Hydrodynamic limit for the Kob-Andersen model

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ABSTRACT. This paper concerns with the hydrodynamic limit of the Kob-Andersen model, an interacting particle system that has been introduced by physicists in order to explain glassy behavior, and widely studied since. We will see that the density profile evolves in the hydrodynamic limit according to a non-degenerate hydrodynamic equation, and understand how the diffusion coefficient decays as density grows.

1. Introduction

The Kob-Andersen (KA) model is an interacting particle system on \mathbb{Z}^d , where each site of the lattice is allowed to contain at most one particle, and particles could jump to an empty neighboring site only under a certain constraint. More precisely, depending on a parameter k, every particle jumps with rate 1 to each of its neighboring sites, provided that the particle has at least k empty neighbors both before and after the jump (so for k = 1 we obtain the symmetric simple exclusion process). This model has been introduced in the physics literature ([16]) as one member of a large family of interacting particle systems called *kinetically constrained lattice gases* (KCLGs), which model certain aspects of glassy behavior (see [12, 20]).

In this paper we will study the hydrodynamic limit of the KA model. Consider a finite box with periodic boundary conditions $\mathbb{T}_N^d = \mathbb{Z}^d/N\mathbb{Z}^d$, and run the KA dynamics inside \mathbb{T}_N^d . The configuration at time s could be described as an empirical measure $\nu_s^{(N)}$ on the continuous torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$: for a rectangle $R \subset [0,1]^d$, seen as a subset of \mathbb{T}^d , $\nu_s^{(N)}(R)$ will count the number of particles in $(NR) \cap \mathbb{T}_N^d$, normalized by N^{-d} (so that the total mass remains independent of N). The initial configuration that we choose will be approximated by some macroscopic profile $\rho_0: \mathbb{T}^d \to [0,1]$, i.e., the measure $\nu_0^{(N)}$ will be close to a measure ν_0 that has density ρ_0 with respect to the Lebesgue measure. A simple example of such initial configuration is given by placing a particle at each site $x \in \mathbb{Z}^d$ independently at random with probability $\rho_0(x/N)$.

In many systems, the relevant time scale over which ν_N^s changes macroscopically is the diffusive time scale N^2 (see, e.g., [15, 23]). That is, fixing a time t, we expect the random measure $\nu_{N^2t}^{(N)}$ to satisfy a law of large numbers, converging to some limiting measure ν_t . We also expect this limiting measure to have a density with respect to the Lebesgue measure, namely $\nu_t = \rho(\theta,t) \mathrm{d}\theta$, which solves the diffusion equation:

$$\frac{\partial}{\partial t}\rho = \nabla D(\rho)\nabla\rho, \quad \rho(\theta, 0) = \rho_0(\theta). \tag{1.1}$$

The parameter $D(\rho)$ is the diffusion coefficient, and when it is non-zero we obtain indeed a macroscopic density profile that changes over diffusive time scales.

Hydrodynamic limits of other KCLGs have been analyzed in [13, 4]. They present two example of *non-cooperative* KCLGs, in which one is able to identify structures (called *mobile clusters*) that could move freely in \mathbb{Z}^d . This way, even though particles could be blocked, mobile clusters behave effectively in an unconstrained manner. In *cooperative* KCLGs there are no such mobile clusters, so in order to move a particle from one site to the other one needs the cooperation of a diverging number of particles. This property has a major contribution to the glassy behavior of many KCLGs, and is responsible for the fast divergence of time scales. See [25].

Unlike the models previously studied in [13, 4], the KA model is cooperative. Due to this cooperative nature, the combinatorics behind the KA model becomes much more complicated. Consider the following question – starting from a stationary measure and assuming that there is a particle at the origin, will this particle eventually move, or could it stay at the origin forever? When the model is non-cooperative the probability to stay forever at the origin is clearly 0 – we know that there is some non-zero density of mobile clusters in \mathbb{Z}^d which diffuse freely, so at some point one of them will reach the origin and move the particle. When the model is cooperative, as in the case of the KA model, already this basic question becomes much more complicated. In some cooperative models the particle might remain blocked forever with positive probability, possibly depending on the density of the initial configuration. In the case of the KA model, it is shown in [25] that all particles will eventually move with probability 1, unless the initial density equals 1.

In the context of the hydrodynamic limit, the techniques used in [13, 4] cannot be simply adapted to cooperative models. It is shown in Appendix A that cooperative KCLGs are nongradient, a fact which makes the analysis of the hydrodynamic limit much more involved. Another property of non-cooperative models used in [4] is that the probability for a site to stay blocked forever for the dynamics in \mathbb{T}_N^d decreases exponentially fast with the volume N^d , since it is bounded by the probability that no mobile cluster is found in \mathbb{T}_N^d . In the KA model, on the other hand, even though this probability decays to 0, the decay is not fast enough.

Recently, a few methods have been developed to overcome some of these difficulties, proving diffusive scaling of the relaxation time [17] and of the motion of a tagged particle [5, 9] in the stationary setting. In both cases, the behavior is the same as that of the simple exclusion process, with time scales that are all slowed down by a factor which diverges quickly as the density approaches 1. For example, in the case k=d=2, the relaxation time at density ρ in a box of side N behaves (roughly) like $e^{C/(1-\rho)}N^2$; and the path of a tagged particle in \mathbb{Z}^2 converges to a standard Brownian motion as the length scale N diverges, when time is scaled (roughly) as $e^{C/(1-\rho)}N^2$.

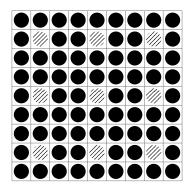


FIGURE 1.1. This is an example of a blocked configuration for the case k=d=2. The filled circles represent occupied sites, while sites marked with a line pattern could be either empty or occupied. In this example particles have at most one empty neighbor, so none of them could move.

The hydrodynamic limit of the KA model has been studied in the physics literature, both heuristically and numerically. In [21] the model has been analyzed, under the (wrong) assumption that the diffusion coefficient $D(\rho)$ vanishes for $\rho > \rho_c \approx 0.88$. [24] studies the diffusion coefficient in two dimensions both numerically and under a mean-field approximation. This approximation yields a diffusion coefficient that behaves polynomially in ρ , and is in rather good agreement with numerical results for low densities. [1] provide a perturbative analysis of the diffusion coefficient in two dimensions, considering finite range effects, and obtaining a polynomial in ρ which approximates $D(\rho)$ very accurately as long as ρ is not too big. In view of other quantities related to the KA model studied in [17, 9], a natural conjecture for the high density regime is that the diffusion coefficient remains positive whenever $\rho < 1$, and as ρ tends to 1 it decays (roughly) as $e^{-C/(1-\rho)}$ (in the case k=d=2). This conjecture has been raised in [1] and was supported by numerical simulations.

The hydrodynamic limit in its full generality, though, cannot exist for this model – consider, for example, the case k=d=2, and an initial density ρ_0 bounded above $\frac{8}{9}$. Fix $N\in 3\mathbb{N}$, and construct the following initial configuration – for every $x\in \mathbb{T}^2_N$, if $x\notin 3\mathbb{Z}^2$ place a particle at x (deterministically). Otherwise, place a particle at x independently at random with probability $9\rho_0(x/N)-8$. See Figure 1.1. These configurations have limiting density $\frac{1}{9}(9\rho_0(x/N)-8)+\frac{8}{9}=\rho_0$, so one may naively expect that, starting the KA dynamics from such a configuration, the particle density will converge to the solution of the hydrodynamic equation (1.1) with initial density ρ_0 . However, observing the initial configuration more carefully, one sees that it is blocked – no site has two empty neighbors, so the constraint is not satisfied. In this case particles do not move, and the dynamics will certainly not follow the hydrodynamic limit. Still, since blocked configurations are very rare ([25]), we may hope that a hydrodynamic limit does exist in a weaker sense, that would allow us to avoid these untypical configurations.

The same problem also appears in [13], and they suggest two solutions – the first is to restrict the initial configuration, e.g., to an independent product of Bernoulli random variables

with parameter $\rho_0(x/N)$. This prevents the issue discussed above, where the configuration is entirely blocked from the beginning, but one must work harder in order to show that blocked configurations are not created later on during the dynamics. Another approach, also considered in [13], is to permit transitions in which the constraint is not satisfied, but with a vanishing rate. Namely, for some $\varepsilon > 0$, we introduce soft constraints, which allow a particle to move with rate 1 when it has k empty neighbors before and after the jump, and with rate ε otherwise. This softening of the constraint enables the system to unblock the blocked configurations, and still the main contribution to the overall dynamics comes from the allowed transitions (where the constraint is satisfies).

This is the approach we will take – consider the KA model with ε -soft constraints, which has a hydrodynamic limit with diffusion coefficient $D^{(\varepsilon)}$. We analyze this coefficient, showing that, as $\varepsilon \to 0$, it converges to a strictly positive limiting coefficient D. This result tells us that when ε is very small, it has a very mild effect on the hydrodynamic limit; and the role it plays (of unblocking configurations), though crucial for the convergence to the hydrodynamic limit, takes a negligible amount of time compared to the hydrodynamic scale. We also analyze the value of D at large densities, finding upper and lower bounds for its decay, which match up to sub-leading corrections. The decay that we obtain is of the same type as the corresponding factor in [17, 9]; so in particular for the case k=d=2, as conjectured is [1], D decays (roughly) as $e^{-C/(1-\rho)}$.

2. Model and main result

The Kob-Andersen model in dimension d is a Markov process on $\Omega = \{0,1\}^{\mathbb{Z}^d}$, depending on a parameter $2 \leq k \leq d$. For a configuration $\eta \in \Omega$, we say that $x \in \mathbb{Z}^d$ is occupied if $\eta(x) = 1$ and empty if $\eta(x) = 0$. The elements of \mathbb{Z}^d are called *sites*, and we will consider the (undirected) graph structure given by the edge set

$$\mathcal{E}(\mathbb{Z}^d) = \left\{ (x, y) \in \mathbb{Z}^d \times \mathbb{Z}^d, y \in x + \{\pm e_1, \dots, \pm e_d\} \right\},\,$$

where e_1, \ldots, e_d are the standard basis vectors. We will sometimes write $x \sim y$ to denote $(x,y) \in \mathcal{E}(\mathbb{Z}^d)$.

For each configuration $\eta \in \Omega$ and edge $(x,y) \in \mathcal{E}(\mathbb{Z}^d)$, we define the constraint

$$c_{x,y}(\eta) = \begin{cases} 1 & \text{if } \sum_{z:y\sim z\neq x} (1-\eta(z)) \ge k-1 \text{ and } \sum_{z:x\sim z\neq y} (1-\eta(z)) \ge k-1, \\ 0 & \text{otherwise.} \end{cases}$$
 (2.1)

The KA dynamics is then defined as the Markov process whose generator, operating on a local function $f: \Omega \to \mathbb{R}$, is given by

$$\mathcal{L}f(\eta) = \sum_{(x,y)\in\mathcal{E}(\mathbb{Z}^d)} c_{x,y}(\eta) \nabla_{x,y} f(\eta), \tag{2.2}$$

where

$$\nabla_{x,y} f(\eta) = f(\eta^{x,y}) - f(\eta),$$

and $\eta^{x,y}$ is the configuration obtained from η by exchanging the occupation at x and at y. This process, for any $\rho \in (0,1)$, is reversible with respect to the measure μ_{ρ} , which is a product measure of Bernoulli random variables with parameter ρ . When clear from the context we will sometimes omit the subscript ρ .

As discussed in the introduction, in order to study the hydrodynamic limit we introduce the *soft constraint* for some $\varepsilon \geq 0$:

$$c_{x,y}^{(\varepsilon)} = \begin{cases} 1 & \text{if } c_{x,y} = 1, \\ \varepsilon & \text{otherwise,} \end{cases}$$
 (2.3)

and the *soft dynamics* defined by the generator

$$\mathcal{L}^{(\varepsilon)}f(\eta) = \sum_{(x,y)\in\mathcal{E}(\mathbb{Z}^d)} c_{x,y}^{(\varepsilon)}(\eta) \nabla_{x,y} f(\eta). \tag{2.4}$$

The introduction of the soft constraints allows us to use the general result of [26]. Fix $\varepsilon \geq 0$, and let

$$D^{(\varepsilon)}(\rho) = \frac{1}{2\rho(1-\rho)} \inf_{f} \mu_{\rho} \left[\sum_{\alpha} c_{0,e_{\alpha}}^{(\varepsilon)} \left(\delta_{\alpha,1} \left(\eta(e_{1}) - \eta(0) \right) - \sum_{x \in \mathbb{Z}^{d}} \nabla_{0,e_{\alpha}} \tau_{x} f \right)^{2} \right], \tag{2.5}$$

where the infimum is taken over all local functions $f:\Omega\to\mathbb{R}$. The operator τ_x is the translation by x, that is,

$$(\tau_x f)(\eta) = f(\tau_x \eta),$$

$$(\tau_x \eta)(y) = \eta(x+y).$$

In this setting, by [11, 3, 26], the density profile of the soft dynamics converges in the hydrodynamic limit to the solution of the hydrodynamic equation (1.1), with diffusion coefficient $D^{(\varepsilon)}(\rho)$.

By equation (2.5) the diffusion coefficient is decreasing with ε , and hence converging to a limit:

$$D(\rho) = \lim_{\varepsilon \to 0} D^{(\varepsilon)}(\rho). \tag{2.6}$$

When taking ε to 0 slowly enough as N grows to infinity, the density profile converges to the solution of the diffusion equation (1.1) with this diffusion coefficient:

Proposition 2.1. Fix a smooth initial density profile $\rho_0 : \mathbb{T}^d \to (0,1)$, and let ν_0 be the measure whose density with respect to the Lebesgue measure is ρ_0 . Consider a sequence of initial conditions $(\eta_0^{(N)})_{N\in\mathbb{N}}$, with $\eta_0^{(N)} \in \{0,1\}^{\mathbb{T}^d_N}$, such that the associated empirical measures $\nu_0^{(N)}$ converge to ν_0 . Let $\rho_t(\theta)$ be the solution of the diffusion equation (1.1), with diffusion coefficient D given by equation (2.6), and ν_t the measure with density ρ_t . For $s \geq 0$, denote by $\nu_s^{(\varepsilon,N)}$ the (random)

empirical measure associated with the Kob-Andersen model on \mathbb{T}_N^d with ε -soft constraints at (microscopic) time s.

Then there exists a sequence ε_N for which $\nu_{N^2s}^{(\varepsilon_N,N)}$ converges in probability to ν_t as $N\to\infty$.

Remark 2.2. In general, the diffusion coefficient is a matrix given by (see [23, Propositions 2.1 and 2.2])

$$D_{\alpha\beta} = \lim_{t \to \infty} \frac{1}{t} \frac{1}{2\rho(1-\rho)} \sum_{x \in \mathbb{Z}^d} x_{\alpha} x_{\beta} \left(\mu_{\rho}(\eta(0) e^{t\mathcal{L}} \eta(x)) - \rho^2 \right).$$

The reason that $D^{(\varepsilon)}(\rho)$ in equation (2.5) is a real number, is that in our case D is a scalar matrix: the dynamics is invariant under inversion of a single coordinate (i.e., $x \mapsto x - (2x \cdot e_{\alpha}) e_{\alpha}$), and therefore, if $\alpha \neq \beta$, the sum $\sum_{x \in \mathbb{Z}^d} x_{\alpha} x_{\beta} (\mu(\eta(0) e^{t\mathcal{L}} \eta(x)) - \rho^2)$ must vanish. That is, D is a diagonal matrix. Since the dynamics is also invariant under permutation of coordinates, all diagonal elements are equal, i.e., D is scalar. This fact is useful for the analysis of the limiting PDE in the proof of Proposition 2.1.

The main result of this paper is that D is strictly positive, so that the hydrodynamic limit is not degenerate, i.e., the density profile evolves over diffusive time scales.

Theorem 2.3. For all $\rho \in (0,1)$,

$$D(\rho) \ge \begin{cases} C/\exp\left(\lambda\log(1/(1-\rho))^2 (1-\rho)^{-1/(d-1)}\right) & k = 2, \\ C/\exp^{k-1}\left(\lambda(1-\rho)^{-1/(d-k+1)}\right) & k \ge 3, \end{cases}$$
$$D(\rho) \le C'/\exp^{k-1}(\lambda'(1-\rho)^{-1/(d-k+1)}),$$

where $\exp^k(\cdot)$ is the k-th iterate of the exponential. The constants C, C', λ, λ' are all strictly positive, and may depend only on d and k.

3. Proof of Proposition 2.1

The proof is based on the results of [11, 3, 26], together with the continuity of the solution $\rho_t(\theta)$ with respect to the diffusion coefficient.

Denote by $\rho_t^{(\varepsilon)}$ the solution of the diffusion equation (1.1) with diffusion coefficient $D^{(\varepsilon)}$ given by equation (2.5). The existence and uniqueness of ρ_t and ρ_t^{ε} , as well the maximum principle, comes from standard theory of parabolic equations (see, e.g., [27]) ¹.

The main tool we use is:

Theorem 3.1 ([11, 3, 26]). For any smooth test function f on \mathbb{T}^d ,

$$\int f(\theta) \, \mathrm{d} \, \nu_{N^2 t}^{(\varepsilon, N)}(\theta) \xrightarrow{N \to \infty} \int f(\theta) \rho_t^{\varepsilon}(\theta) \, \mathrm{d} \, \theta$$

in probability.

¹Most works treat the equation on \mathbb{R}^d rather than the torus. Nonetheless, the results we need hold also for the equation on \mathbb{T}^d , see the discussion in Section 11.5 of [27].

In addition, we need to know that, for small ε , the profile $\rho_t^{(\varepsilon)}$ is close to ρ_t . This problem is analyzed in [2] in a much more complicated setting, where $D(\rho)$ may approach 0 in some points of space. Since we only consider the case where ρ is bounded away from 1, the assumptions of [2] are easily verified, yielding:

Claim 3.2. For all t > 0

$$\rho_t^{(\varepsilon)} \xrightarrow{\varepsilon \to 0} \rho_t$$

in $L^1(\mathbb{T}^d)$.

In order to prove Proposition 2.1, we will fix a dense countable family $\{f_m\}_{m\in\mathbb{N}}$ of bounded functions on \mathbb{T}^d . Then, as discussed in [15, Chapter 4.1], it suffices to show that

$$P\left[\left| \int f_m(\theta) \, \mathrm{d} \, \nu_{N^2 t}^{(\varepsilon_N, N)}(\theta) - \int f_m(\theta) \rho_t(\theta) \, \mathrm{d} \, \theta \right| > \delta \right] \xrightarrow{N \to \infty} 0 \tag{3.1}$$

for any fixed $\delta > 0$ and all $m \in \mathbb{N}$, for an appropriately chosen sequence $\{\varepsilon_N\}$.

An immediate corollary of Theorem 3.1 and Claim 3.2 is:

Corollary 3.3. Fix M > 0. Then there exists $\varepsilon(M)$, N(M) such that, for all $m \leq M$ and $N \geq N(M)$,

$$P\left[\left|\int f_m(\theta) \, \mathrm{d} \, \nu_{N^2 t}^{(\varepsilon(M),N)}(\theta) - \int f_m(\theta) \rho_t(\theta) \, \mathrm{d} \, \theta\right| > \delta\right] \le \frac{1}{M}.$$

Moreover, we may assume $\varepsilon(M) \to 0$ and $N(M) \to \infty$ as $M \to \infty$.

Proof. By Claim 3.2, for all m there exists $\varepsilon^*(m)$ such that

$$\left| \int f_m(\theta) \rho_t^{(\varepsilon)}(\theta) \, \mathrm{d}\, \theta - \int f_m(\theta) \rho_t(\theta) \, \mathrm{d}\, \theta \right| < \delta/2$$

for all $\varepsilon < \varepsilon^*(m)$. We will choose $\varepsilon(M) = \min_{m < M} \varepsilon^*(m) \wedge \frac{1}{M}$.

By Theorem 3.1, for any m and any ε there exists $N(m,\varepsilon)$, such that if $N\geq N(m,\varepsilon)$ then

$$P\left[\left|\int f_m(\theta) \,\mathrm{d}\, \nu_{N^2 t}^{(\varepsilon,N)}(\theta) - \int f_m(\theta) \rho_t^{(\varepsilon)}(\theta) \,\mathrm{d}\, \theta\right| > \delta/2\right] \le \frac{1}{M}.$$

Define $N(M) = \max_{m \leq M} N(m, \varepsilon(M)) \vee M$. This concludes the proof of the corollary. \square

We are now ready to choose our sequence ε_N :

$$M_N = \max\{M : N \ge N(M)\},\$$

 $\varepsilon_N = \varepsilon(M_N).$

Then, indeed,

$$P\left[\left|\int f_m(\theta) \, \mathrm{d} \, \nu_{N^2 t}^{\varepsilon_N, N}(\theta) - \int f_m(\theta) \rho(\theta) \, \mathrm{d} \, \theta\right| > \delta\right] \le \frac{1}{M_N}$$

for all $m \leq M_N$. This concludes the proof of the proposition.

4. Proof of the lower bound

The purpose of this section is to prove

$$D^{(0)} \ge L^{-\lambda},\tag{4.1}$$

$$L = \begin{cases} C \exp\left(\lambda \log(1/q)^2 q^{-1/(d-1)}\right) & k = 2, \\ C \exp^{k-1}\left(\lambda q^{-1/(d-k+1)}\right) & k \ge 3, \end{cases}$$
 (4.2)

where for convenience we denote $1 - \rho = q$. Throughout the section λ and C denote generic positive constants, depending only on k and d, that may be updated from one line to the other. This will prove the first inequality of Theorem 2.3 since $D \ge D^{(0)}$.

The proof is based on a comparison to the diffusion coefficient of a random walk on the infinite component of a percolation cluster. The idea behind the proof, is that even though at small scale particles are blocked, at a large scale there is high probability that somewhere a droplet containing many empty sites could approach the particle allowing it to move; and this is the scale which determines the diffusion coefficient. This mechanism is constructed in [17, 9] using the notion of a *multistep move* – a sequence of exchanges, all allowed for the KA dynamics, moving a particle with the aid of a nearby droplet.

We start by providing the exact definition of a multistep move (see also [17]):

Definition 4.1 (multistep move). Fix $\mathcal{M} \subseteq \Omega$ and $T \in \mathbb{N}$. A T-step move M with domain \mathcal{M} is a function from \mathcal{M} to $\left(\Omega \times \mathbb{Z}^d \times \{\pm e_1, \dots, \pm e_d, 0\}\right)^{T+1}$, described by a sequence of functions $M = \{\eta_t(\eta), x_t(\eta), e_t(\eta)\}_{t=0}^T$, such that, for all $\eta \in \mathcal{M}$,

- (1) $\eta_0(\eta) = \eta$,
- (2) for all $t \in \{1, \dots, T\}$, $\eta_t(\eta) = \eta_{t-1}(\eta)^{x_t, x_t + e_t}$,
- (3) for all $t \in \{1, ..., T\}$, $c_{x_t, x_t + e_t}(\eta_t(\eta)) = 1$, where by convention we set $c_{x,x}(\eta) = 1$ for all x, η .

Definition 4.2. Fix a T-step move M with domain \mathcal{M} . Then, for $t \in \{1, ..., T\}$, the loss of information at time t, denoted $\text{Loss}_t(M)$, is defined as

$$2^{\operatorname{Loss}_t(M)} = \sup_{\eta' \in \mathcal{M}} \# \{ \eta \in \mathcal{M} : \eta_t(\eta) = \eta_t(\eta'), x_t(\eta) = x_t(\eta'), e_t(\eta) = e_t(\eta') \}.$$

We also set $Loss(M) = \sup_t Loss_t(M)$.

The multistep move that we will define will allow us to move a particle at x to the site $x + Le_{\alpha}$ ($\alpha \in \{1, ..., d\}$). The choice of L in equation (4.2) guarantees that such a multistep move could indeed be applied.

We will therefore consider the coarse grained lattice $\mathbb{Z}_L^d = L\mathbb{Z}^d$, and split the configuration η in two – the occupation of the sites of \mathbb{Z}_L^d denoted $\overline{\eta} \in \overline{\Omega} = \{0,1\}^{\mathbb{Z}_L^d}$, and that of the sites outside \mathbb{Z}_L^d denoted $\omega \in \{0,1\}^{\mathbb{Z}^d \setminus \mathbb{Z}_L^d}$. We will also split the measure in two, such that $\overline{\eta}$ distributes according to $\overline{\mu}$ and ω according to ν . The coarse grained lattice has a graph structure

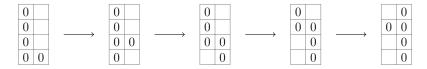


FIGURE 4.1. Droplet propagation. Sites marked with 0 are empty, the other sites could be either empty or occupied. We see that in a sequence of *unconstrained* transitions the empty column moves to the right.

(isomorphic to \mathbb{Z}^d), i.e., two vertices i, j are connected by an edge if $i - j \in \{\pm \overline{e}_1, \dots, \pm \overline{e}_d\}$, where $\overline{e}_{\alpha} = Le_{\alpha}$. We denote the edge set by $\mathcal{E}(\mathbb{Z}^d_L)$.

The multistep move that will allow particles to move on \mathbb{Z}_L^d will require sufficiently many empty sites in the configuration ω , a requirement manifested in a certain percolation process on $\mathcal{E}(\mathbb{Z}_L^d)$.

The combinatorial input that we will use in this section is contained in the following lemma:

Lemma 4.3. There exists a percolation process $\overline{c}(\omega) \in \Pi = \{0,1\}^{\mathcal{E}(\mathbb{Z}_L^d)}$ and T-step moves $M^{\pm \overline{e}_1}, \ldots, M^{\pm \overline{e}_d}$ such that:

- (1) The process \bar{c}_{ij} is stationary and ergodic, and dominates a supercritical Bernoulli percolation process uniformly in q.
- (2) $T \leq CL^{\lambda}$.
- (3) For any $\overline{e} \in \{\pm \overline{e}_1, \dots, \overline{e}_d\}$ consider the move $M^{\overline{e}}$. Then:
 - (a) The domain of $M^{\overline{e}}$, Dom $M^{\overline{e}}$, consists of the configurations in which $\overline{c}_{0,\overline{e}} = 1$.
 - (b) $2^{\operatorname{Loss}(M^{\overline{e}})} < C L^{\lambda}$.
 - (c) For any $\eta \in Dom M^{\overline{e}}$, denoting $M^{\overline{e}} = \{\eta_t(\eta), x_t(\eta), e_t(\eta)\}_{t=0}^T$, at the final configuration

$$\eta_T(\eta) = \eta^{0,\overline{e}}.$$

Proof. The lemma is proven in [9], Lemmas 3.9 and 3.14. See also [17, Section 3.4.1]. The reader may note that in the proof of [9] q is assumed small, but since the relevant probabilities estimated are monotone in q one may discard this assumption by adjusting the constants C, λ in equation (4.2).

Remark 4.4. The reason for the iterated exponential scaling of $D(\rho)$ hides in the proof of Lemma 4.3, and explained in details in [9, 17, 25]. It is based on induction over both k and d, of two different scales. The first scale, l(k,d), is the scale at which cluster of empty sites could typically advance. For k=1, for example, the constraint is always satisfied and l(1,d)=1. Perhaps more interesting is the case k=d=2, where a column of empty sites of length l could move if there is an empty site in a neighboring column (see Figure 4.1). The probability to have a vacancy in the neighboring column is $1-(1-q)^l$, hence this event becomes likely at $l(k,d)\approx 1/q$. This is the scale of the *droplets*, which are those empty clusters of size l that are able to move in \mathbb{Z}^d .

The second scale, L(k,d), is the typical distance of an arbitrary site to a droplet, so $L(k,d) \approx q^{-l(k,d)}$. If we look at a particle and consider its neighborhood at scale L(k,d), we are likely to find a droplet, that would be able to move to the vicinity of that particle and help it jump.

In order to understand the scaling of $D(\rho)$, we should understand the two scales l(k,d) and L(k,d). Consider the set $[1,L(k-1,d-1)]^d$. If we empty the entire boundary of this set, it could serve as a droplet – take, for example, the surface $\{0\} \times [1,L(k-1,d-1)]^{d-1}$. This is a d-1 dimensional surface, and each of its sites has an empty neighbor to the right coming from $[1,L(k-1,d-1)]^d$. Therefore, any move for the KA dynamics with parameters k-1,d-1 could be applied to that surface. Since its size is L(k-1,d-1), it is likely to contain a droplet. Hence, using this droplet, we are able to move freely the sites on the surface. With slightly more careful analysis, it could be shown that by rearranging the sites on $\{0\} \times [1,L(k-1,d-1)]^{d-1}$ the set $[1,L(k-1,d-1)]^d$ could "swallow" this surface, thus moving one step to the left. That is, $[1,L(k-1,d-1)]^d$ is, indeed, a droplet; and so $l(k,d) \approx L(k-1,d-1)$.

The two relations, $L(k,d) \approx q^{-l(k,d)}$ and $l(k,d) \approx L(k-1,d-1)$, show that the two scales indeed behave as an iterated exponential. The scaling of the diffusion coefficient could then be explained heuristically, if we imagine that the particles are mostly blocked, except those in the vicinity of a droplet. Since the sites that are able to move have density L^{-d} , the diffusion coefficient scales polynomially in L.

An immediate consequence of point one of Lemma 4.3 is that the graph induced by the edges for which \bar{c} equals 1 has a unique infinite connected component. Let C denote this infinite component. In [10] (see also [22]), it is shown that the diffusion coefficient of a random walk on C is given by the following variational formula:

$$\overline{D} = \inf_{\psi} \sum_{\alpha} \nu \left[\overline{c}_{0,e_{\alpha}} \left(\delta_{\alpha,1} + \psi(\tau_{\overline{e}_{\alpha}} \overline{c}) - \psi(\overline{c}) \right)^{2} | 0 \in \mathcal{C}, \overline{e}_{\alpha} \in \mathcal{C} \right],$$

where the infimum is taken over function $\psi:\Pi\to\mathbb{R}$ that depend on finitely many edges.

The input we need from [10, 8] is the positivity of the diffusion coefficient:

Lemma 4.5. There exists $\overline{D}_0 > 0$ such that for all $\psi : \Pi \to \mathbb{R}$ and all $\rho \in (0,1)$,

$$\sum_{\alpha} \nu \left[\overline{c}_{0,e_{\alpha}} \left(\delta_{\alpha,1} + \psi(\tau_{\overline{e}_{\alpha}} \overline{c}) - \psi(\overline{c}) \right)^{2} \right] \geq \overline{D}_{0}.$$

Proof. This is a direct consequence of [10, Lemma 2.1] and the first point of Lemma 4.3. □

In order to relate the diffusion coefficient given in equation (2.5) to \overline{D} , we use the following proposition:

Proposition 4.6. Fix a local function $g:\overline{\Omega}\times\Pi\to\mathbb{R}$. Then there exists a local function $\psi:\Pi\to\mathbb{R}$, such that

$$\sum_{\alpha=1}^{d} \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(\delta_{\alpha,1} + \psi(\tau_{\overline{e}_{\alpha}} \overline{c}) - \psi(\overline{c}) \right)^{2} \right] \leq \frac{1}{2\rho(1-\rho)} \times$$

$$\sum_{\alpha=1}^{d} \overline{\mu} \otimes \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(\delta_{\alpha,1}(\overline{\eta}(\overline{e}_{1}) - \overline{\eta}(0)) - \sum_{i \in \mathbb{Z}_{\tau}^{d}} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_{i}\overline{\eta}, \tau_{i}\overline{c}) \right)^{2} \right],$$

where $\overline{\nabla}$ is the gradient operating only on $\overline{\eta}$ (that is, $\overline{\nabla}_{0,\overline{e}_{\alpha}}\,g(\tau_{i}\overline{\eta},\tau_{i}\overline{c})=g(\tau_{i}\,\overline{\eta}^{0,\overline{e}_{\alpha}},\tau_{i}\overline{c})-g(\tau_{i}\overline{\eta},\tau_{i}\overline{c})$).

Proof. Note first that the sum $\sum_{i \in \mathbb{Z}_L^d} \overline{\nabla}_{0,\overline{e}_\alpha} g(\tau_i \overline{\eta}, \tau_i \overline{c})$ is finite (and hence well defined) since g is local. We are therefore allowed, throughout the proof, to replace it by a sum over a large enough torus $\mathbb{T}_L^d = \mathbb{Z}_L^d/N\mathbb{Z}_L^d$ for large N (depending on g). We start by writing the left hand side of the inequality as

$$\begin{split} &\sum_{\alpha=1}^{d} \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(\mathbf{I} + \mathbf{II} + \mathbf{III} \right) \right], \\ &\mathbf{I} = \delta_{\alpha,1}, \\ &\mathbf{II} = 2\delta_{\alpha,1} \left(\psi(\tau_{\overline{e}_{1}}\overline{c}) - \psi(\overline{c}) \right), \\ &\mathbf{III} = \left(\psi(\tau_{\overline{e}_{\alpha}}\overline{c}) - \psi(\overline{c}) \right)^{2}; \end{split}$$

and the right hand side (noting that \overline{c} depends only on ω and not on $\overline{\eta}$) as

$$\sum_{\alpha=1}^{d} \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} (\mathbf{I}' + \mathbf{I}\mathbf{I}' + \mathbf{I}\mathbf{I}\mathbf{I}') \right],$$

$$\mathbf{I}' = \overline{\mu} \left[\delta_{\alpha,1} (\overline{\eta}(\overline{e}_{1}) - \overline{\eta}(0))^{2} \right],$$

$$\mathbf{II}' = -2\delta_{\alpha,1} \overline{\mu} \left[(\overline{\eta}(\overline{e}_{1}) - \overline{\eta}(0)) \sum_{i \in \mathbb{T}_{L}^{d}} \overline{\nabla}_{0,\overline{e}_{1}} g(\tau_{i}\overline{\eta}, \tau_{i}\overline{c}) \right],$$

$$\mathbf{III}' = \overline{\mu} \left[\left(\sum_{i \in \mathbb{T}_{L}^{d}} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_{i}\overline{\eta}, \tau_{i}\overline{c}) \right)^{2} \right].$$

We now compare term by term. The term I, I' do not depend on ψ : $I' = \delta_{\alpha,1} 2\rho(1-\rho)$, so indeed $I \leq \frac{1}{2\rho(1-\rho)}I'$.

For the other terms we need to specify our choice of ψ :

$$\psi(\overline{c}) = 2\overline{\mu} \left[\overline{\eta}(0) \sum_{i \in \mathbb{T}_L^d} g(\tau_i \overline{\eta}, \tau_i \overline{c}) \right].$$

Fix $\overline{e} \in {\overline{e}_1, \dots, \overline{e}_d}$. Then

$$\psi(\tau_{\overline{e}}\overline{c}) = 2\overline{\mu} \left[\overline{\eta}(0) \sum_{i \in \mathbb{T}_L^d} g(\tau_i \overline{\eta}, \tau_{i+\overline{e}}\overline{c}) \right] = 2\overline{\mu} \left[\overline{\eta}(\overline{e}) \sum_{i \in \mathbb{T}_L^d} g(\tau_{i+\overline{e}}\overline{\eta}, \tau_{i+\overline{e}}\overline{c}) \right]$$

$$= 2\overline{\mu} \left[\overline{\eta}(0) \sum_{i \in \mathbb{T}_L^d} g(\tau_i \, \overline{\eta}^{0,\overline{e}}, \tau_i \overline{c}) \right],$$

and thus

$$\psi(\tau_{\overline{e}_{\alpha}}\overline{c}) - \psi(\overline{c}) = \overline{\mu} \left[2\overline{\eta}(0) \sum_{i \in \mathbb{T}_L^d} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_i \, \overline{\eta}, \tau_i \overline{c}) \right]. \tag{4.3}$$

Observe now that $\overline{\eta}(0) = \overline{\eta}(\overline{e}_1)$ implies $\overline{\nabla}_{0,\overline{e}_1} g(\tau_i \overline{\eta}, \tau_i \overline{c}) = 0$, and otherwise $\overline{\eta}(\overline{e}_1) = 1 - \overline{\eta}(0)$, yielding

$$(\overline{\eta}(\overline{e}_1) - \overline{\eta}(0))\overline{\nabla}_{0,\overline{e}_1} g(\tau_i \, \overline{\eta}, \tau_i \overline{c}) = (1 - 2\overline{\eta}(0))\overline{\nabla}_{0,\overline{e}_1} g(\tau_i \, \overline{\eta}, \tau_i \overline{c}).$$

Therefore,

$$\overline{\mu}\left[\left(\overline{\eta}(\overline{e}_1) - \overline{\eta}(0)\right) \sum_{i \in \mathbb{T}_I^d} \overline{\nabla}_{0,\overline{e}_1} g(\tau_i \, \overline{\eta}, \tau_i \overline{c})\right] = \sum_{i \in \mathbb{T}_I^d} \overline{\mu}\left[\overline{\nabla}_{0,\overline{e}_1} g(\tau_i \, \overline{\eta}, \tau_i \overline{c})\right] - (\psi(\tau_{\overline{e}_1} \overline{c}) - \psi(\overline{c})),$$

and noting that $\overline{\mu}\left[\overline{\nabla}_{0,\overline{e}_1} g(\tau_i \, \overline{\eta}, \tau_i \overline{c})\right] = 0$ (the gradient of any function has 0 expected value), we obtain

$$II = II'$$
.

Finally, for the last term we use again equation (4.3), together with Jensen's inequality and the fact that $\overline{\eta}(0)^2 \leq 1$:

$$\operatorname{III} \leq \overline{\mu} \left[\left(2\overline{\eta}(0) \sum_{i \in \mathbb{T}_L^d} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_i \, \overline{\eta}, \tau_i \overline{c}) \right)^2 \right] \leq 4 \operatorname{III}'.$$

Corollary 4.7. For all local $g: \overline{\Omega} \times \Pi \to \mathbb{R}$,

$$\frac{1}{2\rho(1-\rho)}\sum_{\alpha=1}^{d}\overline{\mu}\otimes\nu\left[\overline{c}_{0,\overline{e}_{\alpha}}\left(\delta_{\alpha,1}(\overline{\eta}(\overline{e}_{1})-\overline{\eta}(0))-\sum_{i\in\mathbb{Z}_{L}^{d}}\overline{\nabla}_{0,\overline{e}_{\alpha}}g(\tau_{i}\overline{\eta},\tau_{i}\overline{c})\right)^{2}\right]\geq\overline{D}_{0},$$

where \overline{D}_0 is the positive constant given in Lemma 4.5.

The next step of the proof is to use the multistep move given in Lemma 4.3 in order to compare \overline{D}_0 with D.

Proposition 4.8. Fix a local function $f: \Omega \to \mathbb{R}$. Then there exists a local function $g: \overline{\Omega} \times \Pi \to \mathbb{R}$ such that

$$\mu\left(\sum_{\alpha=1}^{d} c_{0,e_{\alpha}}(\eta) \left(\delta_{\alpha,1}(\eta(e_{\alpha}) - \eta(0)) - \sum_{x \in \mathbb{Z}^{d}} \nabla_{0,e_{\alpha}}(\tau_{x}f)\right)^{2}\right) \geq$$

$$L^{-\lambda} \sum_{\alpha=1}^{d} \overline{\mu} \otimes \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(\delta_{\alpha,1}(\overline{\eta}(\overline{e}_{1}) - \overline{\eta}(0)) - \sum_{i \in \mathbb{Z}_{L}^{d}} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_{i}\overline{\eta}, \tau_{i}\overline{c}) \right)^{2} \right].$$

Proof. Let $g(\overline{\eta},\overline{c})=\mu\left[\frac{1}{L}\sum_{y\in[L]^d}\tau_yf(\eta)\Big|\overline{\eta},\overline{c}\right]$. We use Lemma 4.3 in order to write, for all $x\in\mathbb{Z}^d$ and $\alpha\in\{1,\ldots,d\}$, denoting $M^{\overline{e}_\alpha}=\{\eta_t(\eta),x_t(\eta),e_t(\eta)\}_{t=0}^T$,

$$\overline{\nabla}_{0,\overline{e}_{\alpha}}\tau_{x}f = \sum_{t=1}^{T} \nabla_{x_{t},x_{t}+e_{t}}\tau_{x}f(\eta_{t}) = \sum_{t=1}^{T} \tau_{x_{t}} \nabla_{0,e_{t}}\tau_{x-x_{t}}f(\eta_{t}). \tag{4.4}$$

We also note that the total particle flow (defined as the change in $\sum_x x\eta(x)$) can be decomposed along the T-step move. In more details, using the fact that η_0 and η_T agree outside $\{0, \overline{e}_{\alpha}\}$,

$$\sum_{x} x(\eta_0(x) - \eta_T(x)) = Le_{\alpha} \left(\overline{\eta}(\overline{e}_{\alpha}) - \overline{\eta}(0) \right).$$

On the other hand, at step t the configuration changes only at x_t and $x_t + e_t$, therefore

$$\sum_{t} x(\eta_{t-1}(x) - \eta_t(x)) = e_t(\eta_t(x_t) - \eta_t(x_t + e_t)) = e_t \tau_{x_t}(\eta_t(0) - \eta_t(e_t)),$$

implying

$$\sum_{x} x(\eta_0(x) - \eta_T(x)) = \sum_{t=1}^{T} \sum_{x} x(\eta_{t-1}(x) - \eta_t(x)) = \sum_{t=1}^{T} e_t \tau_{x_t}(\eta_t(0) - \eta_t(e_t)).$$

That is,

$$Le_{\alpha}\left(\overline{\eta}(\overline{e}_{\alpha}) - \overline{\eta}(0)\right) = \sum_{t=1}^{T} e_{t} \tau_{x_{t}} \left(\eta_{t}(e_{t}) - \eta_{t}(0)\right). \tag{4.5}$$

Using these two identities, the Cauchy-Schwarz inequality, and the properties of the move, we obtain

$$\sum_{\alpha=1}^{d} \overline{\mu} \otimes \nu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(e_{1} \cdot e_{\alpha}(\overline{\eta}(\overline{e}_{\alpha}) - \overline{\eta}(0)) - \sum_{i \in \mathbb{Z}_{L}^{d}} \overline{\nabla}_{0,\overline{e}_{\alpha}} g(\tau_{i}\overline{\eta}, \tau_{i}\overline{c}) \right)^{2} \right] \leq$$

$$\frac{1}{L^{2}} \sum_{\alpha=1}^{d} \mu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(e_{1} \cdot Le_{\alpha}(\overline{\eta}(\overline{e}_{1}) - \overline{\eta}(0)) - \sum_{i \in \mathbb{Z}_{L}^{d}} \overline{\nabla}_{0,\overline{e}_{\alpha}} \sum_{y \in [L]^{d}} \tau_{i+y} f(\eta) \right)^{2} \right] =$$

$$\frac{1}{L^{2}} \sum_{\alpha=1}^{d} \mu \left[\overline{c}_{0,\overline{e}_{\alpha}} \left(e_{1} \cdot \sum_{t=1}^{T} e_{t} \tau_{x_{t}} (\eta_{t}(e_{t}) - \eta_{t}(0)) - \sum_{x \in \mathbb{Z}^{d}} \sum_{t=1}^{T} \tau_{x_{t}} \nabla_{0,e_{t}} \tau_{x-x_{t}} f(\eta_{t}) \right)^{2} \right] \leq$$

$$\frac{T}{L^{2}} \sum_{t=1}^{T} \sum_{\alpha=1}^{d} \mu \left[\overline{c}_{0,\overline{e}_{\alpha}} \tau_{x_{t}} c_{0,e_{t}}(\eta_{t}) \left(e_{1} \cdot e_{t} (\eta_{t}(e_{t}) - \eta_{t}(0)) - \sum_{x \in \mathbb{Z}^{d}} \nabla_{0,e_{t}} \tau_{x} f(\eta_{t}) \right)^{2} \right] \leq$$

$$\frac{T}{L^{2}} \sum_{t=1}^{T} \sum_{\alpha=1}^{d} \sum_{\eta \in \Omega} \mu(\eta) \sum_{\eta' \in \Omega} \mathbb{1}_{\eta' = \eta_{t}} \sum_{\beta=1}^{d} \mathbb{1}_{e_{\beta} = e_{t}} c_{0,e_{\beta}}(\eta') \left(e_{1} \cdot e_{\beta} \left(\eta'(e_{\beta}) - \eta'(0) \right) - \sum_{x \in \mathbb{Z}^{d}} \nabla_{0,e_{\beta}} \tau_{x} f(\eta') \right)^{2} \leq$$

$$\frac{T^{2}}{L^{2}} \sum_{\alpha=1}^{d} 2^{\operatorname{Loss}(M^{\overline{e}_{\alpha}})} \sum_{\eta' \in \Omega} \mu(\eta') \sum_{\beta=1}^{d} c_{0,e_{\beta}}(\eta') \left(e_{1} \cdot e_{\beta} \left(\eta'(e_{\beta}) - \eta'(0) \right) - \sum_{x \in \mathbb{Z}^{d}} \nabla_{0,e_{\beta}} \tau_{x} f(\eta') \right)^{2}.$$

The result follows by inserting the bounds for T and Loss(M) given in Lemma 4.3.

The proof of the lower bound (4.1) follows from Proposition 4.8, Corollary 4.7, and the variational characterization of $D^{(0)}$ in equation (2.5).

5. Proof of the upper bound

In order to find the upper bound we will use a process tightly related to the Kob-Andersen model, called the k-neighbor bootstrap percolation (see, e.g., [19]). We start by defining this process, and describing some of its basic properties.

5.1. Bootstrap percolation.

Definition 5.1 (bootstrap percolation). Fix $V \subseteq \mathbb{Z}^d$ and $A \subseteq \mathbb{Z}^d$. The bootstrap percolation in V starting from A is a deterministic process defined for $t = 1, 2, \ldots$ as

$$A_0 = A \cap V,$$

$$A_{t+1} = A_t \cup \{x \in V : \#\{y \in A_t \text{ such that } y \sim x\} \ge k\}.$$

The limit $\bigcup_{t\geq 0} A_t$ is called the *span of* A *in* V, and denoted by $[A]^V$. We say that two sites x and y are connected for the bootstrap percolation in V starting from A if they are connected in $[A]^V$ (thought of as the subgraph of \mathbb{Z}^d induced by the set $[A]^V$), that is, if there is a nearest neighbor path $x = x_1, \ldots, x_n = y$ such that $x_1, \ldots, x_n \in [A]^V$.

For $\eta \in \Omega$, we define

$$A_{\eta} = \{ x \in \mathbb{Z}^d : \eta_x = 0 \}.$$

We may refer to the bootstrap percolation in V starting from A_{η} as the bootstrap percolation starting from η . When context allows we omit the explicit mention of V, A, or both.

We continue with several properties of bootstrap percolation.

Observation 5.2. (monotonicity). Let $U \subseteq V \subseteq \mathbb{Z}^d$, and fix $A \subseteq B \subseteq \mathbb{Z}^d$. Then $[A]^U \subseteq [A]^V$ and $[A]^U \subseteq [B]^U$.

The following observation reveals the the connection between bootstrap percolation and the Kob-Andersen model:

Observation 5.3. Fix $\eta \in \Omega$, and consider a set $V \subset \mathbb{Z}^d$. Assume that, for two neighboring sites $x,y \in V$, the constraint $c_{x,y}$ is satisfied in V, that is, $c_{x,y}(\eta') = 1$ for any η' that agrees with η on V. Then $[A_{\eta}]^V = [A_{\eta^{x,y}}]^V$.

Proof. Assume without loss of generality that $\eta(x)=1$ and $\eta(y)=0$, and note that $[A_{\eta}]^V\subseteq [A_{\eta}\cup\{x\}]^V$. On the other hand, since $c_{x,y}=1$ in V, the site x will be added to A_{η} after a single step of the bootstrap percolation. Denoting the set after that single step by A', $[A_{\eta}\cup\{x\}]^V\subseteq [A']^V=[A_{\eta}]^V$. Therefore $[A_{\eta}]^V=[A_{\eta}\cup\{x\}]^V$. The same argument shows that $[A_{\eta^{x,y}}]^V=[A_{\eta}\cup\{x\}]^V$.

Observation 5.4. Fix $A \subset \mathbb{Z}^d$, $V \subset \mathbb{Z}^d$, and $x \in V$. Let U be the set of sites connected to x in $[A]^V$. Then $[A]^U = U$.

Proof. Let $(A_t)_{t\geq 0}$ denote the bootstrap percolation in V starting with A, and assume by contradiction $[A]^U\subsetneq U$. Since $U\subseteq [A]^V$, there exists a first time t for which some $y\in U\setminus [A]^U$ is contained in A_t . By minimality, $A_{t-1}\cap U\subseteq [A]^U$, and since $y\notin [A]^U$ it has at most k-1 neighbors in $A_{t-1}\cap U$. On the other hand, it has at least k neighbors in A_t . Therefore, it must have at least one neighbor in $V\setminus U$. This is a contradiction, since U is a connected component containing y.

Claim 5.5. Fix $A \subset \mathbb{Z}^d$. Consider two sets $B \subset B' \subset \mathbb{Z}^d$, a site $z \in B$, and any $S \subset \mathbb{Z}^d$. Assume that z is connected to S for the bootstrap percolation in B', but not for the bootstrap percolation in B. Then z is connected to ∂B for the bootstrap percolation in B'.

Proof. Assume that z is not connected to ∂B for the bootstrap percolation in B', so in particular its connected component in $[A]^{B'}$, denoted U, is entirely contained in B. By Observation 5.4 and monotonicity of the bootstrap percolation, $U = [A]^U \subseteq [A]^B$. This is a contradiction, since by assumption $U \cap S \neq \emptyset$ but $[A]^B \cap S = \emptyset$.

5.2. **Analysis of the test function.** We will prove the upper bound by estimating the expression inside the infimum in equation (2.5) for a carefully chosen function f.

Recall $q = 1 - \rho$. The test function we will construct will depend on a scale

$$l = \exp^{k-2}(\lambda q^{-\frac{1}{d-k+1}}). \tag{5.1}$$

Throughout the section λ and C denote generic positive constants.

Definition 5.6 (relevant sites). Fix $\eta \in \Omega$. A site $x \in [-2l, 2l]^d$ is called *relevant* if it is not connected to $\{0, 1\} \times [-2l, 2l]^{d-1}$ for the bootstrap percolation in $[-2l, 2l]^d$; and otherwise it is called *irrelevant*. Denote the set of relevant sites by $\mathcal{R}(\eta)$.

We divide the box $[-l, l]^d$ in two parts – the left part $\Lambda_- = [-l, 0] \times [-l, l]^{d-1}$, and the right part $\Lambda_+ = [1, l] \times [-l, l]^{d-1}$ (see Figure 5.1). The test function we consider is

$$f(\eta) = \frac{1}{2(2l+1)^{d-1}} \left(\sum_{x \in \Lambda_+ \cap \mathcal{R}} \eta(x) - \sum_{x \in \Lambda_- \cap \mathcal{R}} \eta(x) \right). \tag{5.2}$$

Hence, the purpose of this section is to prove that for ε small enough

$$\mu \left[\sum_{\alpha=1}^{d} c_{0,e_{\alpha}}^{(\varepsilon)} \left(\delta_{\alpha,1} \left(\eta(e_1) - \eta(0) \right) - \sum_{x \in \mathbb{Z}^d} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] \le e^{-\lambda l}.$$

Remark 5.7. The choice of f in equation (5.2) seems mysterious at first sight – Observation 5.3 explains the use of bootstrap percolation, but the introduction of relevant sites and the exact form of f are not clear.

One way to gain more intuition on this choice of f is to look more carefully at the variational principle (2.5). Ignoring the contribution of f, we are left with the term

$$c_{0,e_{\alpha}}\left(\delta_{\alpha,1}\left(\eta(e_1)-\eta(0)\right)\right)^2.$$

This could be though of as a contribution of the instantaneous current between the origin and e_1 . The appearance of this term is not surprising – if typically the system has large currents, it is natural to expect the diffusion coefficient to be large.

However, the typical instantaneous current is not sufficient to understand the behavior of the diffusion coefficient – correlations in space and time could also have an important effect. For example, take the Kob-Andersen model with k=d=2, and consider a configuration in which the sites e_1,e_2 and e_1+e_2 are empty, and all other sites (in a large neighborhood of the origin) are occupied. The particle at the origin could jump one step to the right, but any attempt to jump further is not allowed by the constraint. Therefore, if we wait for some time it is likely to jump back to the left. Thus, we see that an instantaneous right current can cause at a later time a current to the left. The role of the function f in equation (2.5) is to compensate for this effect, by adding to $\delta_{\alpha,1} (\eta(e_1) - \eta(0))$ an effective current in the opposite direction.

The example of the last paragraph demonstrates the following heuristic picture – typically, most particles are confined to a very small region; they can move back and forth but never too far. Assume for simplicity that the origin is occupied, and consider the particle there. In view of the heuristic described above, this particle will remain for a very long time in a certain region that we may refer to as the *attainable region*. Recalling Observation 5.3, it is reasonable to approximate this attainable region by the set of sites connected to the origin for the bootstrap percolation in some (large) box. Hence, being *relevant* roughly represents a small attainable region.

As long is this attainable region remains small, we expect that any instantaneous current to the right caused by the particle at the origin will be canceled shortly after by a jump to the left. For a good choice of f, this fact (assuming $c_{0,e_1}(\eta) = 1$) should be expressed as

$$\eta(e_1) - \eta(0) \approx \sum_{x \in \mathbb{Z}^d} \nabla_{0, e_1} \tau_x f(\eta).$$

In the following we will see that the function f defined in equation (5.2) satisfies this approximated relation. The error term corresponds to the possibility that the attainable region is, in fact, large. When the notion of "small" or "large" attainable region is determined according to the scale l given in equation (5.1), we obtain the upper bound of D.

First, observe that since f depends on $(4l+1)^d$ sites and its maximum is smaller than l+1,

$$\mu \left[\sum_{\alpha=1}^{d} \varepsilon \left(\delta_{\alpha,1} \left(\eta(e_1) - \eta(0) \right) - \sum_{x \in \mathbb{Z}^d} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] \le d\varepsilon (1 + (4l+1)^d (l+1))^2 = O(\varepsilon).$$

Therefore, since $c_{0,e_{\alpha}}^{(\varepsilon)}=(1-\varepsilon)c_{0,e_{\alpha}}+\varepsilon$, it suffices to prove

$$\mu \left[\sum_{\alpha=1}^{d} c_{0,e_{\alpha}} \left(\delta_{\alpha,1} \left(\eta(e_1) - \eta(0) \right) - \sum_{x \in \mathbb{Z}^d} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] \le e^{-\lambda l}.$$
 (5.3)

Since the analysis of f will require us to understand when particles enter or exit different boxes (and in particular Λ_{\pm}), we will need to introduce some notation. First, for a set $\Lambda \subset \mathbb{Z}^d$, we say that an (undirected) edge (x,y) is on the *boundary* of Λ , and write $(x,y) \in \overline{\partial} \Lambda$, if one vertex is in Λ and the other outside Λ . The *(inner) boundary* $\partial \Lambda$ are the sites in Λ that have a neighbor outside Λ .

For $\alpha = 1, ..., d$ we define the boundary in the e_{α} direction

$$\partial^{\alpha} \Lambda = \{ x : (x, x - e_{\alpha}) \in \overline{\partial} \Lambda \}.$$

We will write $\Lambda_l = [-l, l]^d$ (and $\Lambda_{2l} = [-2l, 2l]^d$), as well as

$$\Lambda_l^{\alpha} = \left[-l,l\right]^{\alpha-1} \times \left\{0\right\} \times \left[-l,l\right]^{d-\alpha}.$$

Finally, for $x_0 \in \Lambda_l^{\alpha}$, we denote the two boundary sites above and below x_0 as

$$x_0^{+\alpha} = x_0 + (l+1) e_{\alpha},$$

 $x_0^{-\alpha} = x_0 - le_{\alpha}.$

Note that $x_0^{\pm \alpha} \in \partial^{\alpha} \Lambda_l$. See Figure 5.1.

We are now ready to start the analysis of f. In the next proposition we will see, for fixed x, what is the contribution of $\nabla_{0,e_1}\tau_x f$:

Proposition 5.8. Fix an edge (x, x - e) and configuration η such that $c_{0,e} = 1$ and $\nabla_{0,e} \tau_x f \neq 0$. Then one of the following holds:

(1) $0 \in x + (\Lambda_{2l+1} \setminus \Lambda_{2l-2})$ (equivalently $x \in \Lambda_{2l+1} \setminus \Lambda_{2l-2}$), and there exists $y \in x + \partial \Lambda_l$ such that the bootstrap percolation in $x + \Lambda_{2l}$ connects y to $x + \partial \Lambda_{2l-2}$, either for η or $\eta^{0,e}$. In this case $|\nabla_{0,e}\tau_x f| \leq C l$. See Figure 5.2.

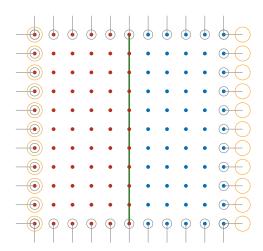


FIGURE 5.1. A sketch of the different sets in Λ_l in two dimensions. The left part Λ_+ are the red vertices; the right part Λ_+ consists of the blue vertices; the boundary $\overline{\partial}\Lambda$ is given by the gray edges; the inner boundary $\partial\Lambda$ contains the sites circled in gray; the boundary in the e_1 direction $\partial^1\Lambda$ is circled in orange; and the set Λ_l^1 is represented by the green line crossing the box. In this picture, for any $x_0 \in \Lambda_l^1$ (i.e., on the green line), the site x_0^{+1} is the orange circle to its right (at distance l+1); and the site x_0^{-1} is the orange circle to its left (at distance l).

(2) $(0,e) \in x + \overline{\partial} \Lambda_l$ (equivalently $(x,x-e) \in \overline{\partial} \Lambda_l$) and -x is relevant for $\tau_x \eta$. In this case

$$\nabla_{0,e}\tau_{x}f = \frac{\eta(e) - \eta(0)}{2(2l+1)^{d-1}} \times \begin{cases}
1 & 0 \in x + \Lambda_{+} \cap \partial [-l, l]^{d} \\
-1 & e \in x + \Lambda_{+} \cap \partial [-l, l]^{d} \\
-1 & 0 \in x + \Lambda_{-} \cap \partial [-l, l]^{d} \\
1 & e \in x + \Lambda_{-} \cap \partial [-l, l]^{d}
\end{cases}$$

$$= \frac{\eta(e) - \eta(0)}{2(2l+1)^{d-1}} \times \begin{cases}
1 & x \in \Lambda_{-} \cap \partial [-l, l]^{d} \\
-1 & x - e \in \Lambda_{-} \cap \partial [-l, l]^{d} \\
-1 & x \in \Lambda_{+} \cap \partial [-l, l]^{d} \\
1 & x - e \in \Lambda_{+} \cap \partial [-l, l]^{d}
\end{cases}$$
(5.4)

Proof. f could only change when the set of relevant sites changes, or when a relevant site changes its occupation.

The first case corresponds to point 1 – for the set of relevant sites for $\tau_x \eta$ to change, $[A_{\eta}]^{x+\Lambda_{2l}}$ must change, and by Observation 5.3 this is only possible if $c_{0,e}$ is only satisfied with the help of sites outside $x + \Lambda_{2l}$. This means that at least one of the vertices 0 or e is in $\partial \Lambda_{el}$, and in particular $0 \in x + (\Lambda_{2l+1} \setminus \Lambda_{2l-2})$.

To understand the second implication, we may assume without loss of generality that there is some site $z \in \Lambda_l$ which is connected to $\{0,1\} \times [-2l,2l]^{d-1}$ in $[A_{\eta}]^{x+\Lambda_{2l}}$ but not in $[A_{\eta^0,e}]^{x+\Lambda_{2l}}$.

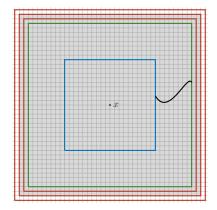


FIGURE 5.2. Illustration of the first case in Proposition 5.8. $x + \Lambda_{2l}$ is the gray square. The origin is on one of the three red lines, which represent $x + \Lambda_{2l+1} \setminus \Lambda_{2l-2}$. The blue square is $x + \partial \Lambda_l$ and the green square is $x + \partial \Lambda_{2l-2}$. These two squares must be connected for the bootstrap percolation.

By monotonicity of bootstrap percolation and using again Observation 5.3, z cannot be connected to $\{0,1\} \times [-2l,2l]^{d-1}$ in $[A_{\eta}]^{\Lambda_{2l-2}}$. Then, by Claim 5.5, z is connected to $\partial \Lambda_{2l-2}$ in $[A_{\eta}]^{x+\Lambda_{2l}}$. To finish the first point, we only need the rough bound $|f(\eta)| \leq \frac{|\Lambda_{+}|+|\Lambda_{-}|}{2(2l+1)^{d-1}}$.

In the second case, we note first if a particle jumps inside Λ_l , and it is originally in $\Lambda_+ \cap \mathcal{R}$, then it will remain in $\Lambda_+ \cap \mathcal{R}$ (and analogously for Λ_-). Therefore, f could only change if a particle jumps into or out of Λ_l , so for $\tau_x f$ to change we must require $(0,e) \in x + \overline{\partial} \Lambda_l$. Moreover, its (shifted) position -x must be relevant for the shifted configuration $\tau_x \eta$. Then, $\nabla_{(0,e)} \tau_x f$ is given by following carefully the four options: moving into Λ_+ , out of Λ_+ , into Λ_- , or out of Λ_- .

In order to control the contribution coming from the first case of Proposition 5.8, we give a name to the event that appears there:

Definition 5.9. Fix an edge (x, x - e). Then $E_{x,x-e}$ is the event, that there exist $y \in x + \partial \Lambda_l$ and $z \in x + \partial \Lambda_{2l-2}$ such that the bootstrap percolation in $x + \Lambda_{2l}$ connects y to z, either for η or $\eta^{0,e}$.

An important tool we will use in order to bound the probability of this event is the following lemma:

Lemma 5.10 ([7, Lemma 5.1]). Let l' < 10l, and fix $y, z \in \Lambda_{l'}$. Then, assuming that the constant λ in equation (5.1) is small enough,

$$\mu(z \text{ connected to } y \text{ in } [A_{\eta}]^{\Lambda_{l'}}) \leq \left(C \|z - y\|_{\infty}^{d-1} q\right)^{\lambda \|z - y\|_{\infty}} \qquad k = 2,$$

$$\mu(z \text{ connected to } y \text{ in } [A_{\eta}]^{\Lambda_{l'}}) \leq q^{\lambda \|z - y\|_{\infty}} \qquad k \geq 3.$$

Claim 5.11. Fix an edge (x, x - e). Then

$$\mu(E_{x,x-e}) \le Ce^{-\lambda l}$$
.

Proof. First, note that there are Cl^{d-1} possible choices of y and Cl^{d-1} choices of z. Note that $||z-y||_{\infty} \geq l-2$. By Lemma 5.10, the probability for y to be connected to z is bounded by $(Cl^{d-1}q)^{\lambda l}$ for k=2 and $q^{\lambda l}$ for $k\geq 3$; both of which are, indeed, smaller than $Ce^{-\lambda l}$.

The last claim covers the first case of Proposition 5.8, and we now move to the second.

When considering that case, we will use certain cancellations in directions perpendicular to e_1 . More precisely, a particle jumping from 0 to e_{α} (for $\alpha \neq 1$) will enter $x + \Lambda_l$ (for an appropriate choice of x) but exit $x' + \Lambda_l$ (for an appropriate choice of x'). We then expect that $\nabla_{0,e_{\alpha}}\tau_x f$ and $\nabla_{0,e_{\alpha}}\tau_{x'} f = 0$ will cancel out, which is indeed the case unless one of the sites is relevant and the other irrelevant. We therefore introduce the following event:

Definition 5.12. Fix $\alpha \in \{2, \dots, d\}$ and $x_0 \in \Lambda_l^{\alpha}$. Let $E_{\alpha}(x_0)$ be the event, that either $-x_0^{+\alpha}$ is relevant for $\tau_{x_0^{+\alpha}}\eta$, or $-x_0^{-\alpha}$ is relevant for $\tau_{x_0^{-\alpha}}\eta$, but not both.

Claim 5.13. Fix $\alpha \in \{2, ..., d\}$ and $x_0 \in \Lambda_l^{\alpha}$. Then for all $\eta \in E_{\alpha}(x_0)$, the origin is connected to $\partial \Lambda_l$ in $[A_n]^{\Lambda_{3l}}$. Moreover,

$$\mu(E_{\alpha}(x_0)) \le Ce^{-\lambda l}$$
.

Proof. We will prove that the origin is connected to $\partial \Lambda_l$ in $[A_{\eta}]^{\Lambda_{3l}}$ for the case where $-x_0^{+\alpha}$ is relevant for $\tau_{x_0^{+\alpha}}\eta$, but $-x_0^{-\alpha}$ is irrelevant for $\tau_{x_0^{-\alpha}}\eta$. The complementing case as analogous.

Let $S=x_0+\{0,1\}\times\mathbb{Z}^{d-1}$, $B_-=x_0^{-\alpha}+\Lambda_{2l}$, $B_+=x_0^{+\alpha}+\Lambda_{2l}$. Saying that $-x_0^{+\alpha}$ is relevant for $\tau_{x_0^{+\alpha}}\eta$ is the same as saying that 0 is connected to $B_+\cap S$ in $[A_\eta]^{B_+}$; and saying that $-x_0^{-\alpha}$ is irrelevant for $\tau_{x_0^{-\alpha}}\eta$ is the same as saying that that 0 is not connected to $B_-\cap S$ in $[A_\eta]^{B_-}$.

In particular, setting z=0, $B=B_-$ and $B'=\Lambda_{3l}$, A_η satisfies the conditions of Claim 5.5. Therefore 0 is connected to ∂B_- in $[A_\eta]^{B'}$, which implies the result since $0 \in \Lambda_l \subset B_-$.

The probability estimate follows from Lemma 5.10.

Claim 5.14. Fix $\alpha \in \{2, \dots, d\}$, and a configuration η such that $\eta \notin \bigcup_{x_0 \in \Lambda_l^{\alpha}} E_{\alpha}(x_0)$ and $c_{0,e_{\alpha}}(\eta) = 1$. Then

$$\sum_{x \in \partial^{\alpha} \Lambda_{l}} \nabla_{0, e_{\alpha}} \tau_{x} f = 0.$$

Proof. We split the sum according to the projection of x on Λ_l^{α} –

$$\sum_{x \in \partial^{\alpha} \Lambda_{l}} \nabla_{0,e_{\alpha}} \tau_{x} f = \sum_{x_{0} \in \Lambda_{l}^{\alpha}} \left(\nabla_{0,e_{\alpha}} \tau_{x_{0}^{+\alpha}} f + \nabla_{0,e_{\alpha}} \tau_{x_{0}^{-\alpha}} f \right).$$

Fix one of these summands. If $-x_0^{+\alpha}$ is irrelevant for $\tau_{x_0^{+\alpha}}\eta$ and $-x_0^{-\alpha}$ is irrelevant for $\tau_{x_0^{-\alpha}}\eta$, then by the Proposition 5.8

$$\nabla_{0,e_{\alpha}}\tau_{x_0^{+\alpha}}f = \nabla_{0,e_{\alpha}}\tau_{x_0^{-\alpha}}f = 0.$$

Otherwise, since $\eta \notin E_{\alpha}(x_0)$, both must be relevant, hence

$$\nabla_{0,e_{\alpha}} \tau_{x_0^{+\alpha}} f = \frac{\eta(e_{\alpha}) - \eta(0)}{2(2l+1)^{d-1}} \times \begin{cases} -1 & x_0 \in \Lambda_-, \\ 1 & x_0 \in \Lambda_+; \end{cases}$$

$$\nabla_{0,e_{\alpha}} \tau_{x_0^{-\alpha}} f = \frac{\eta(e_{\alpha}) - \eta(0)}{2(2l+1)^{d-1}} \times \begin{cases} 1 & x_0 \in \Lambda_-, \\ -1 & x_0 \in \Lambda_+; \end{cases}$$

and their sum is 0.

Claim 5.15. Fix $\alpha \in \{2, \ldots, d\}$. Then

$$\mu \left[c_{0,e_{\alpha}} \left(\sum_{x \in \mathbb{Z}^d} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] \le C e^{-\lambda l}.$$

Proof. We split in the different cases described in Proposition 5.8:

$$\mu \left[c_{0,e_{\alpha}} \left(\sum_{x \in \mathbb{Z}^d} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] \leq 2\mu \left[c_{0,e_{\alpha}} \left(\sum_{x \in \Lambda_{2l+1} \setminus \Lambda_{2l-2}} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right] + 2\mu \left[c_{0,e_{\alpha}} \left(\sum_{x \in \partial^{\alpha} \Lambda_l} \nabla_{0,e_{\alpha}} \tau_x f \right)^2 \right].$$

We can bound the first term using Claim 5.11:

$$\mu \left[c_{0,e_{\alpha}} \left(\sum_{x \in \Lambda_{2l+1} \setminus \Lambda_{2l-2}} \mathbb{1}_{E(x,x-e_{\alpha})} Cl \right)^{2} \right] \leq Cl^{d} \mu \left[\sum_{x} \mathbb{1}_{E(x,x-e_{\alpha})} \right] \leq Ce^{-\lambda l}.$$

The second term, according to Claim 5.14, vanishes unless $\eta \in E_{\alpha}(x_0)$ for some $x_0 \in \Lambda_l^{\alpha}$, so we are left with an error term which by Claim 5.13 is bounded by

$$\mu\left[\left(\frac{|\partial^{\alpha}\Lambda_{l}|}{2(2l+1)^{d-1}}\right)^{2}\sum_{x_{0}\in\Lambda_{l}^{\alpha}}\mathbb{1}_{E_{\alpha}(x_{0})}\right]\leq Ce^{-\lambda l}.$$

The next step is to consider the direction e_1 :

Claim 5.16. Fix $x \in \partial^1 [-l, l]^d$. Then -x is irrelevant for $\tau_x \eta$ with probability smaller than $Ce^{-\lambda l}$.

Proof. For -x to be irrelevant it must be connected to one of $2(4l+1)^{d-1}$ sites on $\{0,1\} \times [-2l,2l]^{d-1}$. All of these sites are at distance at least l-2 from x, and the statement follows by direct application of Lemma 5.10.

Claim 5.17. For $e = e_1$,

$$\mu \left[c_{0,e} \left(\eta(e) - \eta(0) - \sum_{x \in \mathbb{Z}^d} \nabla_{0,e} \tau_x f \right)^2 \right] \le C e^{-\lambda l}.$$

Proof. The proof of the claim consists in showing that each site on $\partial^1 \Lambda_l$ contributes $\frac{\eta(e) - \eta(0)}{|\partial^1 \Lambda_l|}$ to the sum, up to a small error term.

First, using Proposition 5.8, we write

$$\mu \left[c_{0,e} \left(\eta(e) - \eta(0) - \sum_{x \in \mathbb{Z}^d} \nabla_{0,e} \tau_x f \right)^2 \right] \leq 2\mu \left[c_{0,e} \left(\sum_{x \in \Lambda_{2l+1} \setminus \Lambda_{2l-2}} \nabla_{0,e} \tau_x f \right)^2 \right]$$

$$+ 2\mu \left[c_{0,e} \left(\eta(e) - \eta(0) - \sum_{x \in \partial^1 \Lambda_l} \nabla_{0,e} \tau_x f \right)^2 \right].$$

The first term, just as in the proof of Claim 5.15, is bounded by $Ce^{-\lambda l}$ according to Claim 5.11.

In order to bound the second term, we start by assuming that all sites of $-\partial^1 \Lambda_l$ are relevant. In this case,

$$\sum_{x \in \partial^1 \Lambda_l} \nabla_{0,e} \tau_x f = \sum_{x \in \partial^1 \Lambda_l} \frac{\eta(e) - \eta(0)}{2(2l+1)^{d-1}} = \eta(e) - \eta(0),$$

SO

$$\mu \left[c_{0,e} \left(\eta(e) - \eta(0) - \sum_{x \in \partial^1 \Lambda_l} \nabla_{0,e} \tau_x f \right)^2 \mathbb{1}_{-\partial^1 \Lambda_l \subseteq \mathcal{R}} \right] = 0.$$

Finally, since sites of $\partial^1 \Lambda_l$ are at distance at least l from $\{0,1\} \times [-2l,2l]^{d-1}$, by Lemma 5.10 the probability that $\partial^1 \Lambda_l$ contains irrelevant sites is smaller than $Ce^{-\lambda l}$:

$$\mu \left[c_{0,e} \left(\eta(e) - \eta(0) - \sum_{x \in \partial^1 \Lambda_l} \nabla_{0,e} \tau_x f \right)^2 \mathbb{1}_{-\partial^1 \Lambda_l \not\subseteq \mathcal{R}} \right] \le C e^{-\lambda l}.$$

The claim thus follows by summing the contribution of the three terms.

All that is left is to combine claims 5.15 and 5.17, proving inequality (5.3) and hence the second part of Theorem 2.3. \Box

6. Further problems

- Prove convergence to a hydrodynamic limit without the soft constraint from a more restricted family of initial states (as in [13]).
- Improve the bounds on the diffusion coefficient, and in particular find matching upper and lower bound without a logarithmic correction. In the case of the closely related Fredrickson-Andersen model, where similar bounds have been obtained for the spectral gap ([18]), the logarithmic correction could be removed, and, moreover, the exact constant multiplying $1/(1-\rho)^{d-k+1}$ could be identified [14].
- Understand the hydrodynamic limit of more KCLGs. The comparison argument of Section 4 could be used in order to estimate the diffusion coefficient whenever an appropriate multi-step move could be constructed, and may be useful in lager generality than presented here.

• The bounds on the diffusion coefficient may have consequences other than the hydrodynamic limit – in general, we expect the correlation $\mu(\eta(0)e^{t\mathcal{L}}\eta(x))-\rho^2$ to behave like $\rho(1-\rho)(4\pi t\,D)^{-d/2}\,e^{-\frac{x^2}{4tD}}$ (see, e.g., [23]). It has been shown in [6] that, for x=0, this correlation decays at least as fast as $C(\log t)^5/t$ for some unidentified constant C, and any progress towards the predicted $\rho(1-\rho)(4\pi t\,D)^{-d/2}\,e^{-\frac{x^2}{4tD}}$ would be an interesting result.

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Appendix A. The gradient condition in cooperative models

In this appendix we will see that cooperative kinetically constrained lattice gas models (KCLGs) are non-gradient.

A general KCLG is a Markov process with configuration space $\Omega = \{0,1\}^{\mathbb{Z}^d}$, determined by a set of constraints giving each edge $(x,y) \in \mathcal{E}(\mathbb{Z}^d)$ a rate $c_{x,y}(\eta) \in \{0\} \cup [1,\infty)$, for any configuration $\eta \in \Omega$. We will make the following assumptions:

- (1) The model is homogeneous, i.e., the constraint is translation invariant.
- (2) The constraint $c_{x,y}$ depends only on the configuration outside x and y.
- (3) The constraints have finite range, i.e., $c_{x,y}$ depends only on the occupation of sites in the box $x + \Lambda_R$, where R is called the *range*.
- (4) The constraint is non-degenerate, i.e., for every edge (x, y) of \mathbb{Z}^d there exist a configuration η such that $c_{x,y}(\eta) > 0$ and η' such that $c_{x,y}(\eta') = 0$.
- (5) For fixed x, y the constraint $c_{x,y}(\eta)$ is a decreasing function of η , i.e., adding more empty sites could only help the constraint to be satisfied.

With such constraints, the process is given by a generator as in equation (2.2).

Definition A.1 (connected configurations). Fix a KCLG and two configurations η, η' . We say that η' is *connected* to η if there exists a sequence of configuration η_0, \ldots, η_T such that $\eta_0 = \eta$, $\eta_T = \eta'$, and for all $t \in \{0, \ldots, T-1\}$ there exist $x_{t+1} \sim y_{t+1}$ such that $\eta_{t+1} = \eta_t^{x_{t+1}, y_{t+1}}$, with $c_{x_{t+1}, y_{t+1}}(\eta_t) \geq 1$. For any fixed e, we say that η' is e-connected to η if, in addition, $y_{t+1} = x_{t+1} + e$ and $\eta_t(x_t) = 0$, namely, all transitions move a vacancy in the direction e (or, equivalently, a particle in the direction -e). Note that η' is connected to η if and only if η is connected to η' ; and η' is e-connected to η if and only if η is (-e)-connected to η' .

Definition A.2. Let $A \subseteq \mathbb{Z}^d$. The configuration η_A is defined as

$$\eta_A(x) = \begin{cases} 0 & x \in A, \\ 1 & \text{otherwise.} \end{cases}$$

KCLGs could be either *cooperative* or *non-cooperative* (see [6, Definition 1.1]). We remind here that a non-cooperative model is model in which there exists a *mobile cluster*, defined as follows:

Definition A.3 (mobile cluster). Let A be a finite non-empty subset of \mathbb{Z}^d . We say that A is a *mobile cluster* if:

- (1) For all $z \in \mathbb{Z}^d$, the configuration η_A is connected to the configuration η_{z+A} .
- (2) For every edge (x, y), there exists a translation $z \in \mathbb{Z}^d$ such that $c_{x,y}(\eta_{z+A}) \geq 1$.

Remark A.4. The second condition in the above definition is meant to allow, whenever a configuration contains an empty cluster, to move a particle across an edge (x,y) – first move the mobile cluster to its vicinity, guaranteeing that the constraint is satisfied, then exchange $\eta(x)$ with $\eta(y)$, and finally move the mobile cluster back to its initial position. It remains, however, possible, that while moving the mobile cluster the original occupation of x and y has changed, and the resulting configuration will not be $\eta^{x,y}$. Still, our result will also hold replacing this condition with the more restrictive one, that for all η in which the sites of A are empty, and for every edge (x,y), the configurations η and $\eta^{x,y}$ are connected using $O(\|x\|)$ exchanges.

Gradient models are interacting particle systems in which the current is a gradient of some local function, a property which significantly simplifies the analysis of their hydrodynamic limits (see, e.g., [15, Definition 2.5]). The purpose of this appendix is to prove the following result:

Theorem A.5. Cooperative KCLGs are non-gradient.

In order to prove that a model is non-gradient, we will consider the model on a torus, and show that the integral of the current does not always vanish –

Fact A.6. Consider a KCLG, and assume that for N large enough, there exists a configuration on the torus $\eta \in \{0,1\}^{\mathbb{Z}^d/N\mathbb{Z}^d}$, such that

$$\sum_{x,y\in\mathbb{Z}^d/N\mathbb{Z}^d} (x-y)(\eta(x)-\eta(y))c_{x,y}(\eta)\neq 0.$$

Then the model is non-gradient.

The construction of such η for a cooperative KCLG is based on the notion of reachable sites –

Definition A.7 (reachable sites and e-stretch). We say that a site is reachable from a configuration η if it is empty for some η' which is connected to η . For $e \in \{\pm e_1, \ldots, \pm e_d\}$ we say that a site is e-reachable for a configuration η if it is empty for some η' which is e-connected to η . The e-stretch of η is defined as

$$\sup \{e \cdot x : x \text{ is } e\text{-reachable}\}.$$

By the definition of non-cooperative models, it is immediate that if η contains a mobile cluster then for every site x there exists η' connected to η for which $\eta'(x) = 0$. In the next proposition we will see that if we require e-connectivity the converse is also true –

Proposition A.8. Assume that for all $e \in \{\pm e_1, \ldots, \pm e_d\}$ there exists a finite subset A_e of \mathbb{Z}^d , such that the e-stretch of η_{A_e} is infinite. Then the model is non-cooperative.

Before proving this proposition, we will see how it implies Theorem A.5. Consider a cooperative KCLG, so by Proposition A.8 for some $e \in \{\pm e_1, \dots, \pm e_d\}$ and any $L \in \mathbb{N}$, configurations that are entirely filled outside Λ_L have finite e-stretch. We will assume without loss of generality that $e = e_1$.

Since the model is non-degenerate, there exists a configuration η_0 for which $c_{0,e_1}(\eta_0)=1$. Since the model has finite range R, we may assume that this configuration is entirely filled outside Λ_R ; and since the constraint does not depend on the occupation at 0 and e_1 we assume $\eta_0(0)=0$ and $\eta_0(e_1)=1$. We will now construct a sequence of configuration starting at η_0 , so that η_{i+1} is obtained from η_i by moving a 0 to the right, i.e., $\eta_{i+1}=\eta_i^{x_i,x_i+e_1}$ for some x_i such that $c_{x_i,x_i+e_1}(\eta_i)>0$, $\eta_i(x_i)=0$, and $\eta_i(x_i+e_1)=1$. When, for some i, more than one such choice of x is possible, we choose one arbitrarily. We stop when none of the sites satisfy the required conditions.

Since the e_1 -stretch is finite the construction must stop at some step $n < \infty$. On the other hand, we chose η_0 such that $c_{0,e_1}(\eta_0) \ge 1$, $\eta_0(0) = 0$, and $\eta_0(e_1) = 1$, so $n \ge 1$. Hence, for the configuration $\eta = \eta_n$, for all $x \in \mathbb{Z}^d$

$$c_{x,x+e_1}(\eta)(1-\eta(x))\eta(x+e_1)=0,$$

but for $x^* = x_{n-1}$ we know that

$$c_{x^*,x^*+e_1}(\eta)\eta(x^*)(1-\eta(x^*+e_1)) \ge 1.$$

That is,

$$\sum_{x \in \mathbb{Z}^d} (\eta(x) - \eta(x + e_1)) c_{x, x + e_1}(\eta) \ge 1.$$

Since η is filled outside Λ_{R+n} , we may as well sum over x in a large enough torus $\mathbb{Z}^d/(100R+n)\mathbb{Z}^d$. Therefore, by Fact A.6, the model is indeed non-gradient.

We return to the proof of Proposition A.8.

Claim A.9. Fix a finite non-empty $A \subset \mathbb{Z}^d$, and $e \in \{\pm e_1, \dots, \pm e_d\}$. Assume that the e-stretch of η_A is infinite. Then there exists a finite non-empty $A' \subset \mathbb{Z}^d$ and a strictly positive integer n, such that $\eta_{A'}$ is e-connected to $\eta_{ne+A'}$.

Proof. First, we may assume without loss of generality that A has the minimal possible size, among sets for which the e-stretch of η_A is infinite; and for notational convenience we also assume $e = e_1$. Set k = |A|, and fix L such that $A \subset \Lambda_L$.

We will start by showing the following property:

Claim A.10. For all j < k, there exists $s^{(j)}$ such that for all $B \subset (-\infty, 0] \times \mathbb{Z}^{d-1}$ with |B| = j, the e_1 -stretch of η_B is at most $s^{(j)}$. In particular, there exists $L^{(j)}$ such that the maximal possible e_1 -stretch for such a set is obtained for some $B \subset [-L^{(j)}, 0] \times \mathbb{Z}^{d-1}$.

Proof. For j=1 choosing $s^{(1)}=L^{(1)}=0$ suffices since no particle could move. For j>1, let $L^{(j)}=j(h^{(j-1)}+R)$ and $s^{(j)}$ the maximal e_1 -stretch of η_B for any $B\subset [-L^{(j)},0]\times \mathbb{Z}^{d-1}$. Note that $s^{(j)}$ is well defined since particles cannot move in directions orthogonal to e_1 , so we may assume without loss of generality that $B\subset [-L^{(j)},0]\times [-jR,jR]^{d-1}$; and it is finite since j< k.

Assume now that for some $B \subset (-\infty,0] \times \mathbb{Z}^{d-1}$ of size j the e_1 -stretch of η_B is more than $s^{(j)}$. We can assume without loss of generality that $0 \in B$, and by construction there must be a site $x \in B$ outside $[-L^{(j)},0] \times \mathbb{Z}^{d-1}$. Due to our choice of $L^{(j)}$, the set B could be separated by a strip of width $h^{(j-1)} + R$, namely, there exists $n \in \mathbb{Z}$ such that

$$B = B_{-} \cup B_{+},$$

$$B_{-} \subset (-\infty, n] \times \mathbb{Z}^{d},$$

$$B_{+} \subset (n + h^{(j-1)} + R, 0] \times \mathbb{Z}^{d}.$$

However, since the e_1 -stretch of η_{B_-} is at most $h^{(j-1)}$, it would never be able to influence transitions to the right of $n + h^{(j-1)} + R$, thus the e_1 -stretch of B cannot be larger than that of B_- , which is a contradiction.

As a result of this claim, there exists $s < \infty$, such that for any set B of size strictly less than k, the e_1 -stretch of B is at most s plus its maximal e_1 coordinate.

Since the e_1 -stretch of η_A is infinite, there exists an e_1 -reachable site x with $e \cdot x > \binom{(2L+1)^{d-1}k(s+R)}{k} + s + 1$. Consider a sequence of T flips which empties that site. We denote the set of empty sites at step t by A_t , so that $A_0 = A$ and $A_T \ni x$; and a_t denotes the rightmost coordinate of A_t (i.e., $a_t = \max_{y \in A_t} \{e_1 \cdot y\}$). Assume now that at some time t we are able to identify a non-empty set \tilde{A}_t whose rightmost coordinate is \tilde{a}_t , such that all sites of $A_t \setminus \tilde{A}_t$ are at least s + R to the right of \tilde{a}_t , i.e., $a_t < e_1 \cdot y - s - R$ for all $y \in A_t \setminus \tilde{A}_t$. We then know that the 0's coming from \tilde{A}_t will never be able to reach distance R from the sites of $A_t \setminus \tilde{A}_t$, thus the set $A_t \setminus \tilde{A}_t$ moves as if these sites were filled. In particular, it could not go further than distance s, hence s0 (s1) s2. That means that for at least s3 (s2) s3 times s4 with different values of s4,

$$A_t \subset [a_t - k(s+R), a_t] \times [-L, L]^{d-1}$$
.

This box has volume $(2L+1)^{d-1}k(s+R)$, so by the pigeonhole principle there exist t and t' with $a_t < a_{t'}$ such that $A_t - a_t e_1 = A_{t'} - a_{t'} e_1$. This finishes the proof by taking $A' = A_t - a_t e_1$ and $a_t = a_{t'} - a_t$, and using the translation invariance of the model.

Claim A.11. Fix any finite $B \subset \mathbb{Z}^d$ and $e \in \mathbb{Z}^d$, and assume that there exists a finite non-empty $A \subset \mathbb{Z}^d$ such that the e-stretch of η_A is infinite. Then there exist a finite non-empty set $A' \subset \mathbb{Z}^d$ such that for all $m \in \mathbb{N}$, the configuration $\eta_{A'}$ is e-connected to a configuration η_m in which all the sites of me + B are empty. Moreover, we can assume that no site after me + B is empty, i.e., $\eta_m(x) = 1$ whenever $x \cdot e > m + \sup_{u \in B} y \cdot e$.

Proof. By the Claim A.9 there exists $L \in \mathbb{N}$, $A'' \subset \Lambda_L$, and $n \in \mathbb{N}$, such that $\eta_{A''}$ is e-connected to $\eta_{ne+A''}$. Note that we may, equivalently, choose any A'' which is a translation of A_{η} for any η in the path connecting $\eta_{A''}$ with $\eta_{ne+A''}$. We will therefore assume without loss of generality that $0 \in A''$, but $e \cdot x < 0$ for all $x \in A \setminus \{0\}$.

Denote $B = \{b_1, \dots, b_k\}$, with $e \cdot b_1 \ge \dots \ge e \cdot b_k$, and consider the union

$$A_0 = \bigcup_{i=1}^k (b_i + A'' - inLe).$$

This union is disjoint, since $A'' \subset \Lambda_L$, and by repeating L times the sequence of flips required to move A'' to ne + A'', we can move $b_1 + A'' - nLe$ to $b_1 + A''$, reaching a configuration in which b_1 is empty. Then, repeating this sequence again 2L times we can move $b_2 + A'' - 2nLe$ to $b_2 + A''$. This is allowed since during the first sequence we do not changes the configuration at the sites of $b_2 + A'' - 2nLe$; and the in the resulting configuration both b_1 and b_2 are empty. We continue in the same manner, until we reach a configuration η'_0 in which the sites of B are all empty.

Consider now for j = 0, ..., n-1 the set

$$A_i = A_0 - knLje + je$$
.

As before, applying repeatedly the sequence that allowed us to move A'' we can reach a configuration η_j (connected to η'_{A_j}) in which the sites of je+B are empty. Furthermore, A_j and $A_{j'}$ are disjoint for $j \neq j'$, so, indeed, taking

$$A' = \bigcup_{j=0}^{n-1} A_j,$$

for $j=0,\ldots,n-1$, the configuration $\eta_{A'}$ is e-connected to a configuration η_j for which the sites of je+B are empty. Finally, since A' is a disjoint union of copies of A'', we can translate each of them by ne, and if we do that in the right order (starting with $b_1+A''-nLe$ and ending with $b_k+A''-knL(n-1)e+(n-1e)$) they will never intersect. Hence $\eta_{ne+A'}$ is e-connected to $\eta_{A'}$, and the result follows.

Claim A.12. Fix $e \in \{\pm e_1, \dots, \pm e_d\}$ and $L \in \mathbb{N}$. Assume that there exists a finite non-empty $A \subset \mathbb{Z}^d$ such that the e-stretch of η_A is infinite. Then there exists L' and $A' \subset \Lambda_{L'}$ such that for all $x \in [L', \infty] \times [-L, L]^{d-1}$ and every configuration η for which the sites of A' are empty, η is connected to $\eta^{x,x+e}$.

Proof. We assume without loss of generality that $e = e_1$. The first observation needed in order to prove this claim, is that there is a configuration for which the constraint $c_{x,x+e_1}$ is satisfied, but none of the sites to the right of x are empty, i.e., $x + [1, \infty] \times \mathbb{Z}^{d-1}$ is entirely occupied. This is true since, if the e_1 -stretch of η_A is infinite for finite A, at some point the rightmost 0 has to move to the right.

We then find a finite non-empty $B_0 \subset [-\infty,0] \times \mathbb{Z}^{d-1} \setminus \{0\}$ such that $c_{0,e_1}(\eta_{B_0})=1$. Let

$$B = \bigcup_{z \in \{0\} \times [-L,L]^{d-1}} (z + B_0).$$

Then, in particular, $c_{x,x+e_1}(\eta_B) = 0$ for $x \in \{0\} \times [-L,L]^{d-1}$.

We now apply Claim A.11 to find a finite non-empty set $A' \subset \mathbb{Z}^d$ such that for all $m \in \mathbb{N}$, the configuration $\eta_{A'}$ is e-connected to a configuration η_m in which all the sites of me + B are empty. We define L' such that $A' \subset \Lambda_{L'}$, and then, for every $x \in [L', \infty] \times [-L, L]^{d-1}$, taking $m = e_1 \cdot x$ yields $c_{x,x+e_1}(\eta_m) = 1$. Therefore, if we take any configuration η for which A' is empty, by performing the same transitions that connected $\eta_{A'}$ to η_m , we reach a configuration for which $c_{x,x+e_1} = 1$. Note that this is done without changing the configuration neither at x nor at $x + e_1$. We then exchange x and $x + e_1$, and fold back all the transitions we have done before, reaching the configuration $\eta^{x,x+e_1}$.

Claim A.13. Assume that for all $e \in \{e_1, \dots, e_d\}$ there exists a finite set $A_e \subset \mathbb{Z}^d$ such that the e-stretch of η_{A_e} is infinite, and fix $e' \in \{e_1, \dots, e_d\}$. Then there exists $L \in \mathbb{N}$ and $A \subset \Lambda_L$ such that for any η in which the sites of A are empty, and any $x \in [L+1,\infty]^d$, the configuration $\eta^{x,x+e'}$ is connected to η .

Proof. Without loss of generality we fix $e=e_1$. By Claim A.12 we can define $L_1\in\mathbb{N}$ and $A_1\subset\Lambda_{L_1}$ be such that for all $x_1\in[L_1,\infty]\times\{0\}^{d-1}$ and every configuration η for which the sites of A_1 are empty, η is connected to η^{x_1,x_1+e_1} . Using Claim A.11 we can find $L_2\in\mathbb{N}$ and $A_2\in\Lambda_{L_2}$ such that, for every $x_2\in\{0\}\times[L_2,\infty]\times\{0\}^{d-1}$, the configuration η_{A_2} is connected to a configuration η in which the sites of x_2+A_1 are empty, and during the sequence of configurations connecting the two only edges of $[-\infty,-L_2]^d$ were flipped. We continue in the same manner, for $i=1,\ldots,d$, to construct L_i and $A_i\subset\Lambda_{L_i}$ such that for all $x_i\in\{0\}^{i-1}\times[L_i,\infty]\times\{0\}^{d-i}$, the configuration η_{A_i} is connected to a configuration in which the sites of x_i+A_{i-1} are empty, and during the sequence of configurations connecting the two only edges of $[-\infty,-L_i]^d$ were flipped.

Let $L=L_d$, $A=A_d$, and fix η in which the sites of A are empty and $x\in [L+1,\infty]^d$. We write $x=x_1+\cdots+x_d$ for $x_i\in\{0\}^{i-1}\times[L_i,\infty]\times\{0\}^{d-i}$. By our construction of A, η is connected to a configuration η' in which the set $A_1+x_2+\cdots+x_d$ is empty, and during the sequence of configurations connecting the two the sites x and $x+e_1$ remained untouched. Then, by the construction of A_1 , we can connect η' to $\eta'^{x,x+e_1}$. All that is left is to rewind the steps leading to η' , and the proof is complete.

Claim A.14. Assume that for all $e \in \{e_1, \dots, e_d\}$ there exists a finite set $A_e \subset \mathbb{Z}^d$ such that the e-stretch of η_{A_e} is infinite. Then there exists $L \in \mathbb{N}$ and $A \subset \Lambda_L$ such that for any η in which the sites of A are empty, any $x \in [L+1,\infty]^d$, and any $e' \in \{e_1,\dots,e_d\}$, the configuration $\eta^{x,x+e'}$ is connected to η .

Proof. The only difference between this claim and Claim A.13 is that now e' is chosen after A is fixed. In order to achieve that, we apply Claim A.13 d times, with $e' = e_i$ for all $i \in \{1, \ldots, d\}$, obtaining d numbers $L_1, \ldots, L_d \in \mathbb{N}$ and d sets $A_1 \in \Lambda_{L_1}, \ldots, A_d \in \Lambda_{L_d}$. Taking $L = \max_i L_i$ and $A = \bigcup_{i=1}^d A_i$ will suffice – fix η in which the sites of A are empty, every $x \in [L+1, \infty]^d$ and $i \in \{1, \ldots, d\}$. In particular $x \in [L_i + 1, \infty]^d$, and that the sites of A_i are empty in η , so by construction of A_i we know that $\eta^{x,x+e_i}$ is connected to η .

We are now ready to prove Proposition A.8.

Proof of Proposition A.8. We assume that for all $e \in \{\pm e_1, \dots, \pm e_d\}$ there exists a finite set $A_e \subset \mathbb{Z}^d$ such that the e-stretch of η_{A_e} is infinite, and construct a mobile cluster A.

First, use Claim A.14 in order to find $L_+ \in \mathbb{N}$ and $A_+ \subset \Lambda_{L_+}$ such that for any η in which the sites of A_+ are empty, any $x \in [L_+ + 1, \infty]^d$, and any $e \in \{e_1, \dots, e_d\}$, the configuration $\eta^{x,x+e}$ is connected to η . Similarly (by flipping \mathbb{Z}^d), we can find $L_- \in \mathbb{N}$ and $A_- \subset \Lambda_{L_-}$ such that for any η in which the sites of A_- are empty, any $x \in [-\infty, -L_- - 1]^d$, and any $e \in \{-e_1, \dots, -e_d\}$, the configuration $\eta^{x,x+e}$ is connected to η . It will be more convenient to consider translations of these sets,

$$A'_{+} = A_{+} - (L_{+} + 2)e_{1} - \dots - (L_{+} + 2)e_{d},$$

$$A'_{-} = A_{-} + (L_{-} + 2)e_{1} + \dots + (L_{-} + 2)e_{d}.$$

This way, for any η in which the sites of A'_+ are empty, any $x \in [2,\infty]^d$, and any $e \in \{\pm e_1,\ldots,\pm e_d\}$, the configuration $\eta^{x,x+e}$ is connected to η ; and for any η in which the sites of A'_- are empty, any $x \in [-\infty,-2]^d$, and any $e \in \{\pm e_1,\ldots,\pm e_d\}$, the configuration $\eta^{x,x+e}$ is connected to η . Let

$$A = A'_{+} \cup A'_{-}$$

We will show that it is a mobile cluster. Since already A'_+ allows us to flip edges is its vicinity, we only need to show that η_A is connected to η_{e+A} for all $e \in \{\pm e_1, \dots, \pm e_d\}$. To do that, we note that, since the sites of A'_- are all in $[2, \infty]$, the configuration η_A is connected to $\eta_{A'_+\cup(e+A'_-)}$. In this new configuration the sites of $e+A'_-$ are empty, and since the sites of A'_+ are all in $[-\infty, -2]^d + e$ it is connected to $\eta_{(e+A'_+)\cup(e+A'_-)} = \eta_{e+A}$.

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