SELF-REPELLENT BRANCHING RANDOM WALK

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ABSTRACT. We consider a discrete-time binary branching random walk with independent standard normal increments subject to a penalty β for every pair of particles that get within distance ϵ of each other at any time. We give a precise description of the most likely configurations of the particles under this law for N large and β, ϵ fixed. Particles spread out over a distance $2^{2N/3}$, essentially in finite time, and subsequently arrange themselves so that at time $2N/3$ they cover a grid of width ϵ with one particle per site. After time $2N/3$, the bulk of the particles and their descendants do not move anymore, while the particles in a boundary layer of width $2^{N/3}$ form a "staircase" to the particles in the bulk. At time N, each site in the boundary layer is occupied by $2^{N/3}$ particles.

1. INTRODUCTION AND MAIN RESULTS

1.1. **Background.** Both branching Brownian motion (BBM) and branching random walk (BRW) can be seen as elementary models for the evolution of a population of individuals that are subject to birth, death, and motion in space [21, 3]. Of primary interest in these models is the evolution of the spatial distribution of the population over time. Over the past 40 years, BBM and BRW have been investigated from the point of view of extreme-value theory [10, 18, 12, 13, 5, 6, 7, 4, 14, 8].

As models for population dynamics, both BBM and BRW are unrealistic as they lead to uncontrolled exponential growth of the population size and therefore to unsustainably high densities of the population. For instance, the population size of binary BRW at time n grows like 2^n, while the population spreads out over a volume of order n. Several variants have been proposed where, according to some selection rule, offspring is selected in such a way that the total population size remains controlled [11, 20, 15, 19], or competitive interactions between particles are added to suppress the growth [16, 17, 2, 1].

In [9], a BBM is considered that is penalised when any two particles get close to each other at any time. It turns out that the optimal strategy for this process is to delay branching until a late random time, to guarantee that the total number of particles generated remains finite. In short, in this model the optimal strategy is to do nothing for a long time, and branch and diffuse only shortly before the time horizon. In the present paper, we look at a similar process, but in a setting where branching cannot be avoided. Specifically, we consider a BRW where all particles duplicate at each unit of time, jump according to

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independent Gaussian increments, and receive a penalty for every pair of particles that get close to each other at any time.

Sections 1.2 and 1.3 define the model and introduce notation. Section 1.4 defines a subclass of optimal configurations called admissible. Sections 1.5 and 1.6 formulate our main theorems and provide the underlying heuristics. Section 1.7 gives the outline of the remainder of the paper.

1.2. **Model.** Let

$$X = \Big((X_i(n))_{i=1}^{2^n}\Big)_{n\in\mathbb{N}} \tag{1.1}$$

denote the particles of a discrete-time binary BRW whose increments are i.i.d. standard normal random variables. Write $\mathbb{P}$ to denote the law of X. For $N \in \mathbb{N}$ and $\epsilon > 0$, define

$$J_{N,\epsilon}(X) = \sum_{n=1}^{N} \sum_{\substack{1\le i,j\le 2^n \\ i\neq j}} \mathbb{1}_{|X_i(n)-X_j(n)|<\epsilon}, \tag{1.2}$$

which is the total time up to time N that two particles are within distance ϵ of each other. This quantity can be viewed as the *total collision local time* on length scale ϵ of all the particles up to time N. We are interested in the law of X under the tilted probability measure $P_{N,\beta,\epsilon}$ given by

$$P_{N,\beta,\epsilon}(\cdot) = \frac{1}{Z_{N,\beta,\epsilon}}\,\mathbb{E}\Big[\mathbb{1}_{X\in\cdot}\,\mathrm{e}^{-\beta J_{N,\epsilon}(X)}\Big] \tag{1.3}$$

with

$$Z_{N,\beta,\epsilon} = \mathbb{E}\Big[\mathrm{e}^{-\beta J_{N,\epsilon}(X)}\Big] \tag{1.4}$$

the normalising partition function and $\beta > 0$ the *inverse temperature*, i.e., all collisions of all particles up to time N are penalised by a factor $\mathrm{e}^{-\beta}$. To avoid unnecessary complications, we assume throughout this paper that $\beta > \epsilon^2/2$ (the reason will become clear shortly). Note that the birth of particles is *not* penalised: the branching is deterministic and binary.

It is well known that under the law $\mathbb{P}$ the spread of a *typical* particle configuration at time n is of order n. Since there are 2^n particles at time n, the total collision local time in a typical particle configuration at time n is of order $\epsilon\, 2^{2n}/n$. When summed over n this gives a value of $J_{N,\epsilon}$ that is of order $\epsilon\, 2^{2N}/N$.

The situation is *very different* under the law $P_{N,\beta,\epsilon}$. Our main theorems below give a precise description of the most likely configurations of the particles under the law $P_{N,\beta,\epsilon}$ for N large and β, ϵ fixed. Before stating these theorems we need to introduce some notation.

1.3. **Notation.** We denote the infinite binary tree by $\mathbb{T}$ and the finite binary subtree with n generations by $\mathbb{T}^{(n)}$. We label the leaves of $\mathbb{T}$ by an infinite multi-index $\boldsymbol{x} = (x_1x_2\dots) \in \{0,1\}^{\mathbb{N}}$, and write $\boldsymbol{x}^{(n)}$ for the ancestor of $\boldsymbol{x}$ in the n-th generation. The root of $\mathbb{T}$ is denoted by $\emptyset$, and $\mathbb{T}$ is endowed with the natural lexicographic order. Let $h\colon\ \mathbb{T} \to \mathbb{R}$ denote the collection of positions of all the particles in the BRW, i.e., $h(\boldsymbol{x}^{(n)})$ is the position of the ancestor of $\boldsymbol{x}$ in the n-th generation. Then the probability density of a configuration of particles in the first N generations is given by

$$p(h;\mathbb{T}^{(N)}) = \exp\Big(-S_{\mathrm{spr}}(h,\mathbb{T}^{(N)})\Big) \tag{1.5}$$

with

$$S_{\mathrm{spr}}(h,\mathbb{T}^{(N)}) = \sum_{n=0}^{N-1} W_n(h), \tag{1.6}$$

where

$$W_n(h) = \tfrac{1}{2} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \Big(\big(h(z^{(n)}0) - h(z^{(n)}) \big)^2 + \big(h(z^{(n)}1) - h(z^{(n)}) \big)^2 \Big). \tag{1.7}$$

The penalty function reads

$$J_{N,\epsilon}(h, \mathbb{T}^{(N)}) = \sum_{n=1}^{N} I_{n,\epsilon}(h), \tag{1.8}$$

where

$$I_{n,\epsilon}(h) = \sum_{\substack{z^{(n)}, y^{(n)} \in \mathbb{T}^{(n)} \\ z^{(n)} \neq y^{(n)}}} \mathbb{1}_{|h(z^{(n)}) - h(y^{(n)})| < \epsilon}. \tag{1.9}$$

Thus, for given $N \in \mathbb{N}$, the optimal strategy will be given by the configurations minimising the functional

$$S(h, \mathbb{T}^{(N)}) = S_{\mathrm{spr}}(h, \mathbb{T}^{(N)}) + \beta J_{N,\epsilon}(h, \mathbb{T}^{(N)}). \tag{1.10}$$

1.4. **Admissible configurations.** We collect some a priori properties of possible minimising configurations. We begin by showing that $h(z^{(N)})$ takes values only in $\frac{1}{2} + \epsilon\mathbb{Z}$ (so that particles are either at the same location or at a distance at least ϵ from each other). Let h be any configuration such that in generation N at some site $i\epsilon$ there are at least two particles more than at one of the neighbouring sites $j\epsilon$ with $j = i \pm 1$. From h we can obtain a configuration h' by moving one of the particles at site $i\epsilon$ to one of the neighbouring sites $j\epsilon$ without changing anything else. This move entails a cost in the spread W_{N-1} of at most $\epsilon^2/2$ and produces a gain in the interaction I_N of at least 2β. Thus, if $\beta > \epsilon^2/2$, then any minimising configuration h must satisfy the condition that the difference in occupation numbers of any two neighbouring sites in $\epsilon\mathbb{Z}$ is at most one. We call this the set of 'smooth configurations'. We want to find the configurations within this set that minimise the functional in (1.10).

Next, consider configurations that increase linearly over length ϵr, subsequently stay constant over length ϵd, and afterwards decrease linearly over length ϵr again, for some $r \in \mathbb{N}$. The total number of particles in such configurations is $r(r+1) + dr$, which must be equal to 2^N, i.e.,

$$d = (2^N/r) - (r+1). \tag{1.11}$$

We denote the set of such configurations by $\mathcal{H}_{r,d,N}$, and call them *admissible configurations*.

1.5. **Main theorems.** The following theorems identify the *optimal profiles* for N large and will be proved in Section 4. Recall that we assume that $\beta > \epsilon^2/2$.

Theorem 1.1. [The end-profile] *Any h that minimises $S(h, \mathbb{T}^{(N)})$ is an element of $\mathcal{H}_{r,d,N}$ with $r = 2^K$, where K is the integer closest to*

$$\tfrac{N-4}{3} + \tfrac{1}{3}\ln_2(3\epsilon^2/\beta) + O(2^{-N/6}) = \tfrac{N}{3} + O(1), \tag{1.12}$$

and with $d = (2^N/r) - (r+1)$. See Figure 1.

Theorem 1.2. [The post-profile] *Any h that minimises $S(h, \mathbb{T}^{(N)})$ is such that $h(z^{(n)}) \in \mathcal{H}_{r_n,d_n,n}$ for all $N - K \leq n \leq N$, where*

$$r_n = 2^{n-(N-K)}, \tag{1.13}$$

and $d_n = (2^n/r_n) - (r_n + 1)$. See Figure 2.

Theorem 1.3. [The pre-profile] *Any h that minimises $S(h, \mathbb{T}^{(N)})$ is such that*

$$\{h(z^{(n)}) \colon\ 1 \le n \le N-K\} \tag{1.14}$$

is the solution to the Dirichlet problem

$$\begin{aligned} h(z^{(n)}0) + h(z^{(n)}1) + h(z^{(n-1)}) &= 3h(z^{(n)}), \quad 1 \le n < N-K, \\ h(\emptyset) &= 0, \\ h(z^{(N-K)}) &= u(z^{(N-K)}), \end{aligned} \tag{1.15}$$

with boundary condition

$$u(z^{(N-K)}) = \begin{cases} \epsilon \sum_{\ell=2}^{N-K} 2^{(N-K)-\ell} z_\ell + \frac{1}{2}\epsilon, & z_1 = 1, \\ -\epsilon \sum_{\ell=2}^{N-K} 2^{(N-K)-\ell} z_\ell - \frac{1}{2}\epsilon, & z_1 = 0. \end{cases} \tag{1.16}$$

In particular, the position h_n of the right-most particle at time n is

$$h_n = \begin{cases} \epsilon\, 2^{N-K-1}(1 - 2^{-n-1}n), & 2 \le n \ll N-K, \\ \epsilon\, 2^{N-K-3}, & n = 1. \end{cases} \tag{1.17}$$

See Figure 3.

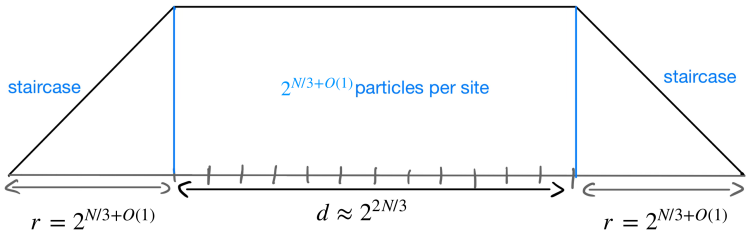

FIGURE 1. The end-profile of a configuration in $\mathcal{H}_{r,d,N}$.

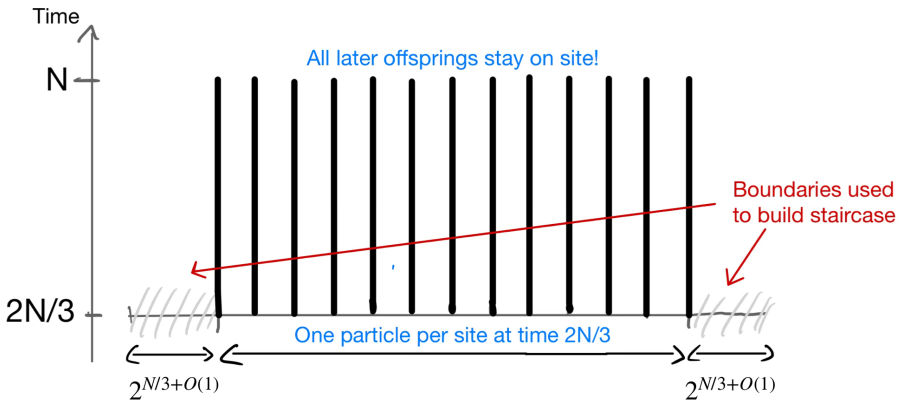

FIGURE 2. The post-profile of a configuration in $\mathcal{H}_{r,d,N}$.

Theorem 1.4. [Cost of the profile] *For $N \to \infty$,*

$$\ln \min_{h\colon\, \mathbb{T}^{(N)} \to \mathbb{R}} S(h, \mathbb{T}^{(N)}) = -2^{5/3}3^{-2/3}(\beta\epsilon)^{2/3}2^{4N/3} + O(2^{7N/6}). \tag{1.18}$$

The following rough picture emerges for the optimal profile:

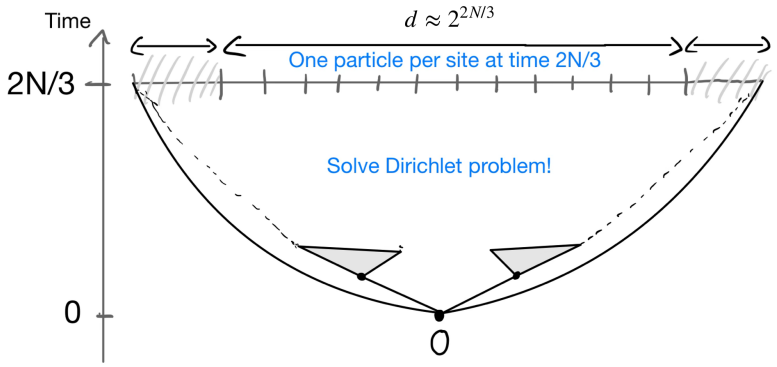

FIGURE 3. The pre-profile of a configuration in $\mathcal{H}_{r,d,N}$.

(i) Until time $2N/3$ particles spread out quickly according to a profile that is captured by a Dirichlet problem.

(ii) At time $2N/3$, there is a single particle on every site in

$$\mathcal{L}_1 = \epsilon \left\{-2^{N-K-1} - \tfrac{1}{2}, \dots, 2^{N-K-1} + \tfrac{1}{2}\right\}. \tag{1.19}$$

(iii) The particles in

$$\mathcal{L}_2 = \epsilon \left\{-2^{N-K-1} - \tfrac{1}{2} + 2^{K-1}, \dots, 2^{N-K-1} + \tfrac{1}{2} - 2^{K-1}\right\} \tag{1.20}$$

and their descendants do not move between time $2N/3$ and time N.

(iv) While the particles in $\mathcal{L}_1 \setminus \mathcal{L}_2$ reproduce, their offspring move minimally to remove increments of height larger than 1.

1.6. **Heuristics.** Before closing this introduction we give a *rough heuristic* for the optimal strategy describing how the particles spread out over space in the course of time. If at time n the particles are evenly distributed over the interval $[-r(n), r(n)]$, then each particle has roughly $\epsilon\, 2^n/r(n)$ particles within distance ϵ (which is possible as long as $\epsilon\, 2^n/r(n) > 1$), and so $J_{N,\epsilon}$ receives a contribution of order $\epsilon\, 2^{2n}/r(n)$. On the other hand, to spread out the offspring, for all $x \in [-1, 1]$, particles that were at a position $xr(n-1)$ at time $n-1$ must move to position $xr(n)$ at time n, which entails a displacement cost of order $\exp(\frac{1}{2}x^2[r(n) - r(n-1)]^2)$ per particle, and hence a total cost of order

$$\exp\left(2^n \int_{-1}^{1} \mathrm{d}x\, \tfrac{1}{2}x^2 (r(n) - r(n-1))^2\right) = \exp\left(2^n \tfrac{1}{3}(r(n) - r(n-1))^2\right). \tag{1.21}$$

We would be tempted to think that, for the optimal choice of $r(n)$, both costs must be equal, i.e.,

$$\beta \frac{\epsilon\, 2^{2n}}{r(n)} = 2^n \tfrac{1}{3}(r(n) - r(n-1))^2. \tag{1.22}$$

Hence

$$r(n)^3 = 2^n\, 3\beta\epsilon \left(1 - \frac{r(n-1)}{r(n)}\right)^{-2}, \tag{1.23}$$

which would give

$$r(n) = C\, 2^{n/3}, \qquad C^3 = \frac{3\beta\epsilon}{(1 - 2^{-1/3})^2}. \tag{1.24}$$

However, the above reasoning is *flawed*: it is *not at all* optimal to optimise the cost in each summand separately. Rather, in anticipation of the fact that the process terminates at time

N, it pays off to *prepare for future expenses at an early stage*, when there are not so many particles yet.

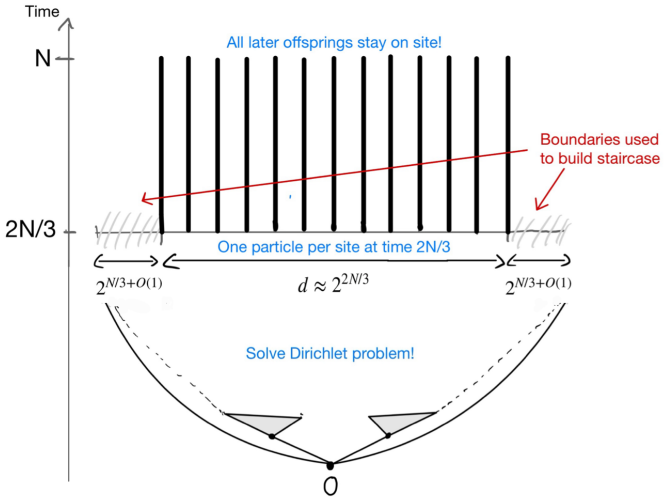

FIGURE 4. Sketch of an optimal configuration.

To get a better answer, we must minimise the functional

$$S(r) = \sum_{n=1}^{N} \left(\beta \frac{\epsilon\, 2^{2n}}{r(n)} + 2^n \tfrac{1}{3} (r(n) - r(n-1))^2 \right). \tag{1.25}$$

Differentiating w.r.t. $r(n)$, we get, for $1 < n < N$,

$$-3\beta\epsilon\, 2^{2n} r(n)^{-2} + 2^{n+1}(r(n) - r(n-1)) - 2^{n+2}(r(n+1) - r(n)) = 0 \tag{1.26}$$

or

$$r(n) - r(n-1) = 3\beta\epsilon\, 2^{n-1} r(n)^{-2} + 2(r(n+1) - r(n)), \tag{1.27}$$

while, for $n = N$,

$$r(N) - r(N-1) = 3\beta\epsilon\, 2^{N} r(N)^{-2}, \tag{1.28}$$

and, for $n = 1$,

$$r(1) = 3\beta\epsilon\, r(1)^{-2} + 2(r(2) - r(1)), \tag{1.29}$$

with $r(0) = 0$. Assume that $2^n r(n)^{-2} \ll 1$ for all $1 \le n \le N$. Then we can neglect the nonlinear term, to get the recursion

$$r(n+1) - r(n) = \tfrac{1}{2}(r(n) - r(n-1)), \tag{1.30}$$

which is the Laplace equation on a binary tree. The solution is

$$r(n) = 2r(1)(1 - 2^{-n}), \tag{1.31}$$

with $r(1)$ a free parameter. Inserting this relation into (1.25), we get

$$\begin{aligned} S_N(r) &= \sum_{n=1}^{N} \left(\beta \frac{\epsilon\, 2^{2n}}{2r(1)(1-2^{-n})} + 2^n \tfrac{4}{3} r(1)^2 2^{-2n} \right) \\ &\sim \tfrac{1}{3}\beta\epsilon\, 2^{2N+1}\, r(1)^{-1} + \tfrac{4}{3} r(1)^2, \end{aligned} \tag{1.32}$$

which takes its minimum for

$$r(1)^3 = \beta\epsilon\, 2^{2N-2}. \tag{1.33}$$

Hence, $2^n r(n)^{-2} \asymp 2^n 2^{-4N/3} \leq 2^{-N/3} \ll 1$, so that our initial assumption is indeed verified. Consequently,

$$S_N(r) \sim \tfrac{2}{3} 2^{2/3} (\beta\epsilon)^{2/3} 2^{4N/3}.$$

This is the same scaling as in Theorem 1.4, but with a different constant (the precise constant is lost in the heuristic argument).

Theorems 1.1–1.4 provide a detailed picture of the underlying particle system (summarised in Figure 4).

1.7. **Outline.** The remainder of this paper is organised as follows. In Section 2 we identify the minimisers of the functional $S_{\rm spr}(h, \mathbb{T}^{(N)})$ in (1.10), which *ignores* the repulsive interaction between the particles. This identification involves a Dirichlet problem and leads to sharp estimates on $S_{\rm spr}(h, \mathbb{T}^{(N)})$. In Section 3 we identify the minimisers of the functional $S(h, \mathbb{T}^{(N)})$ in (1.10), which *includes* the repulsive interaction between the particles. In Section 4 we collect our estimates and prove Theorems 1.1–1.4. The reason why the analysis of $S_{\rm spr}(h, \mathbb{T}^{(N)})$ is crucial is that in the optimal strategy the effect of the repulsive interaction between the particles is simple, as argued in the heuristics in Section 1.6.

2. Optimal strategy without interaction

In this section we identify the optimal strategy for the branching random walk to reach a configuration at time $M \in \mathbb{N}$ where the 2^M particles are distributed at positions such that their distance is just large enough to ensure that there is no penalty to pay yet. In Section 2.1 we represent the optimal strategy as a Dirichlet problem. In Section 2.2 we find the solution to this Dirichlet problem. In Section 2.3 we compute the cost of spreading out the particles. The main results are collected in Lemmas 2.1–2.6 below.

2.1. **Representation of the optimal strategy as a Dirichlet problem.** When we optimise $S_{\rm spr}(h, \mathbb{T}^{(M)})$ under the *boundary conditions*

$$h(\emptyset) = 0, \qquad h(z^{(M)}) = u(z^{(M)}), \qquad u\colon\ \mathbb{T}^{(M)} \to \mathbb{R}, \tag{2.1}$$

the solution is the harmonic function with these boundary conditions, i.e., a solution of the *Dirichlet problem*

$$\begin{aligned} h(z^{(n)}0) + h(z^{(n)}1) + h(z^{(n-1)}) &= 3h(z^{(n)}), \quad 1 \leq n < M, \\ h(\emptyset) &= 0, \\ h(z^{(M)}) &= u(z^{(M)}). \end{aligned} \tag{2.2}$$

It will be convenient to express the latter in terms of the increments of h. For $z \in \mathbb{T}$ and $1 \leq n \leq M$, set

$$a(z^{(n)}) = h(z^{(n)}) - h(z^{(n-1)}). \tag{2.3}$$

Then

$$a(\emptyset) + \sum_{j=1}^{M} a(z^{(j)}) = u(z^{(M)}), \tag{2.4}$$

and, for $1 \leq n \leq M$,

$$a(z^{(n-1)}) = a(z^{(n-1)}0) + a(z^{(n-1)}1). \tag{2.5}$$

Define, for $0 \leq n \leq M$,

$$\Sigma(z^{(n)}) = \sum_{\boldsymbol{y}^{(M-n)} \in \mathbb{T}^{(M-n)}} u(z^{(n)}\, \boldsymbol{y}^{(M-n)}). \tag{2.6}$$

Lemma 2.1. *The unique solution of (2.4)–(2.5) satisfies the recursive equation*

$$\Sigma(z^{(n)}) = 2^{M-n}\left(\sum_{j=1}^{n-1} a(z^{(j)})\right) + \left(2^{M-n+1}-1\right)a(z^{(n)}). \tag{2.7}$$

Proof. Fix $z \in \mathbb{T}$ and $0 \le n \le M$. Sum (2.4) over the descendants of $z^{(n)}$. This gives

$$\begin{aligned}
\Sigma(z^{(n)}) &= \sum_{\boldsymbol{y}^{(M-n)}\in\mathbb{T}^{(M-n)}}\left(a(\emptyset) + \sum_{j=1}^{M} a\Big((z^{(n)}\,\boldsymbol{y}^{(M-n)})^{(j)}\Big)\right)\\
&= 2^{M-n}a(\emptyset) + 2^{M-n}\sum_{j=1}^{n} a(z^{(j)}) + \sum_{j=n+1}^{M}\sum_{\boldsymbol{y}^{(M-n)}\in\mathbb{T}^{(M-n)}} a(z^{(n)}\,\boldsymbol{y}^{(j-n)})\\
&= 2^{M-n}a(\emptyset) + 2^{M-n}\sum_{j=1}^{n} a(z^{(j)}) + \sum_{j=n+1}^{M} 2^{M-j}\sum_{\boldsymbol{y}^{(j-n)}\in\mathbb{T}^{(j-n)}} a(z^{(n)}\,\boldsymbol{y}^{(j-n)})\\
&= 2^{M-n}\,a(\emptyset) + 2^{M-n}\sum_{j=1}^{n} a(z^{(j)}) + \sum_{j=n+1}^{M} 2^{M-j}\,a(z^{(n)})\\
&= 2^{M-n}\,a(\emptyset) + 2^{M-n}\sum_{j=1}^{n-1} a(z^{(j)}) + \left(2^{M-n+1}-1\right)a(z^{(n)}),
\end{aligned} \tag{2.8}$$

where the fourth equality uses (2.5). Since $a(\emptyset) = 0$, this gives (2.7). □

Note that

$$a(z^{(M)}) = h(z^{(M)}) - \sum_{j=1}^{M} a(z^{(j)}). \tag{2.9}$$

The next lemma gives an explicit form of the solution of the recursion in (2.7).

Lemma 2.2. *Set* $b_n = (2^{M-n+1}-1)^{-1}$. *Then*

$$h(z^{(n)}) = b_n\Sigma(z^{(n)}) + \sum_{\ell=1}^{n-1}\frac{b_{n-\ell+1}b_{n-\ell}}{b_{n+1}}\,\Sigma(z^{(n-\ell)}) \tag{2.10}$$

and

$$a(z^{(n)}) \;=\; b_n\Sigma(z^{(n)}) + \sum_{\ell=1}^{n-1} b_{n-\ell}\Sigma(z^{(n-\ell)})\left(\frac{b_{n-\ell+1}}{b_{n+1}} - \frac{b_{n-\ell+1}}{b_n}\right). \tag{2.11}$$

Proof. The recursion (2.7) reads

$$a(z^{(n)}) = b_n\Sigma(z^{(n)}) - b_n 2^{M-n}\sum_{\ell=1}^{n-1} a(z^{(\ell)}) = b_n\Sigma(z^{(n)}) - b_n 2^{M-n}h(z^{(n-1)}), \tag{2.12}$$

or

$$h(z^{(n)}) = b_n\Sigma(z^{(n)}) - \left(b_n 2^{M-n}-1\right)h(z^{(n-1)}) = b_n\Sigma(z^{(n)}) + \frac{b_n}{b_{n+1}}h(z^{(n-1)}). \tag{2.13}$$

A simple iteration gives that (note that $\Sigma(\emptyset) = 0$)

$$h(z^{(n)}) = b_n\Sigma(z^{(n)}) + \sum_{\ell=1}^{n-1}\frac{b_{n-\ell+1}b_{n-\ell}}{b_{n+1}}\Sigma(z^{(n-\ell)}). \tag{2.14}$$

Hence

$$\begin{aligned} a(z^{(n)}) &= b_n\Sigma(z^{(n)}) + \sum_{\ell=1}^{n-1} \frac{b_{n-\ell+1}b_{n-\ell}}{b_{n+1}}\Sigma(z^{(n-\ell)}) \\ &\quad -b_{n-1}\Sigma(z^{(n-1)}) - \sum_{\ell=1}^{n-2} \frac{b_{n-\ell}b_{n-1-\ell}}{b_n}\Sigma(z^{(n-1-\ell)}) \\ &= b_n\Sigma(z^{(n)}) + \sum_{\ell=1}^{n-1} \Sigma(z^{(n-\ell)})\left(\frac{b_{n-\ell+1}b_{n-\ell}}{b_{n+1}} - \frac{b_{n-\ell+1}b_{n-\ell}}{b_n}\right), \end{aligned} \tag{2.15}$$

which gives (2.11). □

For future use, note that

$$\frac{b_{n-\ell+1}}{b_{n+1}} - \frac{b_{n-\ell+1}}{b_n} = 2^{-\ell}\frac{1}{1-2^{-M+n-\ell}}. \tag{2.16}$$

2.2. **Solution of the Dirichlet problem.** In the following we are interested in the Dirichlet problem with boundary conditions that are symmetric around zero and correspond to having single particles at distance ϵ. Hence, we look at

$$u(z^{(M)}) = \begin{cases} \epsilon\sum_{\ell=2}^{M} 2^{M-\ell}z_\ell + \frac{1}{2}\epsilon, & z_1 = 1, \\ -\epsilon\sum_{\ell=2}^{M} 2^{M-\ell}z_\ell - \frac{1}{2}\epsilon, & z_1 = 0. \end{cases} \tag{2.17}$$

For these boundary conditions we compute $a(z^{(n)})$ and $h(z^{(n)})$. We write h^{Dir} for the solution of the Dirichlet problem with boundary condition (2.17).

Lemma 2.3. *The solution of the Dirichlet problem with boundary condition (2.17) is given by*

$$a(z^{(n)}) = \epsilon\, 2^{M-n-2}\left(2 - n + 2\sum_{k=2}^{n} z_k\right) + O(1), \tag{2.18}$$

and, for $M \gg n$,

$$h(z^{(n)}) = \epsilon\, 2^{M-1}\left(n2^{-n-1} + 2\sum_{k=2}^{n}(2^{-k} - 2^{-n-1})z_k\right)(1 + O(2^{-M+n}). \tag{2.19}$$

In particular,

$$h(1^{(n)}) \sim \begin{cases} \epsilon\, 2^{M-1}\left(1 - 2^{-n-1}n\right), & 2 \le n \le M, \\ \epsilon\, 2^{M-3} & n = 1. \end{cases} \tag{2.20}$$

Remark. In the course of the proof we obtain precise formulas for a and h, but we state only the approximate forms in the lemma.

Proof. For $z_1 = 1$,

$$\begin{aligned}\Sigma(\boldsymbol{z}^{(n)}) &= \epsilon \sum_{\boldsymbol{y}^{(M-n)}\in\mathbb{T}^{(M-n)}} \left(\sum_{\ell=2}^{M} 2^{M-\ell} z_\ell + 2^{-1}\right) \\ &= \epsilon \sum_{\boldsymbol{y}^{(M-n)}\in\mathbb{T}^{(M-n)}} \left(\sum_{\ell=2}^{n} 2^{M-\ell} z_\ell + \sum_{\ell=n+1}^{M} 2^{M-\ell} y_\ell + 2^{-1}\right) \\ &= \epsilon\, 2^M \sum_{\ell=2}^{n} 2^{2M-n-\ell} z_\ell + \epsilon\, 2^{M-n-1} \sum_{\ell=n+1}^{M} 2^{-\ell} + \epsilon\, 2^{M-n-1} \\ &= \epsilon\, 2^{2M-n} \left(\sum_{\ell=2}^{n} 2^{-\ell} z_\ell + 2^{-n-1}\right). \end{aligned} \tag{2.21}$$

In particular,

$$\Sigma(1) = -\Sigma(0) = \epsilon\, 2^{2M-3}. \tag{2.22}$$

Consequently

$$b_{n-\ell}\Sigma(\boldsymbol{z}^{(n-\ell)}) = \frac{\epsilon}{2} 2^M \frac{1}{1-2^{-M+n-\ell-1}} \left(\sum_{k=2}^{n-\ell} 2^{-k} z_k + 2^{-n-1}\right) \tag{2.23}$$

and

$$\begin{aligned} a(\boldsymbol{z}^{(n)}) &= \frac{\epsilon}{2} \frac{1}{1-2^{-M+n-1}} \left(\sum_{k=2}^{n} 2^{M-k} z_k + 2^{M-n-1}\right) \\ &\quad -\frac{\epsilon}{2} \sum_{\ell=1}^{n-1} \frac{1}{1-2^{-M+n-\ell-1}} \left(\sum_{k=2}^{n-\ell} 2^{M-k-\ell} z_k + 2^{M-n-1}\right) \frac{1}{1-2^{-M+n-\ell}}. \end{aligned} \tag{2.24}$$

A re-ordering of the summations gives

$$\begin{aligned} a(\boldsymbol{z}^{(n)}) &= \frac{\epsilon}{2} 2^{M-n-1} \left(\frac{1}{1-2^{-M+n-1}} - \sum_{\ell=1}^{n-1} c_\ell\right) \\ &\quad + \frac{\epsilon}{2} 2^M \sum_{k=2}^{n} 2^{-k} z_k \left(\frac{1}{1-2^{-M+n-1}} - \sum_{\ell=1}^{n-k} 2^{-\ell} c_\ell\right) \end{aligned} \tag{2.25}$$

with

$$c_\ell = \frac{1}{(1-2^{-M+n-\ell})(1-2^{-M+n-\ell-1})}. \tag{2.26}$$

Using Wolfram Alpha, we get

$$\frac{1}{1-2^{-M+n-1}} - \sum_{\ell=1}^{n-k} 2^{-\ell} c_\ell = 2^{k-n} \frac{1}{1-2^{-M+k-1}}. \tag{2.27}$$

Hence

$$\begin{aligned} a(\boldsymbol{z}^{(n)}) &= \frac{\epsilon}{2} 2^{M-n-1} \left(\frac{1}{1-2^{-M+n-1}} - \sum_{\ell=1}^{n-1} c_\ell\right) \\ &\quad + \frac{\epsilon}{2} 2^{M-n} \sum_{k=2}^{n} z_k \left(\frac{1}{1-2^{-M+k-1}}\right). \end{aligned} \tag{2.28}$$

We readily verify that, uniformly in $0 \le n \le M$,

$$a(z^{(n)}) = \bar{a}(z^{(n)}) + O(1), \tag{2.29}$$

where we set

$$\bar{a}(z^{(n)}) = \epsilon 2^{M-n-2}\left((2-n) + 2\sum_{k=2}^{n} z_k\right). \tag{2.30}$$

Next, we turn to h. Combining (2.14) with (2.23), we get

$$\begin{aligned} h(z^{(n)}) &= \frac{\epsilon}{2}2^M \frac{1}{1-2^{-M+n-1}}\left(\sum_{k=2}^{n} 2^{-k} z_k + 2^{-n-1}\right) \\ &\quad + \frac{\epsilon}{2}2^M \sum_{\ell=1}^{n-1} \frac{b_{n-\ell+1}}{b_{n+1}} \frac{1}{1-2^{-M+n-\ell-1}}\left(\sum_{k=2}^{n-\ell} 2^{-k} z_k + 2^{-n+\ell-1}\right) \\ &= \frac{\epsilon}{2}2^M \frac{1}{1-2^{-M+n-1}}\left(\sum_{k=2}^{n} 2^{-k} z_k + 2^{-n-1}\right) \\ &\quad + \frac{\epsilon}{2}2^M (1-2^{-M+n}) \sum_{\ell=1}^{n-1} 2^{-\ell} c_\ell \left(\sum_{k=2}^{n-\ell} 2^{-k} z_k + 2^{-n-1+\ell}\right), \end{aligned} \tag{2.31}$$

where we use that (recall the definition of c_ℓ in (2.26)

$$\frac{b_{n-\ell+1}}{b_{n+1}} \frac{1}{1-2^{-M+n-\ell-1}} = 2^{-\ell}(1-2^{-M+n}) c_\ell. \tag{2.32}$$

Re-organising terms, we arrive at

$$\begin{aligned} h(z^{(n)}) &= \frac{\epsilon}{2}2^{M-n-1}\left(\frac{1}{1-2^{-M+n-1}} + (1-2^{-M+n})\sum_{\ell=1}^{n-1} c_\ell\right) \\ &\quad + \frac{\epsilon}{2}2^M \left(\frac{1}{1-2^{-M+n-1}} \sum_{k=2}^{n} 2^{-k} z_k + (1-2^{-M+n}) \sum_{k=2}^{n-1} 2^{-k} z_k \sum_{\ell=1}^{n-k} 2^{-\ell} c_\ell\right). \end{aligned} \tag{2.33}$$

By (2.27), this is equal to

$$\begin{aligned} &\frac{\epsilon}{2}2^{M-n-1}\left(\frac{1}{1-2^{-M+n-1}} + (1-2^{-M+n})\sum_{\ell=1}^{n-1} c_\ell\right) \\ &\frac{\epsilon}{2}2^M\Bigg(\frac{1}{1-2^{-M+n-1}} \sum_{k=2}^{n} 2^{-k} z_k + \frac{1-2^{-M+n}}{1-2^{-M+n-1}} \sum_{k=2}^{n-1} 2^{-k} z_k \\ &-2^{-n} \sum_{k=2}^{n-1} z_k \frac{1-2^{-M+n}}{1-2^{-M+k-1}}\Bigg). \end{aligned} \tag{2.34}$$

Even though this looks rather complicated, it is true that $h(z^{(M)}) = u(z^{(M)})$, as it should be. For $n \ll M$, this simplifies to

$$h(z^{(n)}) = \frac{\epsilon}{2}2^M \left(n2^{-n-1} + 2\sum_{k=2}^{n} 2^{-k} z_k - 2^{-n} \sum_{k=2}^{n} z_k\right)(1 + O(2^{-M+n})), \tag{2.35}$$

and hence, for $n \geq 2$,

$$\begin{aligned} h(1^{(n)}) &= \frac{\epsilon}{2} 2^M \left(n2^{-n-1} + 1 - n2^{-n} \right) (1 + O(2^{-M+n})) \\ &= \frac{\epsilon}{2} 2^M \left(1 - n2^{-n-1} \right) (1 + O(2^{-M+n})), \end{aligned} \tag{2.36}$$

and

$$h(1^{(1)}) = \epsilon 2^{M-3}. \tag{2.37}$$

□

Next, we want to ensure that the spacing between particles decreases as n increases, for which we need the following lemma.

Lemma 2.4. *Suppose that $z_1 = 1$ and $u(\boldsymbol{z}^{(M)}) = \epsilon \sum_{\ell=2}^{M} 2^{M-\ell} z_\ell + \frac{1}{2}\epsilon$. If h is a solution of (2.2), then, for all $0 \leq n \leq M$,*

$$\min_{\substack{z,y \in \mathbb{T}^{(n)} \\ z \neq y}} |h(\boldsymbol{z}^{(n)}) - h(\boldsymbol{y}^{(n)})| \geq \epsilon. \tag{2.38}$$

Proof. Let $\boldsymbol{z}^{(n)} > \boldsymbol{y}^{(n)}$. From (2.34) we get, for $n < M$,

$$\begin{aligned} h(\boldsymbol{z}^{(n)}) - h(\boldsymbol{y}^{(n)}) = \frac{\epsilon}{2} 2^M \Bigg(& \frac{1}{1 - 2^{-M+n-1}} \sum_{k=2}^{n} 2^{-k} (z_k - y_k) + \frac{1 - 2^{-M+n}}{1 - 2^{-M+n-1}} \sum_{k=2}^{n-1} 2^{-k} (z_k - y_k) \\ & - 2^{-n} \sum_{k=2}^{n-1} (z_k - y_k) \frac{1 - 2^{-M+n}}{1 - 2^{-M+k-1}} \Bigg) \\ \geq \frac{\epsilon}{2} 2^M & \frac{1}{1 - 2^{-M+n-1}} 2^{-n} \geq 4\epsilon/3. \end{aligned} \tag{2.39}$$

For $n = M$, the result holds since $h(\boldsymbol{z}^{(M)}) = u(\boldsymbol{z}^{(M)})$. □

2.3. **Cost of spreading out the particles.** We close this section by deriving bounds on the asymptotics of $S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(M)})$ for h^{Dir} satisfying *linear* boundary conditions.

Lemma 2.5. *Let h^{Dir} be the solution to the Dirichlet problem (2.2) with boundary condition u as in Lemma 2.4. Then*

$$\epsilon^2 \frac{2^{2M-6}}{(1 - 2^{-M})^2} \leq S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(M)}) \leq \epsilon^2 \frac{(2^{M-1} + \frac{1}{2})^2}{1 - 2^{-M}}. \tag{2.40}$$

Proof. Obviously,

$$S_{\mathrm{spr}}(h, \mathbb{T}^{(M)}) \geq \frac{1}{2} \sum_{x_1=0}^{1} a(x_1)^2. \tag{2.41}$$

Hence

$$S_{\mathrm{spr}}(h, \mathbb{T}^{(M)}) \geq \frac{\Sigma(0)^2 + \Sigma(1)^2}{2\,(2^M - 1)^2}. \tag{2.42}$$

Since $\Sigma(0) = -\Sigma(1) = \epsilon\, 2^{2M-3}$, this gives the claimed lower bound.

Choose any function that satisfies the boundary condition (2.4). For example, if $h(\boldsymbol{z}^{(M)})$ is linear with $h(0 \ldots 0) = -2^{M-1} - \frac{1}{2}$ and $h(1 \ldots 1) = 2^{M-1} + \frac{1}{2}$, then we can choose

$$a(0) = -\frac{2^{M-1} + \frac{1}{2}}{1 - 2^{-M}} 2^{-1},\ a(00) = -\frac{2^{M-1} + \frac{1}{2}}{1 - 2^{-M}} 2^{-2},\ \ldots,\ a(0 \ldots 0) = -\frac{2^{M-1} + \frac{1}{2}}{1 - 2^{-M}} 2^{-M}. \tag{2.43}$$

Note that

$$a(0) + \cdots + a(0 \dots 0) = -2^{M-1} - \tfrac{1}{2}, \tag{2.44}$$

and choose

$$a(x_1 \dots x_n) = a(0 \dots 0)\,(-1)^{\sum_{i=1}^n x_i}. \tag{2.45}$$

This choice satisfies the boundary conditions and, since

$$\sum_{j=1}^{M} 2^j \left(\frac{2^{M-1} + \frac{1}{2}}{1 - 2^{-M}} \right)^2 2^{-2j} = \frac{(2^{M-1} + \frac{1}{2})^2}{1 - 2^{-M}}, \tag{2.46}$$

gives the claimed upper bound. □

Lemma 2.5 shows that, to leading order in M, the lower bound is $\epsilon^2\, 2^{2M-4}$ and the upper bound is $\epsilon^2\, 2^{2M-2}$, which differ by a factor 4. The next lemma closes this gap.

Lemma 2.6. *As $M \to \infty$,*

$$S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(M)}) = \epsilon^2 2^{2M-3} + O(M^2 2^M). \tag{2.47}$$

Proof. We have that

$$\begin{aligned} S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(M)}) &= \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \tfrac{1}{2} \left(a(z^{(n)}) \right)^2 = \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \tfrac{1}{2} \left(\bar{a}(z^{(n)} + O(1) \right)^2 \\ &= \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \tfrac{1}{2} \left(\bar{a}(z^{(n)} \right)^2 + O(1) \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \bar{a}(z^{(n)}). \end{aligned} \tag{2.48}$$

Since $|\bar{a}(z^{(n)})| \le \epsilon 2^{M-n} n$, the last term is smaller than

$$O(1) \sum_{n=1}^{M} 2^M n = O(1) 2^M M^2. \tag{2.49}$$

The first summand is equal to

$$\begin{aligned} \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \tfrac{1}{2} \left(\bar{a}(z^{(n)}) \right)^2 &= \sum_{n=1}^{M} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \left(\epsilon 2^{M-n-2} \left(2 - n + 2 \sum_{k=2}^{n} z_k \right) \right)^2 \\ &= \epsilon^2 2^{2M-4} \sum_{n=1}^{M} 2^{-2n} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \left(2 - n + 2 \sum_{k=2}^{n} z_k \right)^2 \\ &= \epsilon^2 2^{2M-4} \sum_{n=1}^{M} 2^{-2n} \sum_{z^{(n)} \in \mathbb{T}^{(n)}} \left((2-n)^2 + 4(2-n) \sum_{k=2}^{n} z_k + 4 \sum_{k,k'=2}^{n} z_k z_{k'} \right) \end{aligned} \tag{2.50}$$

Computing the sum over $z^{(n)} \in \mathbb{T}^{(n)}$, we see that this is equal to

$$\begin{aligned} &\epsilon^2 2^{2M-4} \sum_{n=1}^{M} 2^{-2n} \left((2-n)^2 2^{n-1} + (2-n) 2^n (n-1) + (n-1) 2^n + n(n-1) 2^{n-1} \right) \\ = \;& \epsilon^2 2^{2M-4} \sum_{n=1}^{M} 2^{-n} (\tfrac{3}{2} n - 1) = \epsilon^2 2^{2M-4} (2 - 2^{-M-1}(3M+4)). \end{aligned} \tag{2.51}$$

This, together with (2.49), gives the assertion of the lemma. □

3. Optimal strategy with interaction

We next turn to the problem of minimising the full functional $S(h, \mathbb{T}^{(N)})$ in (1.10). In Section 3.1 we derive properties of the optimal configurations. In Section 3.2 we show that optimal configurations are specific admissible configurations. In Section 3.3 we compute the cost of the optimal configurations. The main results in this section are collected in Lemmas 3.1–3.12 below.

3.1. **Properties of optimal configurations.**

First, we show that optimal configurations are restricted to stay on $\epsilon\mathbb{Z}$.

Lemma 3.1. *Fix a range $\mathcal{R} = \epsilon\,[-2^{K-1} - \frac{1}{2}, 2^{K-1} + \frac{1}{2}]$, and let $n \geq K$. Then the minimiser of I_n with range restricted to $\mathcal{R}$ is*

$$h^*(z^{(n)}) = \epsilon\left(\sum_{\ell=0}^{K-1} 2^\ell z_\ell - 2^{K-1} + \tfrac{1}{2}\right). \tag{3.1}$$

Proof. Let h be any configuration of the 2^n particles on $\mathcal{R}$. We first show that $I_n(h) \geq I_n(h^*)$, where

$$h^*(z^{(n)}) = \epsilon(\ell - \tfrac{1}{2}) \quad \text{if} \quad |h(z^{(n)}) - \epsilon(\ell - \tfrac{1}{2})| < \tfrac{1}{2}\epsilon. \tag{3.2}$$

Indeed,

$$\begin{aligned} I_n(h^*) &= \sum_{\substack{z^{(n)},y^{(n)}\in\mathbb{T}^{(n)}\\ z^{(n)}\neq y^{(n)}}} \mathbb{1}_{|h^*(z^{(n)})-h^*(y^{(n)})|<\epsilon} = \sum_{\substack{z^{(n)},y^{(n)}\in\mathbb{T}^{(n)}\\ z^{(n)}\neq y^{(n)}}} \mathbb{1}_{h^*(z^{(n)})=h^*(y^{(n)})} \\ &= \sum_{\substack{z^{(n)},y^{(n)}\in\mathbb{T}^{(n)}\\ z^{(n)}\neq y^{(n)}}} \mathbb{1}_{h^*(z^{(n)})=h^*(y^{(n)})}\,\mathbb{1}_{|h(z^{(n)})-h(y^{(n)})|<\epsilon} \\ &\leq \sum_{\substack{z^{(n)},y^{(n)}\in\mathbb{T}^{(n)}\\ z^{(n)}\neq y^{(n)}}} \mathbb{1}_{|h(z^{(n)})-h(y^{(n)})|<\epsilon} = I_n(h). \end{aligned} \tag{3.3}$$

The last inequality is strict if there is any point that does not lie in $\epsilon\mathbb{Z}$ and there are at least 2^K points, which is the case for $n \geq K$. This shows that any minimiser h must be supported on $\epsilon\mathbb{Z}$. Thus, for any minimiser there must be a_ℓ particles at site $\epsilon(\ell - \frac{1}{2})$, $0 \leq \ell < 2^K$ with $\sum_{\ell=0}^{2^K-1} a_\ell = 2^n$. For such a configuration the interaction energy is equal to

$$I_{n,\epsilon}(a) = \sum_{\ell=0}^{2^K-1} a_\ell(a_\ell - 1). \tag{3.4}$$

Clearly, the constrained minimiser is given by $a_\ell = 2^{n-K}$, which proves the claim. □

Lemma 3.2. *Define the set of configurations*

$$\mathcal{H}_K = \left\{h\colon\ \mathbb{T}^{(N)} \to \epsilon\,[-2^{K-1} + \tfrac{1}{2}, 2^{K-1} - \tfrac{1}{2}]\right\}. \tag{3.5}$$

Set

$$S^K(h, \mathbb{T}^{(N)}) = \sum_{n=N-K}^{N} [I_n(h) + W_n(h)]. \tag{3.6}$$

Let $\bar{h} \in \mathcal{H}_K$ be such that, for any $n \geq N - K$,

$$\bar{h}(z^{(n)}) = h^*(z^{(n)}). \tag{3.7}$$

Then

$$S^K(\bar{h}, \mathbb{T}^{(N)}) = \min_{h\in\mathcal{H}_K} S^K(h, \mathbb{T}^{(N)}). \tag{3.8}$$

Proof. By Lemma 3.1, $\bar{h}$ minimises I_n for all $0 \le n \le N-K$. Moreover, $W_n(h) = 0$ for all $n \ge N-K$ (recall (1.7)), which proves the claim. □

The next lemma controls the range of optimal configurations.

Lemma 3.3. *Suppose that h minimises $S(h, \mathbb{T}^{(N)})$ and that the range of $h(\mathbf{z}^{(N)})$ is 2^K. Then, for any $0 \le n \le N$, the range of $h(\mathbf{z}^{(n)})$ is at most 2^K.*

Proof. Assume that, for some $0 \le n < N$, there exist a z such that $h(\mathbf{z}^{(n)}) > \epsilon\,(2^{M-1} + \frac{1}{2})$. Compare the cost of *moving this particle and all its offspring* back to positions $\le \epsilon\,(2^{M-1} + \frac{1}{2})$ to the cost of just leaving one particle at $h(\mathbf{z}^{(n)})$. Clearly, the former is smaller than the latter, because it costs nothing not to move the particle, while the cost of the interaction is lowered because the particle does not get with distance ϵ of any other particle. □

The next lemma identifies the optimal configurations that also optimise the interaction cost in the last generation.

Lemma 3.4. *Let*

$$u(\mathbf{z}^{(M)}) = \epsilon\left(\sum_{\ell=1}^{M} 2^{M-\ell} z_\ell - 2^{M-1} + \tfrac{1}{2}\right). \tag{3.9}$$

Let $h^{\mathrm{Dir}}(z)$ be the solution to the Dirichlet problem in (2.2) with boundary condition u. Set

$$h^{**}(\mathbf{z}^{(n)}) = \begin{cases} h^{\mathrm{Dir}}(\mathbf{z}^{(n)}), & 0 \le n \le M, \\ u(\mathbf{z}^{(M)}), & n \ge M. \end{cases} \tag{3.10}$$

If $M = 2N/3$, then

$$S(h^{**}, \mathbb{T}^{(N)}) = \beta\left(\tfrac{1}{3}2^{4N/3+2} - 2^{N+1} + \tfrac{2}{3}2^{2N/3}\right) + S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(2N/3)}), \tag{3.11}$$

where

$$S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(2N/3)}) = \epsilon^2\, 2^{4N/3-3} + O(N 2^{2N/3}). \tag{3.12}$$

Proof. The claim is straightforward from Lemma 3.3. Use Lemma 2.6 with $M = 2N/3$. □

Lemma 3.4 essentially states that there exists a configuration h^{**} with total cost

$$S(h^{**}, \mathbb{T}^{(N)}) \sim \left(\tfrac{4}{3}\beta + 2^{-3}\epsilon^2\right) 2^{4N/3}. \tag{3.13}$$

At this stage we may be tempted to believe that the configurations h^{**} in Lemma 3.4 are optimisers. However, this is *not* the case.

Lemma 3.5. *Let h be any configuration such that at time N there exists a point ϵk for which $|a_k - a_{k+1}| \ge 2$. Then h cannot minimise $S(h, \mathbb{T}^{(N)})$.*

Proof. Assume w.l.o.g. that $a_k = a_{k+1} + m$ with $m \ge 2$. Then one of the m extra particles can be moved at cost $\le \epsilon^2$ from k to $k+1$ from time $N-1$ to time N. But then the contribution to I_N from this site changes from $(a_{k+1}+m)(a_{k+1}+m-1) + a_{k+1}(a_{k+1}-1)$ to $(a_{k+1}+m-1)(a_{k+1}+m-2) + (a_{k+1}+1)a_{k+1}$. Consequently, the interaction cost is reduced by $2(m-1)\beta \ge 2\beta$, which offsets the cost of the displacement because we assumed that $\beta > \epsilon^2/2$. Hence such a configuration cannot be a minimiser. □

Remark. Lemma (3.5) is the reason we impose the condition $\beta > \epsilon^2/2$. If β is smaller than that, one cannot exclude steps size larger than one. In fact, as β gets smaller, increasingly larger steps become admissible. This will lead to optimal configurations where the boundary staircases become increasingly steep.

3.2. **Admissible configurations.** We have seen that without the restriction on the increments to be at most 1, the optimal configurations are constants. The next lemma identifies the optimal configurations under this restrictions.

Lemma 3.6. *Consider the functional $I_{n,\epsilon}(a)$ from (3.4). Then the minimiser of $I_{n,\epsilon}(a)$ with range $\{1,\dots,L\}$ for $L \in \mathbb{N}_0$, under the constraint $\sum_{\ell=0}^{L} a_\ell = 2^n$ and with the restriction $|a_{\ell+1} - a_\ell| \le 1$, $1 \le \ell < L$, is given by*

$$a_\ell = \min\left(\tfrac{1}{2}(\lambda^* + 1), \min(\ell, L + 1 - \ell)\right), \tag{3.14}$$

where

$$\lambda^* = L - \sqrt{(L+1)^2 - 2^{n+2}}. \tag{3.15}$$

Proof. The constrained optimisation problem without the restriction on the increments amounts to finding the critical point of the functional

$$F(a,\lambda) = I_{n,\epsilon}(a) - \lambda\left(\sum_{\ell=1}^{L} a_\ell - 2^n\right). \tag{3.16}$$

The gradient of F has the components

$$\begin{aligned} \frac{\partial}{\partial a_\ell} F(a,\lambda) &= 2a_\ell - 1 - \lambda, \quad 1 \le \ell \le L, \\ \frac{\partial}{\partial \lambda} F(a,\lambda) &= \sum_{\ell=1}^{L} a_\ell - 2^n. \end{aligned} \tag{3.17}$$

We claim that in order to take the restriction on the increments into account, it is enough to impose the weaker constraints

$$0 \le a_\ell \le \min(\ell, L + 1 - \ell). \tag{3.18}$$

We search for a and λ such that the gradient vanishes except on the boundary of the admissible region. For given λ this means that a is given by

$$a = a_\ell^\lambda = \min\left(\tfrac{1}{2}(\lambda + 1), \min(\ell, L + 1 - \ell)\right), \tag{3.19}$$

and λ by

$$2\sum_{\ell=1}^{(\lambda+1)/2} \ell + \tfrac{1}{2}(L - \lambda - 1)(1 + \lambda) - 2^n = 0. \tag{3.20}$$

The latter has the unique solution

$$\lambda^* = L - \sqrt{(L+1)^2 - 2^{n+2}}, \tag{3.21}$$

and $a = a^{\lambda^*}$. □

As a consequence, the configuration that minimises I_N with range $\mathcal{R}_N = L$ is in $\mathcal{H}_{r_N,d_N,N}$ with

$$r_N = \tfrac{1}{2}(\lambda^* + 1), \tag{3.22}$$

and $d_N = L - 2r_N$.

Lemma 3.7. *The configuration at time $n-1$ that optimises $I_{n-1,\epsilon}$ with a range that allows to obtain the configuration in $\mathcal{H}_{r_n,d_n,n}$ for some given r_n at time n is the configuration in $\mathcal{H}_{r_n/2,d_n+r_n,n-1}$ with minimal spreading cost.*

Proof. Consider a configuration in $\mathcal{H}_{r_n/2,d_n+r_n,n-1}$. At time n, each of the particles splits into two and without moving (i.e., without any spreading cost), we obtain a configuration where the occupation number at each site is doubled. This configuration is not smooth. Now, we can apply the procedure described in Lemma 3.5 to move particles in steps each of which lowers the interaction energy by more than the spreading cost involved in this move. This involves moving particles only in the staircase and a strip of width $\frac{1}{4}r_n$ from each side of the central part.

The total number of particles in the staircase on the r_n sites is given by $\frac{1}{2}r_n(r_n+1)$. As $r_{n-1} = \frac{1}{2}r_n$, a staircase of width r_{n-1} contains $\frac{1}{4}r_n(\frac{1}{2}r_n+1)$ particles, which produce $\frac{1}{2}r_n(\frac{1}{2}r_n+1)$ offsprings in the next generation. The remaining $\frac{1}{2}r_n^2$ particles come from the central part. In total, these are

$$\tfrac{1}{2}r_n(\tfrac{1}{2}r_n+1) + \tfrac{1}{4}r_n^2 = \tfrac{1}{2}r_n(r_n+1) \tag{3.23}$$

particles for each of the two staircases of width r_n. The resulting configuration is in $\mathcal{H}_{r_n,d_n,n}$, in particular it is the optimal configuration for $I_{n,\epsilon}$ with range $2r_n + d_n$. Thus, moving any more particles would increase the spreading cost and could not reduce the interaction cost without increasing the range. Note that

$$d_{n-1} = d_n + \tfrac{1}{2}r_n, \tag{3.24}$$

and hence

$$L_{n-1} = d_{n-1} + 2r_{n-1} = d_n + \tfrac{3}{2}r_n = L_n - \tfrac{1}{2}r_n. \tag{3.25}$$

□

Lemma 3.8. *Let h be a minimiser of $S(h, \mathbb{T}^{(N)})$ such that its range is L_N. Then for $M \le n \le N$, with M such that $2^{-(N-M)}r_N = 1$, $h(\mathbb{T}^{(n)})$ is as described above, i.e., it is the minimising admissible configuration with range*

$$L_n = L_N - 2r_N + (1 - 2^{-(N-n)})\tfrac{1}{2}r_N + 2^{-(N-n)+1}r_N. \tag{3.26}$$

Proof. The structure of the proof is as follows.

- Let h be a minimiser of $S(h, \mathbb{T}^{(N)})$. Assume that the range of h at time N is L_N. We will show that then the range of h at times $n < N$ is not larger than some L_n. This L_n will be determined by the fact that if the range at time n were larger than L_n, then we could construct a configuration with a smaller total cost and a range at time N larger than L_N, in contradiction with the assumption that the optimal configuration has range L_N. This procedure ends at time M when $L_M = \epsilon 2^M$ and the interaction cost is zero for the configuration with a single particle at each site.
- At times before time M, the best configuration is given by the solution of the Dirichlet problem discussed in Section 2. Given these constraints on the ranges, the configuration that minimises the total interaction cost is realised if, for any $M \le n \le N$, $h(\mathbf{z}^{(n)})$ is such that it minimises $I_{n,\epsilon}$ over all admissible configurations with range at most L_n, which implies that the range is equal to L_n.
- Finally, we show that from such a configuration at time n after doubling all particles, we can arrive at the configuration at time $n+1$ by moving particles in such a way that total cost is reduced in each step.

We will first establish the existence of a sequence L_n and a configuration h as described above. If h minimises I_n with range L_n, then we know that $L_n = d_n + 2r_n$ and $h(\mathbf{z}^{(n)}) \in \mathcal{H}_{r_n,d_n,n}$. It follows from Lemma 3.7 that $r_n = r_N 2^{-N+n}$. It is also clear that r_N is a power of 2, say $r_N = 2^K$, and then $M = N - K$. Following the procedure in Lemma 3.7, we obtain h such that, for each $M \le n \le N$, $h(\mathbf{z}^{(n)}) \in \mathcal{H}_{r_n,d_n,n}$. Since there is no way to further reduce

the interaction energies without increasing the final range L_N, and any further move would increase the spreading costs, this h optimises the total cost from time M to time N. Finally, for times up to M, choosing for h the solution of the Dirichlet problem also minimises the cost during this time. As a consequence, we have obtained the minimiser under the assumption that its range is L_N. □

3.3. **Cost of the optimal configurations.** In Lemma 3.8, we have identified the candidate minimisers h assuming that the range of h at time N is $2r_N + d_N = L_N$. We denote these configurations by h^*_r, is $r_N = r$. We still have to determine the value of r_N. To do so, we must compute very precisely the total cost of such a configuration.

Lemma 3.9. *The interaction cost of a configuration h^*_r is given by*

$$J_{N,\epsilon}(h^*_r, \mathbb{T}^{(N)}) = \tfrac{1}{3}2^{N+2} + 2r - 2^{N+1} + O(r^2). \tag{3.27}$$

Proof. The interaction energy at generation n of a configuration in $\mathcal{H}_{r,d,n}$ is

$$2\sum_{j=1}^{r}(j^2 - j) + dr(r-1) = \tfrac{1}{3}r(r+1)(2r+1) - r(r+1) + dr(r-1). \tag{3.28}$$

Hence, by (1.11) and (3.24),

$$\begin{aligned} I_{N-k,\epsilon}(h^*_r) &= \tfrac{1}{3}r_k(r_k+1)(2r_k+1) - r_k(r_k+1) + d_k r_k(r_k-1) \\ &= \tfrac{2}{3}r_k^3 - \tfrac{2}{3}r_k + d_k r_k(r_k-1) \\ &= \tfrac{2}{3}r^3 2^{-3k} - \tfrac{2}{3}r2^{-k} + (d + r(1-2^{-k})(r^2 2^{-2k} - r2^{-k}). \end{aligned} \tag{3.29}$$

Summing this over k from 0 to $N - M$, we get the total interaction energy

$$\begin{aligned} &J_{N,\epsilon}(h^*_r, \mathbb{T}^{(N)}) = \sum_{k=0}^{N-M} I_{N-k} \\ &= \tfrac{2}{3}r^3\tfrac{1}{7}(8 - 8^{-(N-M)}) - \tfrac{2}{3}r(2 - 2^{-(N-M)}) + (d+r)\left(r^2\tfrac{1}{3}(4 - 4^{-(N-M)}) - r(2 - 2^{-(N-M)})\right) \\ &\quad -r^3\tfrac{1}{7}(8 - 8^{-(N-M)}) + r^2\tfrac{1}{3}(4 - 4^{-(N-M)}). \end{aligned} \tag{3.30}$$

Since $2^{-(N-M)} = 1/r$, we can neglect all terms with powers $-(N-M)$. Using that $d = (2^N/r) - r - 1$, we get

$$J_{N,\epsilon}(h^*_r, \mathbb{T}^{(N)}) = \tfrac{4}{3}\,2^N r - \tfrac{8}{21}\,r^3 - 2^{N+1} + O(r^2). \tag{3.31}$$

□

To compute the total cost of a configuration h^*_r, it remains to compute the spreading cost. This consists of two parts. First, there is the spreading cost from the Dirichlet problem up to time M, which is estimated in Lemma 2.6. The second part is the spreading cost from time M to time N. We do not have a precise formula for this, but we know that it is smaller than the difference between the interaction cost of h^*_r and the configuration obtained from not moving particles any more after time M.

Lemma 3.10. *With the notation above,*

$$0 \le S_{\mathrm{spr}}(h^*_r, \mathbb{T}^{(N)}) - S_{\mathrm{spr}}(h^{\mathrm{Dir}}, \mathbb{T}^{(M)}) \le O(r^3). \tag{3.32}$$

Proof. The cost of a configuration where particles only reproduce and do not move from time M to time N is

$$2^M \sum_{k=1}^{N-M} 2^k(2^k - 1) = \tfrac{1}{3}2^{2N-M+2} - 2^{N+1} + \tfrac{2}{3} = \tfrac{1}{3}2^{N+2}r - 2^{N+1} + \tfrac{2}{3}, \tag{3.33}$$

where $r = 2^{N-M}$. This yields the assertion of the lemma. □

Collecting these result, we get the following lemma.

Lemma 3.11.

$$S_N(h_r^*, \mathbb{T}^{(N)}) = \beta\left(\tfrac{4}{3}2^N r - 2^{N+1}\right) + \epsilon^2 2^{2N-3} r^{-2} + O(r^3). \tag{3.34}$$

Lemma 3.11 allows us to obtain sharper bounds on r as stated in Theorem 1.1.

Lemma 3.12. *Let h be any minimiser of $S(h, \mathbb{T}^{(N)})$. Then $h \in \mathcal{H}_{r,d,N}$ with*

$$|r - r^*| \le O(2^{N/6}), \tag{3.35}$$

where

$$r^* = \arg\min_r \left(\beta\left(\tfrac{1}{3}2^{N+2} r - 2^{N+1}\right) + \epsilon^2 2^{2N-3} r^{-2}\right). \tag{3.36}$$

Moreover,

$$r^* = (3\epsilon^2/\beta)^{1/3} 2^{(N-4)/3} \tag{3.37}$$

and

$$S(h_{r^*}^*, \mathbb{T}^{(N)}) = 2(\beta\epsilon/3)^{2/3} 2^{4N/3+2/3} + O(2^N). \tag{3.38}$$

Proof. The computing of r^* is straightforward, while (3.35) follows from an elementary perturbation argument. Note that, for the minimising h, the interaction cost and the spreading cost are the same. □

4. Proof of the main theorems

We are now ready to prove the main theorems.

Proof of Theorem 1.1. Lemma 3.1 shows that any optimising configuration at time N has particles only on $\epsilon\mathbb{Z}$. Lemmas 3.5–3.6 shows that such configurations must be admissible and belong to some $\mathcal{H}_{r,d,N}$. Lemma 3.12 provides a control on the value of r. Taking the logarithm, we get

$$\ln_2(r) = \ln_2\left(3\epsilon^2/\beta)^{1/3} 2^{(N-4)/3} + O(2^{N/6})\right) = \tfrac{1}{3}(N-4) + \tfrac{1}{3}\ln_2(3\epsilon^2/\beta) + \ln_2\left(1 + O(2^{-N/6})\right), \tag{4.1}$$

which implies Theorem 1.1 as $\ln_2\left(1 + O(2^{-N/6})\right) = O(2^{-N/6})$. □

Proof of Theorem 1.2. Theorem 1.2 is a direct consequence of Lemmas 3.7 and 3.12. □

Proof of Theorem 1.3. Theorem 1.3 is a direct consequernce of Lemmas 3.7 and 2.3. □

Proof of Theorem 1.4. Theorem 1.4 is a direct consequence of Lemma 3.12. □

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