partial x_i \partial x_j} = \begin{cases} -e''(x_j - x_i), & i \neq j, \\ \sum\limits_{1 \leq k \leq N, k \neq i} e''(x_k - x_i), & i = j, \end{cases}$$

where $e''(x) = \frac{\alpha_1 \pi^2}{N^2 l^2} \left[ \frac{3r}{N^2} - \left(1 + \frac{2r}{N^2}\right) \sin^2 \frac{\pi x}{Nl} \right] \left( \sin \frac{\pi x}{Nl} \right)^{-4}$ (see (18)). Note that each row of $H_{ij}$ sums up to 0.

By assumption, $\text{dist}(x_i, x_j) > l_{**}$ for $1 \leq i \leq n$ and $n + 1 \leq j \leq N$. Hence,

$$H_{ij} = -e''(x_j - x_i) > -e''(l_{**}) = 0.$$

Therefore $\sum_{i=1}^{n} \sum_{j=n+1}^{N} H_{ij} > 0$. By Lemma 2, $H$ is not positive semidefinite, and hence the step profile $X$ is not stable. ∎

As another application of Lemma 2, we apply this method to show the instability of the uniform step train for $N \gg 1$. This instability is also studied by Tersoff et al. [18] using linear stability analysis.

PROPOSITION 6 (instability of the uniform step train). *Let $X$ be a uniform step train with $x_i = (i - 1)l$ for all $i = 1, 2, \ldots, N$. Then the Hessian matrix $H$ is not positive semidefinite for $N \gg 1$. In other words, the uniform step train is unstable.*

We remark that from Lemma 2, the proposition is true if $l > l_{**}$. The point here is that we can in fact prove the instability for any value of $l$.

*Proof.* Without loss of generality, we assume $N$ is even. We apply Lemma 2 to the case of $m = n = \frac{N}{2}$. Now we estimate

$$\sum_{1 \leq i \leq \frac{N}{2}, \frac{N}{2}+1 \leq j \leq N} e''(x_j - x_i) = \frac{N}{2} e'' \left( \frac{Nl}{2} \right) + 2 \sum_{m=1}^{\frac{N}{2}-1} \sum_{k=m}^{\frac{N}{2}-1} e''(kl)$$

$$\leq \frac{N}{2} \cdot \frac{\alpha_1 \pi^2}{N^2 l^2} \left( \frac{3r}{N^2} - \left( 1 + \frac{2r}{N^2} \right) \right) + \frac{2 \alpha_1 \pi^2}{N^2 l^2} \sum_{m=1}^{\frac{N}{2}-1} \sum_{k=m}^{\frac{N}{2}-1} \left[ \frac{3r}{N^2} \cdot \frac{N^4}{16 k^4} - \left( 1 + \frac{2r}{N^2} \right) \frac{N^2}{4k^2} \right]$$

$$\leq -\frac{\alpha_1 \pi^2}{2Nl^2} \left( 1 + \frac{r}{N^2} \right) + \frac{\alpha_1 \pi^2}{2l^2} \sum_{m=1}^{\frac{N}{2}-1} \sum_{k=m}^{\frac{N}{2}-1} \left[ \frac{3r}{4} \cdot \frac{1}{k^4} - \frac{1}{k^2} \right].$$

For $k \geq 4$, note that $\frac{1}{k^4} \leq \frac{1}{3} [\frac{1}{(k-3)(k-2)(k-1)} - \frac{1}{(k-2)(k-1)k}]$. Thus we have

$$\frac{3r}{4} \sum_{m=4}^{\frac{N}{2}-1} \sum_{k=m}^{\frac{N}{2}-1} \frac{1}{k^4} \leq \frac{r}{4} \sum_{m=4}^{\frac{N}{2}-1} \frac{1}{(m-3)(m-2)(m-1)} \leq \frac{r}{16},$$

$$\frac{3r}{4}\sum_{m=1}^{3}\sum_{k=m}^{\frac{N}{2}-1}\frac{1}{k^4} \le \frac{3r}{4}\sum_{k=1}^{\infty}\frac{1}{k^2} \le \frac{3r}{2},$$

$$\text{and } \sum_{m=1}^{\frac{N}{2}-1}\sum_{k=m}^{\frac{N}{2}-1} -\frac{1}{k^2} \le \sum_{m=1}^{\frac{N}{2}-1}\left(-\frac{1}{m}+\frac{2}{N}\right) \le 1-\sum_{m=1}^{\frac{N}{2}-1}\frac{1}{m} \le 2+\gamma-\log\frac{N}{2},$$

where $\gamma$ is Euler constant.

Collecting the above estimates, for $N \gg 1$, we have

$$\sum_{1\le i\le \frac{N}{2},\, \frac{N}{2}+1\le j\le N} e''(x_j-x_i)$$
$$\le -\frac{\alpha_1\pi^2}{2Nl^2}\left(1+\frac{r}{N^2}\right)+\frac{\alpha_1\pi^2}{2l^2}\left[\frac{3r}{2}+\frac{r}{16}+2+\gamma-\log\frac{N}{2}\right] < 0.$$

Therefore $\sum_{1\le i\le \frac{N}{2},\, \frac{N}{2}+1\le j\le N} H_{ij} = -\sum_{1\le i\le \frac{N}{2},\, \frac{N}{2}+1\le j\le N} e''(x_j-x_i) > 0$. Then apply Lemma 2 to complete the proof. □

**6. Lower bounds for terrace lengths.** In contrast to section 5, which considers the second variation of $E$, here we analyze the vanishing condition of the first variation (32), i.e., force balance $D_X E = 0$. Therefore, all the results in this section hold for any critical point of $E$. Our main results are lower bounds for the terrace lengths (Theorem 5(a) and (b)).

PROPOSITION 7. *Let $X$ be a critical point of $E$. For any $\frac{2}{3} < \alpha < 1$, there exists $N_\alpha$ such that for all $N > N_\alpha$, we have $l^{(1)} \ge N^{-\alpha}$.*

*Proof.* We prove the statement by contradiction. Suppose, for any sufficiently large $N_\alpha$, there is some $N > N_\alpha$ with $l^{(1)} < N^{-\alpha} < l_{**}$. Recall that $e'(\cdot)$ is increasing on $(0, l_{**})$. We estimate $e'(l^{(1)})$ as follows:

$$\begin{aligned} e'(l^{(1)}) \le e'(N^{-\alpha}) &= \frac{\alpha_1\pi}{Nl}\left[1-\frac{r}{N^2}\left(\sin\frac{\pi N^{-\alpha}}{Nl}\right)^{-2}\right]\frac{1-2\sin^2\frac{\pi N^{-\alpha}}{2Nl}}{\sin\frac{\pi N^{-\alpha}}{Nl}} \\ &\le \frac{\alpha_1\pi}{Nl}\left[1-\frac{rl^2N^{2\alpha}}{\pi^2}\right]\frac{1-\frac{\pi^2N^{-2\alpha}}{2N^2l^2}}{\frac{\pi N^{-\alpha}}{Nl}} \\ &= \frac{\alpha_1}{N}\left[1-\frac{rl^2N^{2\alpha}}{\pi^2}\right]N^{1+\alpha}\left(1-\frac{\pi^2N^{-2-2\alpha}}{2l^2}\right). \end{aligned}$$

Note that $1-\frac{rl^2}{\pi^2}N^{2\alpha} \le -\frac{1}{2}\frac{rl^2}{\pi^2}N^{2\alpha}$ and $1-\frac{\pi^2}{2l^2}N^{-2-2\alpha} \ge \frac{1}{2}$ for $N > N_\alpha \gg 1$. Therefore

$$e'(l^{(1)}) \le -\frac{\alpha_1 rl^2}{4\pi^2}N^{3\alpha}. \tag{47}$$

Next we estimate $\max\{e'(l_j+\cdots+l_k)\}$. Note that $l \le l_N$ and hence

$$l_j+\cdots+l_k \le l_1+\cdots+l_{N-1} = Nl-l_N \le Nl-l = (N-1)l. \tag{48}$$

Thus by the monotonicity property of $e'(\cdot)$ (see Figure 4), we have

$$e'(l_j+\cdots+l_k) \le \max\{e'(l_{**}), e'((N-1)l)\}.$$

Now,

$$e'(l_{**}) = \frac{\alpha_1\pi}{Nl}\left[1 - \frac{r}{N^2}\frac{N^2+2r}{3r}\right]\frac{\sqrt{1-\frac{3r}{N^2+2r}}}{\sqrt{\frac{3r}{N^2+2r}}} \le \frac{2\alpha_1\pi}{3\sqrt{3r}l}, \tag{49}$$

$$\begin{aligned} e'((N-1)l) &= \frac{\alpha_1\pi}{Nl}\left[\frac{r}{N^2}\frac{1}{\sin^2\frac{\pi}{N}} - 1\right]\frac{1-2\sin^2\frac{\pi}{2N}}{\sin\frac{\pi}{N}} \\ &\le \frac{\alpha_1\pi}{Nl}\left[\frac{r}{N^2}\frac{N^2}{4}+1\right]\frac{3N}{2} \;=\; \frac{\alpha_1 3\pi(r+4)}{8l}. \end{aligned} \tag{50}$$

Hence, for $1 \le j \le i \le k \le N-1$ with $j < k$, we have

$$\begin{aligned} e'(l_j + \cdots + l_k) &\le \max\{e'(l_{**}), e'((N-1)l)\} \\ &\le \max\left\{\frac{2\alpha_1\pi}{3\sqrt{3r}l}, \frac{\alpha_1 3\pi(r+4)}{8l}\right\} \\ &\le \frac{\alpha_1\pi}{l}\left[\frac{2}{3\sqrt{3r}} + \frac{3(r+4)}{8}\right]. \end{aligned} \tag{51}$$

Let $l_i = l^{(1)}$. Combining (47) and (51), for $N > N_\alpha \gg 1$, we have

$$\begin{aligned} \sum_{1\le j\le i\le k\le N-1} e'(l_j + \cdots + l_k) &= e'(l_i) + \sum_{1\le j\le i\le k\le N-1, j<k} e'(l_j + \cdots + l_k) \\ &\le -\frac{\alpha_1 r l^2}{4\pi^2}N^{3\alpha} + \frac{N^2\alpha_1\pi}{4l}\left[\frac{2}{3\sqrt{3r}} + \frac{3(r+4)}{8}\right] < 0, \end{aligned}$$

where we have used the fact that the number of $(j,k)$ pairs is no more than $\frac{N^2}{4}$. This contradicts force balance (32). ∎

Next, we introduce an iteration scheme to improve the exponents in the above estimates.

Proposition 8 (iteration scheme). *Let $X$ be a critical point of $E$. Suppose there exist $\alpha$ and $N_\alpha$ such that for any $N > N_\alpha$, we have $l^{(1)} \ge N^{-\alpha}$. Then, for any $\beta$ satisfying $\frac{\alpha+1}{3} < \beta < 1$, there exists $N_{\alpha,\beta}$ such that for $N > N_{\alpha,\beta}$, we have $l^{(1)} \ge N^{-\beta}$.*

We begin the proof with a lemma which gives an upper bound for the force exerted by a step chain.

Lemma 3. *Suppose for some $\alpha$ satisfying $0 < \alpha < 1$ and for all $N > N_\alpha$, we have $N^{-\alpha} \le l^{(1)}$. Then, for all $1 \le k \le N-1$, we have*

$$\max_{0<\xi_1<\xi_2<\cdots<\xi_k\le(N-1)l}\{e'(\xi_1) + e'(\xi_2) + \cdots + e'(\xi_k)\} \le C_\alpha N^\alpha \log N, \tag{52}$$

*where $\xi_i$ are constrained by $\xi_{i+1} - \xi_i \ge l^{(1)}$ for all $i = 1, 2, \ldots, k-1$ and the constant $C_\alpha > 0$.*

Later this lemma will be applied to $\xi_1 = l_j + \cdots + l_i, \xi_2 = l_j + \cdots + l_{i+1}, \ldots, \xi_k = l_j + \cdots + l_{i+k-1}$. The appearance of $(N-1)l$ is due to the estimate (48): $l_j + \cdots + l_{i+k-1} \le l_1 + \cdots + l_{N-1} = Nl - l_N \le (N-1)l$.

*Proof.* Let

$$\begin{aligned}k_1 &= \#\{i : 0 < \xi_i \le l_{**}\},\\ k_2 &= \#\{i : l_{**} < \xi_i \le Nl - l_{**}\},\\ k_3 &= \#\{i : Nl - l_{**} < l_i \le (N-1)l\}.\end{aligned}$$

Thus $k_1 + k_2 + k_3 = k$. Without loss of generality, assume $k_1, k_2, k_3 \ge 1$. (If any of them is 0, we still have the similar estimates and the result remains the same.) Recall that $e'(\cdot)$ is monotone increasing on $(0, l_{**})$, $(Nl - l_{**}, (N-1)l)$ and monotone decreasing on $(l_{**}, Nl - l_{**})$. Then

$$\begin{aligned}&e'(\xi_1) + \cdots + e'(\xi_k)\\ &\le e'(l_{**}) + e'(l_{**} - l^{(1)}) + \cdots + e'(l_{**} - (k_1-1)l^{(1)})\\ &\quad + e'(l_{**}) + e'(l_{**} + l^{(1)}) + \cdots + e'(l_{**} + (k_2-1)l^{(1)})\\ &\quad + e'((N-1)l) + e'((N-1)l - l^{(1)}) + \cdots + e'((N-1)l - (k_3-1)l^{(1)})\\ &\le 2e'(l_{**}) + e'((N-1)l) + \frac{1}{l^{(1)}}\int_{l_{**}-(k_1-1)l^{(1)}}^{l_{**}} e'(x)\mathrm{d}x\\ &\quad + \frac{1}{l^{(1)}}\int_{l_{**}}^{l_{**}+(k_2-1)l^{(1)}} e'(x)\mathrm{d}x + \frac{1}{l^{(1)}}\int_{(N-1)l-(k_3-1)l^{(1)}}^{(N-1)l} e'(x)\mathrm{d}x\\ &= 2e'(l_{**}) + e'((N-1)l) + \frac{1}{l^{(1)}}\Big\{e(l_{**} + (k_2-1)l^{(1)}) - e(l_{**} - (k_1-1)l^{(1)})\\ &\quad + e((N-1)l) - e((N-1)l - (k_3-1)l^{(1)})\Big\}.\end{aligned}$$

Recall (49), (50) and estimate the following terms:

$$\begin{aligned}e(l_{**} + (k_2-1)l^{(1)}) &< e(\tfrac{L}{2}) = O(1),\\ -e(l_{**} - (k_1-1)l^{(1)}) &\le -e(l_*) = \alpha_1 \log N + O(1),\\ e((N-1)l) &= -\alpha_1 \log N + O(1),\\ -e((N-1)l - (k_3-1)l^{(1)}) &\le -e(l_*) = \alpha_1 \log N + O(1).\end{aligned}$$

Collecting these estimates, we have

$$\max_{0<\xi_1<\xi_2<\cdots<\xi_k\le(N-1)l} \{e'(\xi_1) + e'(\xi_2) + \cdots + e'(\xi_k)\} \le C_\alpha N^\alpha \log N. \qquad \square$$

*Proof of Proposition* 8. Again we prove this proposition by contradiction. Suppose for any sufficiently large $N_{\alpha,\beta}$, there is some $N > N_{\alpha,\beta}$ such that $l^{(1)} < N^{-\beta}$. Let $l_i = l^{(1)}$. Applying Lemma 3 with $\alpha$ and $k = N - i$ to $\xi_1 = l_j + \cdots + l_i, \xi_2 = l_j + \cdots + l_{i+1}, \ldots, \xi_k = l_j + \cdots + l_{N-1}$, we obtain

$$e'(l_j + \cdots + l_i) + e'(l_j + \cdots + l_{i+1}) + \cdots + e'(l_j + \cdots + l_{N-1}) \le C_\alpha N^\alpha \log N.$$

By (47), $e'(l_i) \le -\frac{\alpha_1 r l^2}{4\pi^2} N^{3\beta}$. Thus for $N > N_{\alpha,\beta} \gg 1$, by force balance (32), we have

$$\begin{aligned}0 &= \sum_{1\le j\le i\le k\le N-1} e'(l_j + \cdots + l_i + \cdots + l_k)\\ &= e'(l_i) + [e'(l_i + l_{i+1}) + \cdots + e'(l_i + \cdots + l_{N-1})]\end{aligned}$$

$$
\begin{aligned}
&+\sum_{j=1}^{i-1}[e'(l_j+\cdots+l_i)+e'(l_j+\cdots+l_{i+1})+\cdots+e'(l_j+\cdots+l_{N-1})]\\
&\le -\frac{\alpha_1 r l^2}{4\pi^2}N^{3\beta}+iC_\alpha N^\alpha \log N\\
&\le -\frac{\alpha_1 r l^2}{4\pi^2}N^{3\beta}+C_\alpha N^{1+\alpha}\log N\\
&< 0.
\end{aligned}
$$

This contradiction completes the proof. ∎

PROPOSITION 9. *Let $X$ be a critical point of $E$. For any $\delta > 0$, there exists $N_\delta$ such that for all $N > N_\delta$, we have $N^{-\frac{1}{2}-\delta} \le l^{(1)}$.*

*Proof.* Choose any $\delta_0$ such that $0 < \delta_0 < \frac{1}{3}$. Let

$$\beta_n = \frac{1}{2} + \left(\frac{2}{3}\right)^{n-1}\left(\frac{1}{6}+\delta_0\right).$$

Note that $\frac{2}{3} < \beta_1 = \frac{2}{3}+\delta_0 < 1$, $\frac{\beta_n+1}{3} < \beta_{n+1}$ and $\beta_n$ is decreasing in $n$.

By Proposition 7, $l^{(1)} \ge N^{-\beta_1}$ for sufficiently large $N$. Applying Proposition 8, we have $l^{(1)} \ge N^{-\beta_2}$ and by induction, $l^{(1)} \ge N^{-\beta_n}$ for sufficiently large $N > N_{\beta_n}$. After a finite number of iterations, we have $\beta_{n_*} < \frac{1}{2}+\delta$ for $n_* \ge \min\{1, [\log \frac{\delta}{1/6+\delta_0} / \log \frac{2}{3}] + 2\}$. Hence $l^{(1)} \ge N^{-\beta_{n_*}} \ge N^{-\frac{1}{2}-\delta}$ for all $N > N_{\beta_{n_*}}$ completing the proof. ∎

Based on this proposition, we are able to show the lower bounds of $l_1$ as well as $l^{(N-1)}$.

PROPOSITION 10. *Let $X$ be a critical point of $E$. For any $\delta > 0$, there exists $N_\delta$ such that for all $N > N_\delta$ have $N^{-\frac{1}{6}-\delta} \le l_1$ and hence $N^{-\frac{1}{6}-\delta} \le l^{(N-1)}$.*

*Proof.* We prove the proposition by contradiction. Suppose there is some $\delta \in (0, \frac{1}{2})$, and for $N > N_\delta$, we have $l_1 < N^{-\frac{1}{6}-\delta} < l_{**}$. Proposition 9 shows that $N^{-\frac{1}{2}-\delta} \le l^{(1)}$ for $N > N_\delta \gg 1$. Applying Lemma 3, we have $\sum_{k=2}^{N-1} e'(l_1+\cdots+l_k) \le C_\delta N^{\frac{1}{2}+\delta}\log N$. Note that $e'(\cdot)$ is increasing on $(0, l_{**})$. Thus we have $e'(l_1) \le e'(N^{-\frac{1}{6}-\delta}) \le -\frac{\alpha_1 r l^2}{4\pi^2}N^{\frac{1}{2}+3\delta}$ for $N > N_\delta \gg 1$ (see also the proof of (47)). Combining these results, we have

$$
\begin{aligned}
\sum_{k=1}^{N-1} e'(l_1+\cdots+l_k) &= e'(l_1) + \sum_{k=2}^{N-1} e'(l_1+\cdots+l_k)\\
&\le -\frac{\alpha_1 r l^2}{4\pi^2}N^{\frac{1}{2}+3\delta} + C_\delta N^{\frac{1}{2}+\delta}\log N\\
&< 0,
\end{aligned}
$$

which contradicts force balance $\sum_{k=1}^{N-1} e'(l_1+\cdots+l_k) = 0$. This completes the proof for $N^{-\frac{1}{6}-\delta} \le l_1$. Hence $N^{-\frac{1}{6}-\delta} \le l_1 \le l^{(N-1)}$. ∎

Essentially, we have already proved the lower bounds in Theorem 5(a) and (b). The remaining parts of Theorem 5 will be completed in section 11.

**7. Energy minimizing bunch concentrated in half period.** In this section, we are going to show the second result (Theorem 3(b)) for the one bunch structure which is also the foundation of the proofs in the remaining sections. Note that we use distance on a circle in the periodic setting. If we can show that all steps indeed concentrate in the half period, then the distance equals the one-dimensional Euclidean distance. Hence the monotonicity of $e(\cdot)$ and $e'(\cdot)$ can be applied. Physically, the result is also important in the sense that all steps concentrate in a band whose width is less than half of the period. Later we will have the stronger result that the relative width of this band vanishes as $N \to \infty$.

We start with several useful lemmata.

LEMMA 4. *If $N^2 > r$, then $e(l_* + x) < e(l_* - x)$ for all $0 < x < l_*$.*

*Proof.* Let $g(x) = e(l_*+x)-e(l_*-x)$. Then $g(0) = 0$, $g'(x) = e'(l_*+x)+e'(l_*-x)$, $g'(0) = 0$, and

$$\begin{aligned} g''(x) &= e''(l_* + x) - e''(l_* - x) \\ &= \frac{\alpha_1 \pi^2}{N^2 l^2} \left[ \left( \sin \frac{\pi(l_* + x)}{Nl} \right)^{-2} - \left( \sin \frac{\pi(l_* - x)}{Nl} \right)^{-2} \right] \\ &\quad \cdot \left\{ \frac{3r}{N^2} \left[ \left( \sin \frac{\pi(l_* + x)}{Nl} \right)^{-2} + \left( \sin \frac{\pi(l_* - x)}{Nl} \right)^{-2} \right] - \left( 1 + \frac{2r}{N^2} \right) \right\}. \end{aligned}$$

Since $0 < \frac{\pi(l_*-x)}{Nl} < \frac{\pi(l_*+x)}{Nl}$ and $\frac{\pi(l_*-x)}{Nl} < \pi - \frac{\pi(l_*+x)}{Nl}$, we have

$$\left( \sin \frac{\pi(l_* + x)}{Nl} \right)^{-2} - \left( \sin \frac{\pi(l_* - x)}{Nl} \right)^{-2} < 0$$

and

$$\begin{aligned} &\frac{3r}{N^2} \left[ \left( \sin \frac{\pi(l_* + x)}{Nl} \right)^{-2} + \left( \sin \frac{\pi(l_* - x)}{Nl} \right)^{-2} \right] - \left( 1 + \frac{2r}{N^2} \right) \\ &> \frac{3r}{N^2} \left( \sin \frac{\pi(l_* - x)}{Nl} \right)^{-2} - \left( 1 + \frac{2r}{N^2} \right) > \frac{3r}{N^2} \left( \sin \frac{\pi l_*}{Nl} \right)^{-2} - \left( 1 + \frac{2r}{N^2} \right) \\ &= 3 - \left( 1 + \frac{2r}{N^2} \right) = \frac{2(N^2 - r)}{N^2} > 0. \end{aligned}$$

Therefore $g''(x) < 0$ for all $0 < x < l_*$. For $0 < x < l_*$, we have $g(x) = g(0)+g'(0)x+\frac{g''(\xi)}{2}x^2 < 0$, where $\xi \in (0, x)$. Hence $e(l_* + x) < e(l_* - x)$. ◻

LEMMA 5. *Suppose $N^{-\beta} \le l^{(1)}$ for some $0 < \beta < 1$ and for all $N > N_\beta$. Then, for all $1 \le k \le N - 1$, we have*

$$\min_{0<\xi_1<\xi_2<\cdots<\xi_k\le\frac{Nl}{2}} \{e(\xi_1) + e(\xi_2) + \cdots + e(\xi_k)\} \ge \alpha_1 k \log k N^{-1-\beta} + O(k), \tag{53}$$

*where $\xi_i$'s are constrained by $\xi_{i+1} - \xi_i \ge l^{(1)}$ for all $i = 1, 2, \ldots, k - 1$.*

*Proof.* For $k = 1$, $\min_{0<\xi_1\le\frac{Nl}{2}} e(\xi_1) \ge -\alpha_1 \log N + O(1)$. For any $2 \le k \le N - 1$, suppose $(\xi_1, \ldots, \xi_k)$ minimize $\sum_{i=1}^{k} e(\xi_i)$ with constraints: $0 < \xi_1$, $\xi_k \le \frac{Nl}{2}$ and $\xi_{i+1} - \xi_i \ge l^{(1)}$ for all $i = 1, 2, \ldots, k - 1$. It is easy to see that, by mononocity of $e(\cdot)$, we must have

$$\xi_2 - \xi_1 = \xi_3 - \xi_2 = \cdots = \xi_k - \xi_{k-1} = l^{(1)}, \ \ \xi_1 \le l_* \ \text{ and } \ l_* < \xi_k.$$

Suppose $\xi_j \leq l_* < \xi_{j+1}$. Then $1 \leq j \leq k-1$. Then for all $1 \leq i < i+k-1 \leq N-1$ and $2 \leq k \leq N-1$, using Lemma 4, we have

$$\begin{aligned}\sum_{i=1}^{k} e(\xi_i) &\geq e(l_*) + e(l_* - l^{(1)}) + \cdots + e(l_* - (j-1)l^{(1)}) \\ &\quad + e(l_*) + e(l_* + l^{(1)}) + \cdots + e(l_* + (k-j-1)l^{(1)}) \\ &\geq e(l_*) + e(l_* + l^{(1)}) + \cdots + e(l_* + (j-1)l^{(1)}) \\ &\quad + e(l_*) + e(l_* + l^{(1)}) + \cdots + e(l_* + (k-j-1)l^{(1)}) \\ &\geq 2e(l_*) + \frac{1}{l^{(1)}} \int_{l_*}^{l_*+(j-1)l^{(1)}} e(x)\mathrm{d}x + \frac{1}{l^{(1)}} \int_{l_*}^{l_*+(k-j-1)l^{(1)}} e(x)\mathrm{d}x.\end{aligned}$$

Notice that for $n = j-1$ and $n = k-j-1$, we have

$$\begin{aligned}\int_{l_*}^{l_*+nl^{(1)}} e(x)\mathrm{d}x &\geq \int_{l_*}^{l_*+nl^{(1)}} \left(\alpha_1 \log \frac{2x}{Nl} + \frac{\alpha_1 r l^2}{2\pi^2 x^2}\right) \mathrm{d}x \\ &= \left[\alpha_1 \left(\log \frac{2}{Nl}\right) x + \alpha_1 x \log x - \alpha_1 x - \frac{\alpha_1 r l^2}{2\pi^2 x}\right]\Bigg|_{l_*}^{l_*+nl^{(1)}} \\ &= \left(\alpha_1 \log \frac{2}{Nle}\right) nl^{(1)} + \alpha_1 (l_* + nl^{(1)}) \log(l_* + nl^{(1)}) \\ &\quad - \alpha_1 l_* \log l_* - \frac{\alpha_1 r l^2}{2\pi^2} \left(\frac{1}{l_* + nl^{(1)}} - \frac{1}{l_*}\right) \\ &\geq \alpha_1 nl^{(1)} \log \frac{2}{Nle} + \alpha_1 (l_* + nl^{(1)}) \log(l_* + nl^{(1)}) - \alpha_1 l_* \log l_*.\end{aligned}$$

Collecting these estimates,

$$\begin{aligned}\sum_{i=1}^{k} e(\xi_i) &\geq 2e(l_*) + \alpha_1 (j-1) \log \frac{2}{Nle} \\ &\quad + \frac{\alpha_1 (l_* + (j-1)l^{(1)})}{l^{(1)}} \log(l_* + (j-1)l^{(1)}) - \frac{2\alpha_1 l_*}{l^{(1)}} \log l_* \\ &\quad + \alpha_1 (k-j-1) \log \frac{2}{Nle} + \frac{\alpha_1 (l_* + (k-j-1)l^{(1)})}{l^{(1)}} \log(l_* + (k-j-1)l^{(1)}).\end{aligned}$$

Note that $\frac{1}{2}(j-1+k-j-1) = \frac{k}{2} - 1$ and by convexity of function $x \log x$, we have

$$\begin{aligned}&\frac{\alpha_1 (l_* + (j-1)l^{(1)})}{l^{(1)}} \log(l_* + (j-1)l^{(1)}) \\ &+ \frac{\alpha_1 (l_* + (k-j-1)l^{(1)})}{l^{(1)}} \log(l_* + (k-j-1)l^{(1)}) \\ &\geq \frac{2\alpha_1 (l_* + \frac{k-2}{2} l^{(1)})}{l^{(1)}} \log\left(l_* + \frac{k-2}{2} l^{(1)}\right).\end{aligned}$$

Hence,

$$\sum_{i=1}^{k} e(\xi_i) \geq 2e(l_*) + \alpha_1 (k-2) \log \frac{2}{Nle}$$

$$
\begin{aligned}
&+ \frac{2\alpha_1(l_* + \frac{k-2}{2}l^{(1)})}{l^{(1)}} \log\left(l_* + \frac{k-2}{2}l^{(1)}\right) - \frac{2\alpha_1 l_*}{l^{(1)}} \log l_* \\
&\geq \alpha_1\left(\log\frac{r}{N^2} + 1\right) - \alpha_1(k-2)\log N + \alpha_1(k-2)\log\frac{2}{le} \\
&+ \alpha_1(k-2)\log\left(l_* + \frac{k-2}{2}l^{(1)}\right) + \frac{2\alpha_1 l_*}{l^{(1)}}\log\frac{l_* + \frac{k-2}{2}l^{(1)}}{l_*} \\
&\geq \alpha_1\left(\log\frac{r}{N^2} + 1\right) - \alpha_1(k-2)\log N + \alpha_1(k-2)\log\frac{2}{le} \\
&+ \alpha_1(k-2)\log\left(\frac{k-2}{2}l^{(1)}\right) \\
&\geq -\alpha_1 k\log N + \alpha_1(k-2)\log(k-2)N^{-\beta} + O(k) \\
&= \alpha_1 k\log kN^{-1-\beta} + O(k). \qquad \square
\end{aligned}
$$

LEMMA 6. *For any $a, b$ satisfying $1 \leq a \leq b \leq N$ and for all $\beta \in \mathbb{R}$, we have*

$$\sum_{k=a}^{b} k\log\left(kN^{-1-\beta}\right) \geq -\frac{\beta(a+b)(b-a+1)}{2}\log N - \frac{1}{e}N^2 \tag{54}$$

*for all $N$.*

*Proof.* The lemma can be proved by direct computation,

$$
\begin{aligned}
\sum_{k=a}^{b} k\log\left(kN^{-1-\beta}\right) &= N\sum_{k=a}^{b}\frac{k}{N}\log\frac{k}{N} + \sum_{k=a}^{b} k\log N^{-\beta} \\
&\geq N\sum_{k=a}^{b} -\frac{1}{e} - \beta\sum_{k=a}^{b} k\log N \\
&\geq -\frac{\beta(a+b)(b-a+1)}{2}\log N - \frac{1}{e}N^2. \qquad \square
\end{aligned}
$$

Now we are ready to prove Theorem 3(b), which basically states $l_1 + l_2 + \cdots + l_{N-1} \leq \frac{1}{2}Nl$.

*Proof of Theorem* 3(b). We prove the statement by contradiction. Suppose $x_N - x_1 > \frac{Nl}{2}$. Without loss of generality, we assume that $x_1 = 0$. Then $x_N > \frac{Nl}{2}$. Let $I$ be the step index set and $P$ be the ordered step pair index set:

$$I = \{1, 2, \ldots, N\}, \tag{55}$$
$$P = \{(i, j) : 1 \leq i < j \leq N\}. \tag{56}$$

We partition $I$ and $P$ into six and three nonintersecting subsets:

$$I_j = \left\{i : \frac{j-1}{6}Nl \leq x_i < \frac{j}{6}Nl\right\} \quad k_j = \#I_j, \text{ for } j = 1, 2, \ldots, 6, \tag{57}$$
$$P_1 = \{(i,j) \in P : i, j \in I_k \text{ for some } k\}, \tag{58}$$
$$P_2 = \{(i,j) \in P : i \in I_k, j \in I_{k+1} \text{ for some } k = 1, 2, \ldots, 5 \text{ or } i \in I_6, j \in I_1\}, \tag{59}$$
$$P_3 = \{(i,j) \in P : (i,j) \in P\backslash(P_1 \cup P_2)\}. \tag{60}$$

Recalling Proposition 9, for any $0 < \delta < \frac{1}{2}$, we have $l^{(1)} \geq N^{-\frac{1}{2}-\delta}$ for $N \gg 1$.

First, we estimate the energy contributions from $(i,j) \in P_1 \cup P_2$. For example, if $i \in I_1$, $j \in I_1 \cup I_2$ and $i < j$, then we apply Lemma 5 with $\beta = \frac{1}{2} + \delta$, $k = k_1 + k_2 - i$ to the step chain $x_i, x_{i+1}, \ldots, x_{i+k}$ with $\{\xi_m = x_{i+m} - x_i,\ m = 1, 2, \ldots, k\}$. This gives

$$\sum_{j=i+1}^{k_1+k_2} e(x_j - x_i) \geq \alpha_1 k \log k N^{-\frac{3}{2}-\delta} + O(k).$$

Now applying Lemma 6 with $a = k_2$, $b = k_1 + k_2 - 1$, and $\beta = \frac{1}{2} + \delta$, we have

$$\begin{aligned}
\sum_{i \in I_1, j \in I_1 \cup I_2} e(x_j - x_i) &= \sum_{i=1}^{k_1} \sum_{j=i+1}^{k_1+k_2} e(x_j - x_i) \\
&\geq \sum_{k=k_2}^{k_1+k_2-1} \alpha_1 k \log k N^{-\frac{3}{2}-\delta} + O(k) \\
&= -\left(\frac{\alpha_1}{2} + \alpha_1 \delta\right) \frac{k_1(k_1 + 2k_2 - 1)}{2} \log N + O(N^2) \\
&= -\left(\frac{\alpha_1}{4} + \frac{\alpha_1 \delta}{2}\right) \left(k_1^2 + 2k_1 k_2\right) \log N + O(N^2).
\end{aligned}$$

Similarly, we can estimate the energy contribution from $i \in I_2$, $j \in I_2 \cup I_3$, $i < j$, etc. Collecting all these contribution, we have

$$\begin{aligned}
&\sum_{(i,j) \in P_1 \cup P_2} e(x_j - x_i) \\
&= \sum_{i \in I_1, j \in I_1 \cup I_2} e(x_j - x_i) + \sum_{i \in I_2, j \in I_2 \cup I_3} e(x_j - x_i) + \sum_{i \in I_3, j \in I_3 \cup I_4} e(x_j - x_i) \\
&\quad + \sum_{i \in I_4, j \in I_4 \cup I_5} e(x_j - x_i) + \sum_{i \in I_5, j \in I_5 \cup I_6} e(x_j - x_i) + \sum_{i \in I_6, j \in I_6 \cup I_1} e(x_j - x_i) \\
&\geq -\left(\frac{\alpha_1}{4} + \frac{\alpha_1 \delta}{2}\right) \left(k_1^2 + 2k_1 k_2 + k_2^2 + 2k_2 k_3 + k_3^2 + 2k_3 k_4\right. \\
&\quad \left. + k_4^2 + 2k_4 k_5 + k_5^2 + 2k_5 k_6 + k_6^2 + 2k_6 k_1\right) \log N + O(N^2).
\end{aligned} \tag{61}$$

Second, we estimate the energy contributions from $(i,j) \in P_3$. For example, $i \in I_1$, $j \in I_3 \cup I_4 \cup I_5$. Then $\mathrm{dist}(x_i, x_j) \geq \frac{Nl}{6}$, and hence

$$\begin{aligned}
\sum_{i \in I_1, j \in I_3 \cup I_4 \cup I_5} e(x_j - x_i) &\geq \sum_{i \in I_1, j \in I_3 \cup I_4 \cup I_5} e\left(\frac{Nl}{6}\right) \\
&= \frac{\alpha_1}{2} \left(k_1 k_3 + k_1 k_4 + k_1 k_5\right) \left(\log \frac{1}{4} + \frac{4r}{N^2}\right).
\end{aligned}$$

Similarly, we estimate the energy contribution from $i \in I_2$, $j \in I_4 \cup I_5 \cup I_6$, $i < j$, etc. Collecting all these contribution, we have

$$\begin{aligned}
&\sum_{(i,j) \in P_3} e(x_j - x_i) \\
&= \frac{1}{2} \left( \sum_{i \in I_1, j \in I_3 \cup I_4 \cup I_5} + \sum_{i \in I_2, j \in I_4 \cup I_5 \cup I_6} + \sum_{i \in I_3, j \in I_5 \cup I_6 \cup I_1} \right.
\end{aligned}$$

$$+\sum_{i\in I_4,j\in I_6\cup I_1\cup I_2}+\sum_{i\in I_5,j\in I_1\cup I_2\cup I_3}+\sum_{i\in I_6,j\in I_2\cup I_3\cup I_4}\Bigg) e(x_j-x_i)$$

$$\geq \frac{\alpha_1}{2}\,(k_1k_3+k_1k_4+k_1k_5+k_2k_4+k_2k_5+k_2k_6+k_3k_5+k_3k_6+k_3k_1+k_4k_6$$

$$+k_4k_1+k_4k_2+k_5k_1+k_5k_2+k_5k_3+k_6k_2+k_6k_3+k_6k_4)\,\frac{1}{2}\left(\log\frac{1}{4}+\frac{4r}{N^2}\right), \tag{62}$$

where we have divided the sum by 2 to avoid double counting.

Finally, we combine (61) and (62) to obtain

$$\begin{aligned}
&\sum_{1\leq i<j\leq N} e(x_j-x_i)\\
&\geq \sum_{(i,j)\in P_1\cup P_2} e(x_j-x_i)+\sum_{(i,j)\in P_3} e(x_j-x_i)\\
&\geq -\left(\frac{\alpha_1}{4}+\frac{\alpha_1\delta}{2}\right)\left(k_1^2+2k_1k_2+k_2^2+2k_2k_3+\cdots+k_6^2+2k_6k_1\right)\log N\\
&\quad+\frac{\alpha_1}{2}\,(k_1k_3+k_1k_4+k_1k_5+\cdots+k_6k_2+k_6k_3+k_6k_4)\,\frac{1}{2}\left(\log\frac{1}{4}+\frac{4r}{N^2}\right)+O(N^2)\\
&= -\left(\frac{\alpha_1}{4}+\frac{\alpha_1\delta}{2}\right)[k_1+\cdots+k_6]^2\log N\\
&\quad+\frac{\alpha_1}{2}\,[(k_1k_3+k_1k_4+k_1k_5)+\cdots]\left[(1+2\delta)\log N+\log\frac{1}{2}+\frac{2r}{N^2}\right]+O(N^2)\\
&\geq -\left(\frac{\alpha_1}{4}+\frac{\alpha_1\delta}{2}\right)N^2\log N+\frac{\alpha_1}{2}k_1k_3(1+2\delta)\log N+O(N^2),
\end{aligned}$$

where we used $k_1+\cdots+k_6=N$ in the last equality.

For $N\gg 1$, we have $k_1 l_*\geq x_{k_1+1}-x_1\geq \frac{Nl}{6}$. By (21), we have $l_*=\frac{\sqrt{r}l}{\pi}+O(N^{-2})\leq\frac{\sqrt{r}l}{3}$ for $N\gg 1$. Hence $k_1\geq\left(\frac{Nl}{6}\right)/l_*\geq\frac{N}{2\sqrt{r}}$. Similarly, $k_3\geq\frac{N}{2\sqrt{r}}$. Thus $k_1k_3\geq\frac{N^2}{4r}$. Therefore

$$\begin{aligned}
-\frac{\alpha_1}{4}N^2\log N+O(N^2)\geq E(X)&=\sum_{1\leq i<j\leq N} e(x_j-x_i)-E_N^0\\
&\geq\left[-\frac{\alpha_1}{4}+\frac{\alpha_1}{2}\left(-\delta+\frac{1+2\delta}{4r}\right)\right]N^2\log N+O(N^2)\\
&\geq\left(-\frac{\alpha_1}{4}+\delta\right)N^2\log N+O(N^2).
\end{aligned}$$

The last inequality leads to a contradiction upon choosing $\delta$ small enough such that $\delta\leq\frac{\alpha_1}{2}\left(-\delta+\frac{1+2\delta}{4r}\right)$. This shows that we must have $l_N>\frac{Nl}{2}$ for $N\gg 1$. ∎

**8. Lower bound for bunch size.** In this section, we prove Theorem 4(a), which provides a lower bound for bunch size. The proof makes use of the notion of the distribution for terrace lengths $\left\{l^{(k)}, k=1,2,\ldots,N-1\right\}$.

PROPOSITION 11 (terrace length distribution). *Let $X$ be a global minimizer of $E$. There exists a constant $C$, independent of $N$ and $k$, such that*

$$\#\left\{j: l_j>Ck^{1/2}N^{-1}(\log N)^{-1/2},\, 1\leq j\leq N-1\right\}\geq N-k \tag{63}$$

*for $N\geq 2$ and $1\leq k\leq N-1$.*

*Proof.* By (21), there exists a constant $C$, independent of $N$ and $k$, such that

$$l_* > CN^{-1/2}(\log N)^{-1/2}$$

for $N \geq 2$. If $l^{(k)} > l_*$, then

$$l^{(j)} \geq l^{(k)} > l_* > Ck^{1/2}N^{-1}(\log N)^{-1/2}, \;\; j = k, k+1, \dots, N-1. \tag{64}$$

This implies (63). In the following, we assume that $k$ satisfies $l^{(k)} \leq l_*$. (Indeed, we will see that by Theorem 5(b), this is the case for $N \gg 1$ and for all $k = 1, 2, \dots, N-1$.) Then we have

$$\begin{aligned} -cN^2 \log N \geq E(X) &\geq \sum_{i=1}^{k} e(l^{(i)}) + \frac{\alpha_1}{2}\left[\frac{N(N-1)}{2} - k\right]\left(\log \frac{r}{N^2} + 1\right) - E_N^0 \\ &\geq ke(l^{(k)}) - CN^2 \log N. \end{aligned}$$

The last inequality is due to the monotonicity of $e(\cdot)$: $e(l^{(i)}) \geq e(l^{(k)})$ for $0 < l^{(i)} \leq l^{(k)} \leq l_*$. Therefore, with some $C > 0$,

$$CN^2 \log N \geq ke(l^{(k)}) = \frac{\alpha_1}{2} k \left[\log \sin^2 \frac{\pi l^{(k)}}{Nl} + \frac{r}{N^2}\left(\sin \frac{\pi l^{(k)}}{Nl}\right)^{-2}\right].$$

Choosing $\delta = \frac{1}{4}$ in Proposition 9, we obtain that $l^{(1)} \geq CN^{-\frac{3}{4}}$ for all $N$. In addition, note that $0 < l^{(k)} \leq \frac{Nl}{2}$. Thus

$$\frac{\alpha_1}{2} k \log \sin^2 \frac{\pi l^{(k)}}{Nl} \geq \frac{\alpha_1}{2} N \log \sin^2 \frac{\pi l^{(1)}}{Nl} \geq \alpha_1 N \log \frac{2l^{(1)}}{Nl} \geq -CN \log N.$$

Therefore,

$$CN^2 \log N \geq \frac{\alpha_1}{2} k \frac{r}{N^2}\left(\sin \frac{\pi l^{(k)}}{Nl}\right)^{-2} \geq \frac{\alpha_1}{2} k \frac{rl^2}{\pi^2}\left(l^{(k)}\right)^{-2}$$

leading to

$$l^{(k)} > Ck^{1/2}N^{-1}(\log N)^{-1/2}.$$

Hence for $k = 1, 2, \dots, N-1$, we have

$$\#\left\{j : l_j > Ck^{1/2}N^{-1}(\log N)^{-1/2}, 1 \leq j \leq N-1\right\} \geq N-k. \tag{65}$$

□

Now, we are going to use this distribution result to show the lower bound of the bunch size.

*Proof of Theorem* 4(a). Choose $k = \left[\frac{1}{2}N\right]$ in Proposition 11. Then we have

$$\#\left\{j : l_j > CN^{-1/2}(\log N)^{-1/2}, 1 \leq j \leq N-1\right\} \geq \frac{N}{2}.$$

Therefore, $l_1 + l_2 + \cdots + l_{N-1} \geq \frac{N}{2}CN^{-1/2}(\log N)^{-1/2} = CN^{1/2}(\log N)^{-1/2}$ for $N \geq 2$. □

*Remark* 4. By Proposition 9, we have $l^{(1)} \geq C_\delta N^{-\frac{1}{2}-\delta}$ for all $N$. This implies that $l_1 + \cdots + l_{N-1} \geq C_\delta N^{\frac{1}{2}-\delta}$ for all $N$. Hence Theorem 4(a) is a somewhat stronger version of this estimate.

**9. Energy scaling law: Strong version.** Based on Proposition 11, we can improve the minimum energy lower bound in Proposition 5.

*Proof of Theorem* 2. Given any $\delta > 0$, for any $0 < s < 1$ and any $\alpha > 0$ let $k = [sN]$. Then (63) implies

$$\#\left\{j : l_j > s^{1/2} C_\alpha N^{-1/2-\alpha/2}, 1 \le j \le N-1\right\} \ge (1-s)N. \tag{66}$$

Let $P = \{(i,j) : j - i \ge 2sN\}$, then $\#P = \frac{(1-2s)^2N^2}{2} + O(N)$. For $(i,j) \in P$, we have

$$x_j - x_i \ge sN \cdot s^{1/2} C_\alpha N^{-1/2-\alpha/2} + sN \cdot 0 = s^{3/2} C_\alpha N^{1/2-\alpha/2} > l_*$$

for $N > N_{\alpha,s} \gg 1$. Theorem 3(b) implies $x_j - x_i \le \frac{Nl}{2}$ for $N \gg 1$. Thus, by the monotonicity of $e(\cdot)$ on $(l_*, \frac{Nl}{2})$, we have

$$\begin{aligned}
e(x_j - x_i) &\ge e(s^{3/2} C_\alpha N^{1/2-\alpha/2}) \\
&\ge 2\log\left(\frac{2s^{3/2}C_\alpha}{l} N^{-1/2-\alpha/2}\right) + \frac{rl^2}{\pi^2 s^3 C_\alpha^2} N^{-1+\alpha} \\
&= -(1+\alpha)\log N + O(1).
\end{aligned}$$

Therefore,

$$\begin{aligned}
E(X) &= \sum_{1 \le i < j \le N} e(x_j - x_i) - E_N^0 \\
&\ge \frac{\alpha_1}{2}\left\{\left[\frac{(1-2s)^2N^2}{2} + O(N)\right][-(1+\alpha)\log N + O(1)]\right. \\
&\quad \left. + \left[\frac{N(N-1)}{2} - \frac{(1-2s)^2N^2}{2} - O(N)\right]\left(\log\frac{r}{N^2} + 1\right)\right\} - E_N^0 \\
&= \frac{\alpha_1}{2}\left[\frac{1-\alpha}{2}(1-2s)^2 - 1\right] N^2 \log N + O(N^2) \\
&\ge -\left(\frac{\alpha_1}{4} + \delta\right) N^2 \log N - c_\delta N^2.
\end{aligned}$$

The last inequality holds for sufficiently small $s$ and $\alpha$.

So far, this improved lower bound holds for $N > N_{\alpha,s} \gg 1$. It is easy to revise the coefficients and obtain the same statement for all $N$. ∎

**10. Upper bound for bunch size.** In this section, we complete the proof of the upper bound for bunch size. We prove the following proposition, from which Theorem 4(b) is an immediate consequence.

PROPOSITION 12. *Let $X$ be any global minimizer of $E$. Suppose that $l^{(1)} \ge N^{-\beta}$ for some $\frac{1}{2} < \beta < 1$ and for sufficiently large $N$, i.e., $N > N_\beta$. Then for any $s, \alpha$ satisfying $0 < s < 1 - \sqrt{\frac{\beta - 1/2}{\beta}}$ and $0 < \alpha < \beta - \frac{\beta-1/2}{(1-s)^2}$, there exists $N_{\alpha,\beta}$, for all $N > N_{\alpha,\beta}$,*

$$\min_{1 \le i \le N-[sN]} x_{i+[sN]} - x_i < N^{1-\alpha}.$$

*Proof of Theorem* 4(b). Let $\beta$ and hence $\alpha$ be sufficiently close to $\frac{1}{2}$; then Proposition 12 immediately implies Theorem 4(b). ∎

*Proof of Proposition* 12. Given $\beta$, from the definition of $\alpha$, we have $0 < \alpha < \frac{1}{2} < \beta < 1$. Suppose the statement is false. Then for any $N_{\alpha,\beta}$, there exists an $N > N_{\alpha,\beta}$ satisfying

$$\min_{1\le i\le N-[sN]} x_{i+[sN]} - x_i \ge N^{1-\alpha}. \tag{67}$$

Let $P = \{(i,j) : 1 \le i < j \le N\}$. We partition $P$ into three nonintersecting subsets $P = P_1 \cup P_2 \cup P_3$, where

$$\begin{aligned} P_1 &= \{(i,j) \in P : j - i \ge [sN]\}, \\ P_2 &= \{(i,j) \in P : j - i < [sN], i \le N - [sN]\}, \\ P_3 &= \{(i,j) \in P : j - i < [sN], i > N - [sN]\}. \end{aligned}$$

Then

$$\#P_1 = \frac{(1-s)^2N^2}{2} + O(N), \ \#P_2 = s(1-s)N^2 + O(N), \ \text{ and } \ \#P_3 = \frac{s^2N^2}{2} + O(N).$$

For $(i,j) \in P_1$, $j - i \ge [sN]$, $x_j - x_i \ge N^{1-\alpha} > l_*$. Recall that $x_j - x_i \le l_1 + \cdots + l_{N-1} \le \frac{Nl}{2}$ for $N \gg 1$. The monotonicity of $e(\cdot)$ on $(l_*, \frac{Nl}{2})$ leads to

$$e(x_j - x_i) \ge e(N^{1-\alpha}) \ge \alpha_1 \log \frac{2N^{1-\alpha}}{Nl} + \frac{\alpha_1 r}{2N^2}\left(\frac{\pi N^{1-\alpha}}{Nl}\right)^{-2} = -\alpha_1\alpha \log N + O(1).$$

Summing up all these pairs $(i,j) \in P_1$ leads to

$$\sum_{(i,j)\in P_1} e(x_j - x_i) \ge -\alpha_1\alpha\frac{(1-s)^2}{2}N^2 \log N + O(N^2).$$

Now we consider $(i,j) \in P_2 \cup P_3$. For each $i$, applying Lemma 5 to the step chain $x_i, x_{i+1}, \ldots, x_{i+k}$ with $\{\xi_m = x_{i+m} - x_i,\ m = 1, 2, \ldots, k\}$ gives

$$e(x_{i+1} - x_i) + e(x_{i+2} - x_i) + \cdots + e(x_{i+k} - x_i) \ge \alpha_1 k \log kN^{-1-\beta} + O(k).$$

We then estimate the contribution from $P_2$,

$$\begin{aligned} \sum_{(i,j)\in P_2} e(x_j - x_i) &\ge (N - [sN]) \cdot \left[\alpha_1 k \log kN^{-1-\beta} + O(k)\right]\Big|_{k=[sN]-1} \\ &= -\alpha_1\beta s(1-s)N^2 \log N + O(N^2). \end{aligned}$$

For contribution from $P_1$, we apply Lemma 6 with $a = 1, b = [sN] - 1$,

$$\begin{aligned} \sum_{(i,j)\in P_3} e(x_j - x_i) &\ge \sum_{k=1}^{[sN]-1} \left[\alpha_1 k \log kN^{-1-\beta} + O(k)\right] \\ &\ge -\alpha_1\beta\frac{s^2}{2}N^2 \log N + O(N^2). \end{aligned}$$

Now let $\delta = (\beta - \alpha)\frac{(1-s)^2}{2} - \frac{1}{2}\left(\beta - \frac{1}{2}\right) > 0$. Then the above estimates give

$$\begin{aligned} E(X) &\ge \alpha_1 \left\{-\alpha\frac{(1-s)^2}{2} - \beta s(1-s) - \beta\frac{s^2}{2}\right\} N^2 \log N + O(N^2) \\ &= \alpha_1 \left(-\frac{1}{4} + \delta\right) N^2 \log N + O(N^2). \end{aligned}$$

This contradicts the energy upper bound $-\frac{\alpha_1}{4}N^2 \log N + O(N^2) \ge E(X)$ for $N \gg 1$. Hence the original statement is true. ∎

**11. Upper bound for terrace length.** Here we combine the previous results to prove Theorem 5.

*Proof of Theorem* 5(a). Proposition 9 provides a lower bound for $l^{(1)}$. Here we only need to show the upper bound for $l^{(1)}$. Let $s = \frac{1}{2}(1 - \frac{1}{\sqrt{2}}) \in (0, 1)$. We prove the statement by contradiction. Suppose that for any $N_\delta$, there exists $N > N_\delta$ such that $N^{-\frac{1}{2}+\delta} < l^{(1)}$. Now suppose $N_\delta \gg 1$. Let

$$P_1 = \{(i, j) : 1 \leq i < j \leq N, j - i \geq [sN]\}.$$

Then $\#P_1 = \frac{(1-s)^2 N^2}{2} + O(N)$. For $(i, j) \in P_1$, it holds that

$$\frac{Nl}{2} \geq x_j - x_i \geq sNl^{(1)} \geq sN^{\frac{1}{2}+\delta} > l_*.$$

The monotonicity of $e(\cdot)$ on $(l_*, \frac{Nl}{2})$ leads to

$$\begin{aligned} e(x_j - x_i) \geq e(sN^{\frac{1}{2}+\delta}) &\geq \alpha_1 \log \frac{2sN^{\frac{1}{2}+\delta}}{Nl} + \frac{\alpha_1 r}{2N^2} \left( \frac{\pi s N^{1/2+\delta}}{Nl} \right)^{-2} \\ &\geq -\frac{\alpha_1}{2}(1 - 2\delta) \log N + \alpha_1 \log \frac{2s}{l}. \end{aligned}$$

Therefore

$$\begin{aligned} E(X) \geq\ & \frac{\alpha_1}{2} \left\{ \left[ \frac{(1-s)^2 N^2}{2} + O(N) \right] \left[ -(1-2\delta) \log N + 2 \log \frac{2s}{l} \right] \right. \\ & \left. + \left[ \frac{N(N-1)}{2} - \frac{(1-s)^2 N^2}{2} + O(N) \right] \left( \log \frac{r}{N^2} + 1 \right) \right\} - E_N^0 \\ =\ & \frac{\alpha_1}{2} \left[ -(1-s)^2 \left( \frac{1}{2} - \delta \right) - 2s + s^2 \right] N^2 \log N + O(N^2) \\ \geq\ & \left( -\frac{\alpha_1}{4} + \frac{\delta}{2} \right) N^2 \log N + O(N^2), \end{aligned}$$

leading to a contradiction with $-\frac{\alpha_1}{4} N^2 \log N + CN^2 \geq E(X)$ for $N \gg 1$. ∎

*Proof of Theorem* 5(b). Proposition 10 provides the lower bound for $l^{(N-1)}$. Here we only need to show the upper bound for $l^{(N-1)}$. By Theorem 3(b), we have $l_N > \frac{Nl}{2}$ for $N \gg 1$. We will prove $l^{(N-1)} \leq l_*$ for $N \gg 1$ by contradiction. Suppose $l_i > l_*$ for some $i$, $1 \leq i \leq N - 1$.

Note that $0 < l_i \leq l_j + \cdots + l_i + \cdots + l_k \leq \frac{Nl}{2}$. Therefore

$$\begin{aligned} & \sum_{1 \leq j \leq i \leq k \leq N-1} e'(l_j + \cdots + l_k) \\ = & \sum_{1 \leq j \leq i \leq k \leq N-1} \frac{\alpha_1 \pi}{Nl} \left( 1 - \frac{r}{N^2} \left( \sin \frac{\pi(l_j + \cdots + l_k)}{Nl} \right)^{-2} \right) \cot \frac{\pi(l_j + \cdots + l_k)}{Nl} \\ \geq & \sum_{1 \leq j \leq i \leq k \leq N-1} \frac{\alpha_1 \pi}{Nl} \left( 1 - \frac{r}{N^2} \left( \sin \frac{\pi l_i}{Nl} \right)^{-2} \right) \cot \frac{\pi(l_j + \cdots + l_k)}{Nl} \\ > & \ 0, \end{aligned}$$

contradicting the force balance (32). Therefore, $l^{(N-1)} \leq l_*$ for $N \gg 1$ and $l^{(N-1)} \leq O(1)$ for all $N$. ∎

*Remark* 5. If $N \gg 1$, the lower bound in Theorem 5(b) is stronger than the one in Theorem 3(a) because $l_* < l_{**}$. However, the latter holds for all $N$.

Finally, we complete the proof for Theorem 3(c).

*Proof of Theorem* 3(c). For any $0 < s < 1$, Theorems 4(b) and 5(b) together imply

$$0 \leq \limsup_{N\to\infty} \frac{l_1 + \cdots + l_{N-1}}{l_N} \leq \limsup_{N\to\infty} \frac{C_{\delta,s}N^{1/2+\delta} + (1-s)Nl_*}{\frac{1}{2}Nl} \leq 2(1-s).$$

Therefore $\lim_{N\to\infty} \frac{l_1+\cdots+l_{N-1}}{l_N} = 0$. ∎

**12. Extensions.** There are several extensions of our results, including the same model with the Neumann boundary condition, a particle system with generic pairwise interactions, and higher dimensional problems. Here we state only the results corresponding to the same pairwise interaction with the Neumann boundary condition.

In the setting with the Neumann boundary condition, the total energy can be written as

$$E(X) = \sum_{1\leq i<j\leq N} e(x_i - x_j), \quad \text{where} \quad e(x) = \alpha_1 \log x + \frac{\alpha_2}{2x^2}. \tag{68}$$

We have $l_* = \sqrt{\frac{\alpha_2}{\alpha_1}}$ and $l_{**} = \sqrt{\frac{3\alpha_2}{\alpha_1}}$. Our results are stated as follows.

THEOREM 6 (energy scaling law with Neumann boundary condition). *For any $\delta > 0$, there exist constants $c_\delta$ and $C$ such that*

$$\left(\frac{\alpha_1}{4} - \delta\right) N^2 \log N - c_\delta N^2 \leq \inf_{X\in\mathbb{R}^N} E(X) \leq \frac{\alpha_1}{4} N^2 \log N + CN^2 \tag{69}$$

*for all $N$. Consequently, $\lim_{N\to+\infty} \frac{\inf E(X)}{N^2 \log N} = \frac{\alpha_1}{4}$.*

THEOREM 7 (size of the bunch with Neumann boundary condition). *For the global minimizer of $E$, we have the following:*

(a) (Lower bound) *There exists $C$ such that for all $N$, we have*

$$CN^{1/2} (\log N)^{-1/2} \leq l_1 + \cdots + l_{N-1}. \tag{70}$$

(b) (Upper bound) *For any $\delta > 0$ and any $0 < s < 1$, there exists $C_{\delta,s}$ such that for all $N$, we have*

$$\min_i \left\{l_i + \cdots + l_{i+[sN]}\right\} \leq C_{\delta,s} N^{1/2+\delta}. \tag{71}$$

THEOREM 8 (slope of the bunch profile, with Neumann boundary condition). *For the global minimizer of $E$, we have the following:*

(a) (Estimates on minimal terrace length $l^{(1)}$) *For any $\delta > 0$, there exist constants $c_\delta$ and $C_\delta$ such that for all $N$, we have*

$$c_\delta N^{-1/2-\delta} \leq l^{(1)} \leq C_\delta N^{-1/2+\delta}. \tag{72}$$

(b) (Estimates on next-maximal terrace length $l^{(N-1)}$) *For any $\delta > 0$, there exists a constant $c_\delta$ such that for all $N$, we have*

$$c_\delta N^{-1/6-\delta} \leq l^{(N-1)} \leq l_* = O(1). \tag{73}$$

These results are almost the same as the ones in the periodic setting. It is straightforward if we notice that we are using the Euclidean distance $|x_i - x_j|$ instead of the distance on a circle, i.e., $\mathrm{dist}(x_i, x_j)$. Indeed, the energy in the Neumann boundary setting can be obtained by replacing $\sin x$ with $x$, and the model is somewhat "linearized." The length scales of the bunch size and the minimal terrace remain the same. However, we should emphasize the following two modifications for the case with the Neumann boundary condition:

1. There is no reference state and hence no reference energy $E_N^0$.
2. The leading order of the minimum energy scaling law is $\frac{\alpha_1}{4} N^2 \log N$ instead of $-\frac{\alpha_1}{4} N^2 \log N$. The missing $-\frac{\alpha_1}{2} N^2 \log N$ can be understood in the following way. For each pair $x_i, x_j$, the difference between $\frac{\alpha_1}{2} \log \sin^2 \frac{\pi(x_i - x_j)}{Nl}$ and $\alpha_1 \log |x_i - x_j|$ is $-\log N + O(1)$. Totally, we have $\frac{N(N-1)}{2}$ such pairs.

Our method can also be applied to more general $(m, n)$-type pairwise interactions, where the pairwise force is given by

$$f(x) = \left(\alpha_1 |x|^{-m-1} - \alpha_2 |x|^{-n-1}\right) \frac{x}{|x|}. \tag{74}$$

The corresponding total energy is

$$E(X) = \sum_{1 \le i < j \le N} e(x_i - x_j), \tag{75}$$

where

$$e(x) = \begin{cases} -\frac{\alpha_1}{m} |x|^{-m} + \frac{\alpha_2}{n} |x|^{-n}, & -1 < m < n, m \neq 0, n \neq 0, \\ \alpha_1 \log |x| + \frac{\alpha_2}{n} |x|^{-n}, & 0 = m < n, \\ -\frac{\alpha_1}{m} |x|^{-m} - \alpha_2 \log |x|, & -1 < m < n = 0. \end{cases} \tag{76}$$

Here $m, n$ can be nonintegers. For $-1 < m < 1$ and $1 < n < +\infty$, we can also obtain the minimum energy scaling law, the size of the system, and fine-structure length scales of the system. This will be reported in a future work.

Other possible generalizations of the present work include the proof of the analogous results for the continuum model as derived in [19, 20] and the analysis of the dynamical equations and the temporal and spatial coarsening behaviors of the solutions. These will be explored in the future works.

**Appendix A. Derivations of $f_i$ and $E$.** We derive (6)–(8) in this appendix. Note that $\cot x = \sum_{k \in \mathbb{Z}} \frac{1}{x + k\pi}$. Then we have

$$\sum_{k \in \mathbb{Z}} \frac{1}{x + kL} = \frac{\pi}{L} \cot\left(\frac{\pi x}{L}\right),$$

$$\sum_{k \in \mathbb{Z}} \frac{1}{(x + kL)^2} = \frac{\pi^2}{L^2} \left(\sin \frac{\pi x}{L}\right)^{-2},$$

$$\sum_{k \in \mathbb{Z}} \frac{1}{(x + kL)^3} = \frac{\pi^3}{L^3} \left(\cot \frac{\pi x}{L}\right) \left(\sin \frac{\pi x}{L}\right)^{-2}.$$

Recall that, without loss of generality, we assume $0 \le x_1 < x_2 < \cdots < x_N < lN = L$. Then we have the explicit form of $f_i$ and $E$. For $i = 1, 2, \ldots, N$,

$$f_i = -\sum_{j \in \mathbb{Z}, j \neq i} \left[\frac{\alpha_1}{x_j - x_i} - \frac{\alpha_2}{(x_j - x_i)^3}\right]$$

$$= - \sum_{1 \le j \le N, j \ne i} \sum_{k \in \mathbb{Z}} \left[ \frac{\alpha_1}{x_j - x_i + kL} - \frac{\alpha_2}{(x_j - x_i + kL)^3} \right]$$
$$= - \sum_{1 \le j \le N, j \ne i} \left[ \alpha_1 \frac{\pi}{L} \cot \frac{\pi(x_j - x_i)}{L} - \alpha_2 \frac{\pi^3}{L^3} \cot \frac{\pi(x_j - x_i)}{L} \left( \sin \frac{\pi(x_j - x_i)}{L} \right)^{-2} \right].$$

Let

$$E = \sum_{1 \le i < j \le N} \left[ \frac{\alpha_1}{2} \log \sin^2 \frac{\pi(x_j - x_i)}{L} + \frac{\alpha_2}{2} \frac{\pi^2}{L^2} \left( \sin \frac{\pi(x_j - x_i)}{L} \right)^{-2} \right] - E_N^0$$

Here $E_N^0$ is some constant satisfying $E(\text{uniform step train}) = 0$. It is easy to check that

$$\frac{\partial E}{\partial x_i} = - \sum_{1 \le j \le N, j \ne i} \left[ \alpha_1 \frac{\pi}{L} \cot \frac{\pi(x_j - x_i)}{L} - \alpha_2 \frac{\pi^3}{L^3} \cot \frac{\pi(x_j - x_i)}{L} \left( \sin \frac{\pi(x_j - x_i)}{L} \right)^{-2} \right]$$
$$= f_i.$$

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