



Homogeneous nucleation for two-dimensional Kawasaki dynamics

Simone Baldassarri, Alexandre Gaudillière, Frank Den Hollander, Francesca Romana Nardi, Enzo Olivieri, Elisabetta Scoppola

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Homogeneous nucleation for two-dimensional Kawasaki dynamics

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Abstract

This is the third in a series of three papers in which we study a lattice gas subject to Kawasaki dynamics at inverse temperature $\beta > 0$ in a large finite box $\Lambda_\beta \subset \mathbb{Z}^2$ whose volume depends on β . Each pair of neighbouring particles has a *negative binding energy* $-U < 0$, while each particle has a *positive activation energy* $\Delta > 0$. The initial configuration is drawn from the grand-canonical ensemble restricted to the set of configurations where all the droplets are subcritical. Our goal is to describe, in the metastable regime $\Delta \in (U, 2U)$ and in the limit as $\beta \rightarrow \infty$, how and when the system nucleates, i.e., creates a critical droplet somewhere in Λ_β that subsequently grows by absorbing particles from the surrounding gas.

In the first paper we showed that subcritical droplets behave as quasi-random walks. In the second paper we used the results in the first paper to analyse how subcritical droplets form and dissolve on multiple space-time scales when the volume is *moderately large*, namely, $|\Lambda_\beta| = e^{\theta\beta}$ with $\Delta < \theta < 2\Delta - U$. In the present paper we consider the setting where the volume is *very large*, namely, $|\Lambda_\beta| = e^{\Theta\beta}$ with $\Delta < \Theta < \Gamma - (2\Delta - U)$, where Γ is the energy of the critical droplet in the local model with fixed volume, and use the results in the first two papers to identify the nucleation time and the tube of typical trajectories towards nucleation. We will see that in a very large volume critical droplets appear more or less independently in boxes of moderate volume, a phenomenon referred to as *homogeneous nucleation*. One of the key ingredients in the proof is an estimate showing that no information can travel between these boxes on relevant time scales. Prior to nucleation, the dynamics inside the moderately large boxes spends most of its time in configurations consisting of a single quasi-square surrounded by free particles, and makes transitions between these configurations at rates that depend on the linear sizes of the quasi-square in a computable manner.

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1 Introduction and main results

1.1 Background

The present paper is the third in a series of three papers dealing with *nucleation* in a *super-saturated lattice gas* in a large volume. In particular, we consider a two-dimensional lattice gas at low density and low temperature that evolves under Kawasaki dynamics, i.e., particles hop around randomly subject to hard-core repulsion and nearest-neighbour attraction. We are interested in how the gas *nucleates* in large volumes, i.e., how the particles form and dissolve subcritical droplets until they manage to build a critical droplet that is large enough to trigger the nucleation.

In the first paper [6] we showed that subcritical droplets behave as quasi-random walks. In the second paper [1] we used the results in the first paper to analyse how subcritical droplets form and dissolve *on multiple space-time scales* when the volume is *moderately large*. In large volumes the evolution of the Kawasaki lattice gas is much more involved than in finite volumes treated earlier [9], [10]. The main difficulty in analysing the metastable behaviour is a proper description of the interaction between the droplets and the surrounding gas. As part of the nucleation process, droplets grow and shrink by exchanging particles with the gas around them, as is typical for conservative dynamics.

Our focus is on both the *nucleation time* and the *tube of typical trajectories prior to nucleation*. In Section 1.4 we discuss the importance of the results obtained in the present paper and the two preceding papers, and their relevance within the literature on metastability of interacting particle systems. To derive our main theorems we distinguish between *moderate volumes* and *large volumes*. We first consider moderate volumes and use the results obtained in [1] to describe the escape from metastability. In particular, we show that this escape occurs via nucleation rather than via coalescence. Subsequently, we consider large volumes and exploit the work in [7] that derives an upper bound on the velocity of front propagation, from which we deduce that essentially no information can travel between distant volumes on appropriate space-time scales. This in turn implies that the nucleation in large volumes is *homogeneous*, i.e., occurs independently and with equal probability in disjoint moderate volumes that are essentially independent.

We refer the reader to [1] for a description of what is achieved in the three papers together (see [1, Items (1)–(7) in Section 1.1]) and what are the key challenges associated with Kawasaki dynamics in large volumes (see [1, Remarks 1.1–1.3]). For more background on metastability for interacting particle systems, we refer the reader to the monographs [11], [2] and references therein.

1.2 Kawasaki dynamics

• **Hamiltonian, generator and equilibrium.** Let $\beta > 0$ denote the inverse temperature. Let $\Lambda_\beta \subset \mathbb{Z}^2$ be the square box with volume

$$|\Lambda_\beta| = e^{\Theta\beta}, \quad \Theta > 0, \quad (1.1)$$

centered at the origin with periodic boundary conditions. With each $x \in \Lambda_\beta$ associate an occupation variable $\eta(x)$, assuming the values 0 or 1. A lattice gas configuration is denoted by $\eta \in \mathcal{X}_\beta = \{0, 1\}^{\Lambda_\beta}$. With each configuration η associate an energy given by the Hamiltonian

$$H(\eta) = -U \sum_{\{x,y\} \in \Lambda_\beta^*} \eta(x)\eta(y), \quad (1.2)$$

where Λ_β^* denotes the set of bonds between nearest-neighbour sites in Λ_β , i.e., there is a *binding energy* $-U < 0$ between neighbouring particles. Let

$$|\eta| = \sum_{x \in \Lambda_\beta} \eta(x) \quad (1.3)$$

be the number of particles in Λ_β in the configuration η , and let

$$\mathcal{X}_N = \{\eta \in \mathcal{X}_\beta : |\eta| = N\} \quad (1.4)$$

be the set of configurations with N particles.

We define Kawasaki dynamics as the continuous-time Markov chain $X = (X(t))_{t \geq 0}$ with state space \mathcal{X}_N given by the generator

$$(\mathcal{L}f)(\eta) = \sum_{\{x,y\} \in \Lambda_\beta^*} c(x,y,\eta)[f(\eta^{x,y}) - f(\eta)], \quad \eta \in \mathcal{X}_\beta, \quad (1.5)$$

where

$$\eta^{x,y}(z) = \begin{cases} \eta(z) & \text{if } z \neq x, y, \\ \eta(x) & \text{if } z = y, \\ \eta(y) & \text{if } z = x, \end{cases} \quad (1.6)$$

and

$$c(x,y,\eta) = e^{-\beta[H(\eta^{x,y}) - H(\eta)]_+}. \quad (1.7)$$

Equations (1.5)–(1.7) represent the standard *Metropolis dynamics* associated with H , and is *conservative* because it preserves the number of particles, i.e., $|X(t)| = |X(0)|$ for all $t > 0$. The *canonical Gibbs measure* μ_N defined as

$$\mu_N(\eta) = \frac{e^{-\beta H(\eta)} 1_{\mathcal{X}_N}(\eta)}{Z_N}, \quad Z_N = \sum_{\eta \in \mathcal{X}_N} e^{-\beta H(\eta)}, \quad \eta \in \mathcal{X}_\beta, \quad (1.8)$$

is the reversible equilibrium of this stochastic dynamics for any N :

$$\mu_N(\eta) c(x,y,\eta) = \mu_N(\eta^{x,y}) c(x,y,\eta^{x,y}). \quad (1.9)$$

We augment the energy $H(\eta)$ of configuration η by adding a term $\Delta|\eta|$, with $\Delta > 0$ an *activation energy* per particle. This models the presence of an external reservoir that keeps the density of particles in Λ_β fixed at $e^{-\beta\Delta}$.

• **Subcritical, critical and supercritical droplets.** The initial configuration is chosen according to the *grand-canonical Gibbs measure* restricted to the set of subcritical droplets. More precisely, denote by

$$\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil \quad (1.10)$$

the critical length introduced in [9] for the *local model* where $\Lambda_\beta = \Lambda$ does not depend on β (see Fig. 1). The energy of the critical droplet in the local model equals

$$\Gamma = -U[(\ell_c - 1)^2 + \ell_c(\ell_c - 2) + 1] + \Delta[\ell_c(\ell_c - 1) + 2] \quad (1.11)$$

By defining a cluster as a connected component of nearest-neighbours particles, define

$$\mathcal{R} = \{\eta \in \mathcal{X}_\beta : \text{all clusters of } \eta \text{ have volume at most } \ell_c(\ell_c - 1) + 2\} \quad (1.12)$$

and put

$$\mu_{\mathcal{R}}(\eta) = \frac{e^{-\beta[H(\eta) + \Delta|\eta|]}}{Z_{\mathcal{R}}} 1_{\mathcal{R}}(\eta), \quad \eta \in \mathcal{X}_\beta, \quad (1.13)$$

where

$$Z_{\mathcal{R}} = \sum_{\eta \in \mathcal{R}} e^{-\beta[H(\eta) + \Delta|\eta|]} \quad (1.14)$$

is the normalising partition sum. Write P_η for the law of X given $X(0) = \eta$. The initial configuration $X(0)$ is drawn from $\mu_{\mathcal{R}}$, i.e., the initial law is $P_{\mu_{\mathcal{R}}} = \int_{\mathcal{X}_\beta} \mu_{\mathcal{R}}(d\eta) P_\eta$.

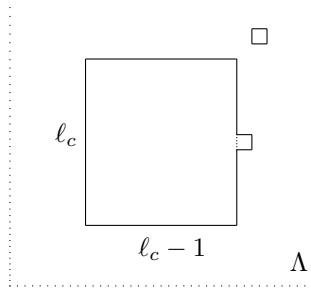


Figure 1: A critical droplet in a finite volume Λ : a protocritical droplet, consisting of an $(\ell_c - 1) \times \ell_c$ quasi-square with a single protuberance attached to one of the longest sides, and a free particle nearby. When the free particle attaches itself to the protuberance, the droplet becomes supercritical.

We will be interested in the regime

$$\Delta \in (U, 2U), \quad \beta \rightarrow \infty. \quad (1.15)$$

which corresponds to *metastable behaviour*. In this regime, droplets with side length smaller than ℓ_c have a tendency to shrink, while droplets with a side length larger than ℓ_c have a tendency to grow. We will refer to the former as *subcritical droplets* and to the latter as *supercritical droplets*.

1.3 Main theorems

• **Nucleation time.** Let

$$\tau_{\mathcal{R}^c} = \inf\{t \geq 0 : X(t) \notin \mathcal{R}\}. \quad (1.16)$$

Theorem 1.1 [Nucleation time] *Subject to (1.15), for every $\Delta < \Theta < \Gamma - (2\Delta - U)$ and every $\delta > 0$,*

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln P_{\mu_{\mathcal{R}}} \left(\tau_{\mathcal{R}^c} \notin \left[\frac{e^{\Gamma\beta}}{|\Lambda_\beta|} e^{-\delta\beta}, \frac{e^{\Gamma\beta}}{|\Lambda_\beta|} e^{\delta\beta} \right] \right) < 0. \quad (1.17)$$

• **Tube of typical trajectories.** We define *quasi-squares* as clusters of sizes $\ell_1 \times \ell_2$ in the set

$$\text{QS} = \{(\ell_1, \ell_2) \in \mathbb{N}^2 : \ell_1 \leq \ell_2 \leq \ell_1 + 1\}$$

and let $\lambda(\beta)$ be an unbounded but slowly increasing function of β satisfying

$$\lambda(\beta) \log \lambda(\beta) = o(\log \beta), \quad \beta \rightarrow \infty, \quad (1.18)$$

e.g. $\lambda(\beta) = \sqrt{\log \beta}$.

Theorem 1.2 [Tube of typical trajectories] *Subject to (1.15), for every $\Delta < \Theta < \Gamma - (2\Delta - U)$ and starting from the initial measure $\mu_{\mathcal{R}}$, with a probability that is exponentially close to 1 the system nucleates a growing cluster that visits the full increasing sequence of quasi-squares, and after the exit from \mathcal{R} grows in the same way up to a $\sqrt{\lambda(\beta)/8} \times \sqrt{\lambda(\beta)/8}$ -square. This square is reached after the exit from \mathcal{R} in a time that is exponentially smaller than the time needed to reach \mathcal{R}^c .*

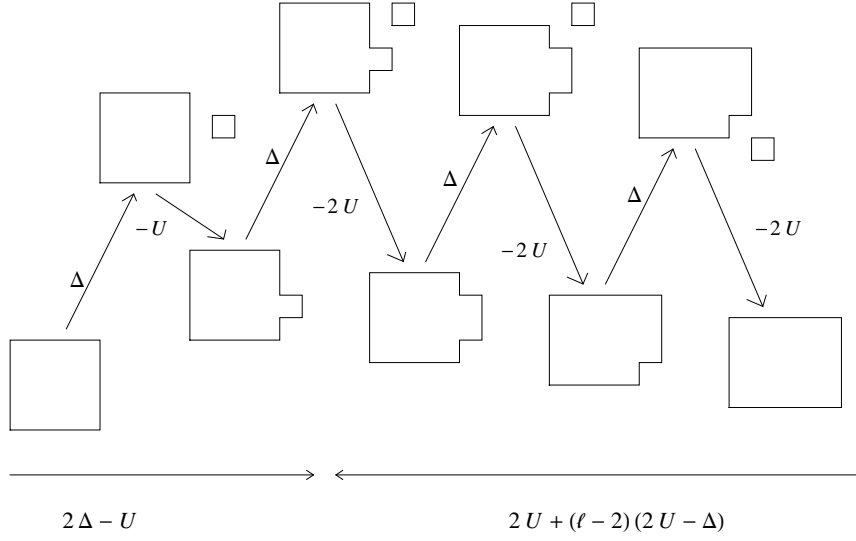


Figure 2: Cost of adding or removing a row of length ℓ in a finite volume.

In the proof of Theorems 1.1 and 1.2 the parameter Θ will play a crucial role. Indeed, in Section 5 we will see that the analysis for *large volumes*, i.e., $\Theta > \theta$, can be reduced to that for *moderate volumes*, i.e., $\Theta \leq \theta$, by using their near-independence, where the parameter θ is defined as follows. Let $r(\ell_1, \ell_2)$ be the *resistance* of the $\ell_1 \times \ell_2$ quasi-square with $1 \leq \ell_1 \leq \ell_2$ given by (see Fig. 2)

$$r(\ell_1, \ell_2) = \min\{(2U - \Delta)\ell_1 - U + 2\Delta - U, 2\Delta - U\}. \quad (1.19)$$

Let $\theta = 2\Delta - U - \gamma$ be the resistance of the largest subcritical quasi-square. Since this quasi-square has sizes $(\ell_c - 1) \times \ell_c$, we have $\theta = 2U + (\ell_c - 3)(2U - \Delta)$, and so

$$\gamma = (\Delta - U) - (\ell_c - 2)(2U - \Delta) > 0. \quad (1.20)$$

Remark 1.3 With the techniques developed in [1] it is possible to show that the growing cluster in Theorem 1.2 triggering the nucleation is *wandering*, i.e., when the cluster has size $\ell_1 \times \ell_2$ with $|\ell_1 - \ell_2| \leq 1$ it exits any finite box around it with a volume that does not depend on β within a time of order $e^{r(\ell_1, \ell_2)\beta}$.

1.4 Conclusion

1. Theorems 1.1–1.2 provide a detailed description of the *escape from metastability* for Kawasaki dynamics in moderate and large volumes, in particular, how subcritical droplets form and dissolve *on multiple space-time scales*, and concludes the work initiated in [6] and [1]. The escape occurs *via nucleation and not via coalescence*. The nucleation is *homogeneous*, in the sense that a supercritical droplet appears for the first time more or less independently and with equal probability in disjoint boxes of moderate volume, and trigger the nucleation. The configurations in moderately large boxes behave as if they are *essentially independent* and as if the surrounding gas is *ideal*. The asymptotics of the nucleation time is identified on a time scale that is exponential in β and depends on an *entropic factor* related to the size of the box. We find that the

probability to deviate from the lower bound is exponentially small in β , while the probability to deviate from the upper bound is $\text{SES}(\beta)$, where we write $\text{SES}(\beta)$ for any function of β that decays to zero faster than any exponential of β . This asymmetry is due to the fact that nucleation after a given time can only happen when an exponentially large number of particles does not manage to trigger the nucleation before that time.

2. In [3] the average nucleation time was identified including a *sharp prefactor*, but only for a specific starting distribution called *the last-exit-biased distribution*, which is tuned to the potential-theoretic approach to metastability. This distribution is *unphysical*, in the sense that it is unclear how to prepare a low-density gas so that it starts from this distribution. In contrast, the *Gibbs distribution restricted to subcritical droplets* in (1.13) employed here as starting distribution is *physical*, because it can be obtained by rapidly cooling down a low-density gas. With extra work the prefactor found in [3] can in principle be obtained here as well, but we do not push this point.

3. In [8] the transitions between the different ground states are analysed in a regime where there is no pure-gas metastable state and the process is started from a large square droplet with no surrounding gas. In that setting the interaction between the gas and the droplet, which is at the core of the present work, is largely avoided.

4. Our theorems only concern the *initial phase* of the nucleation, until the critical droplet grows into a droplet that is roughly $\sqrt{\lambda(\beta)}$ times the size of the critical droplet. They provide no information on what happens *afterwards*, when the droplet grows even further and becomes macroscopically large. In that regime the gas around the droplet becomes depleted, smaller droplets move around and coalesce into larger droplets, etc. It remains a major challenge to describe what precisely happens in this regime, which lies *beyond* metastability.

Outline. The rest of the paper is organised as follows. In Section 2 we recall some definitions and notations that will be used throughout the paper. In Section 3 we provide the lower bound for the nucleation time for all $\Delta < \Theta < \Gamma - (2\Delta - U)$, while in Section 4 (respectively, Section 5) we provide the upper bound for the nucleation time and the tube of typical trajectories for all $\Delta < \Theta \leq \theta$ (respectively, $\theta < \Theta < \Gamma - (2\Delta - U)$). In Sections 3 and 4 we use technical arguments that are explained in more detail in [1], and focus on the relevant estimates only. The lower bound for the nucleation time can be obtained for arbitrarily large volumes because it requires the construction of a nucleation event only. The upper bound is much harder.

2 Definitions and notations

In this section we introduce some definitions and notations that will be needed throughout the sequel.

Definition 2.1

1. As in [6], [1], α and d are two positive parameters that can be chosen as small as desired, and $\lambda(\beta)$ is an unbounded but slowly increasing function of β that satisfies (1.18). Moreover, C^* is a positive parameter that can be chosen as large as desired. Once chosen, α , d , λ and C^* are fixed. We write $O(\delta)$, $O(\alpha)$ and $O(d)$ for quantities with an absolute value that can be bounded by a constant times $|\delta|$, $|\alpha|$ and $|d|$, for small enough values of these parameters. We write $O(\delta, \alpha, d)$ for the sum of three such quantities.

2. We use short-hand notation for a few quantities that depend on the old parameters $\Delta \in (\frac{3}{2}U, 2U)$, $\Theta \in (\Delta, \Gamma - (2\Delta - U))$ and the new parameters α, d . Recall that

$$\epsilon = 2U - \Delta, \quad \ell_c = \left\lceil \frac{U}{\epsilon} \right\rceil, \quad \gamma = \Delta - U - (\ell_c - 2)\epsilon, \quad \theta = 2\Delta - U - \gamma, \quad (2.1)$$

and

$$D = U + d, \quad \Delta^+ = \Delta + \alpha,$$

and abbreviate

$$S = \frac{4\Delta - \theta}{3} - \alpha. \quad (2.2)$$

For $C > 0$, write T_C for the time scale $T_C = e^{C\beta}$.

3. For convenience we identify a configuration $\eta \in \mathcal{X}_\beta$ with its support $\text{supp}(\eta) = \{z \in \Lambda_\beta : \eta(z) = 1\}$ and write $z \in \eta$ to indicate that η has a particle at z . For $\eta \in \mathcal{X}_\beta$, denote by η^{cl} the *clusterised part* of η :

$$\eta^{cl} = \{z \in \eta : \|z - z'\| = 1 \text{ for some } z' \in \eta\}. \quad (2.3)$$

Call *clusters of η* the connected components of the graph drawn on η^{cl} obtained by connecting nearest-neighbour sites that are not a singleton.

4. Denote by $B(z, r)$, $z \in \mathbb{R}^2$, $r > 0$, the open ball on \mathbb{R}^2 with center z and radius r in the ℓ_∞ -norm defined by

$$\|\cdot\|_\infty : (x, y) \in \mathbb{R}^2 \mapsto |x| \vee |y|. \quad (2.4)$$

We denote by $\text{dist}(\cdot, \cdot)$ the distance induced by this norm.

5. The closure of $A \subset \mathbb{R}^2$ is denoted by \bar{A} . For $A \subset \mathbb{Z}^2$ and $s > 0$, put

$$[A, s] = \bigcup_{z \in A} \overline{B(z, e^{\frac{s}{2}\beta})} \cap \mathbb{Z}^2. \quad (2.5)$$

Call A a rectangle on \mathbb{Z}^2 if there are $a, b, c, d \in \mathbb{R}$ such that

$$A = [a, b] \times [c, d] \cap \mathbb{Z}^2. \quad (2.6)$$

Write $\text{RC}(A)$ to denote the intersection of all the rectangles on \mathbb{Z}^2 containing A , called the *circumscribed rectangle* of A . Denote by \mathcal{R} the set of all finite collections of rectangles on \mathbb{Z}^2 .

7. Given $\sigma \geq 0$ and $\bar{S} = \{R_1, \dots, R_{|\bar{S}|}\} \in \mathcal{R}$, two rectangles R and R' in \bar{S} are said to be in the same equivalence class if there exists a finite sequence R_1, \dots, R_k of rectangles in \bar{S} such that

$$R = R_1, \quad R' = R_k, \quad \text{dist}(R_j, R_{j+1}) < \sigma \quad \forall 1 \leq j < k.$$

Let C be the set of equivalent classes, define the map

$$\bar{g}_\sigma : \bar{S} \in \mathcal{R} \mapsto \left\{ \text{RC} \left(\bigcup_{j \in c} R_j \right) \right\}_{c \in C} \in \mathcal{R},$$

and let $(\bar{g}_\sigma^{(k)})_{k \in \mathbb{N}_0} \in \mathcal{R}^{\mathbb{N}}$ be the sequence of iterates of \bar{g}_σ . Define

$$g_\sigma(\bar{S}) = \lim_{k \rightarrow \infty} \bar{g}_\sigma^{(k)}(\bar{S}). \quad (2.7)$$

As discussed in [5], the sequence $(\bar{g}_\sigma^{(k)}(\bar{S}))_{k \in \mathbb{N}_0}$ ends up being a constant, so the limit is well defined.

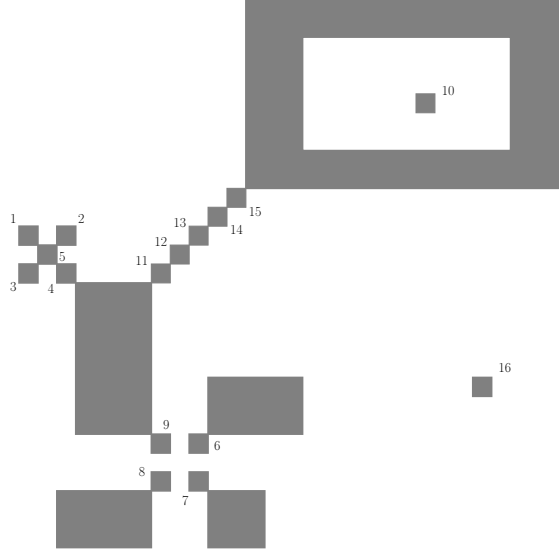


Figure 3: Each particle is represented by a unit square. A particle is free when it is not touching any other particles and can be moved to infinity without doing so. A particle is clusterised when it is part of a cluster. Particles 1–5 and 16 are free, particles 6–9, 10, 11–15 are not free. All other particles are clusterised.



As in [6], [1], the notion of *active* and *sleeping* particles will be crucial. For the precise definition we refer to [1, Section 4.3.1]. The division of particles into active and sleeping is related to the notion of free particles. Intuitively, a particle is *free* if it does not belong to a cluster and can be moved to infinity without clusterisation, i.e., by moving non-clusterised particles only (see Figure 3). For $t > e^{D\beta}$, a particle is said to be *sleeping* at time t if it was not free during the time interval $[t - e^{D\beta}, t]$. Non-sleeping particles are called *active*. Note that being active or sleeping depends on the history of the particle.

Recall the definition of the local energy $\bar{H}_i(\bar{\eta}_i)$ given in [1, Section 2.3].

Definition 2.2 For any time $t \geq 0$, given a configuration $\eta_t = X(t) \in \mathcal{X}_\beta$ and the collection $\bar{\Lambda}(t) = (\bar{\Lambda}_i(t))_{1 \leq i \leq k(t)}$ of finite boxes in Λ_β constructed in [1, Definition 1.4], we say that η_t is 0-reducible (respectively, U -reducible) if for some i the local energy of $\bar{\eta}_i$ can be reduced along the dynamics with constant $\bar{\Lambda}(t)$ without exceeding the energy level $\bar{H}_i(\bar{\eta}_i) + 0$ (respectively, $\bar{H}_i(\bar{\eta}_i) + U$). If η_t is not 0-reducible or U -reducible, then we say that η_t is 0-irreducible or

U -irreducible, respectively. We define

$$\begin{aligned}
\mathcal{X}_0 &= \{\eta_t \in \mathcal{X}^* : \eta_t \text{ is } 0\text{-irreducible}\}, \\
\mathcal{X}_U &= \{\eta_t \in \mathcal{X}_0 : \eta_t \text{ is } U\text{-irreducible}\}, \\
\mathcal{X}_D &= \{\eta_t \in \mathcal{X}_U : \text{all the particles in } \Lambda(t) \text{ are sleeping}\}, \\
\mathcal{X}_S &= \{\eta_t \in \mathcal{X}_D : \text{each box of volume } e^{S\beta} \text{ contains three active particles at most}\}, \\
\mathcal{X}_{\Delta+} &= \left\{ \eta_t \in \mathcal{X}_S : \begin{array}{l} \bar{\eta}_t \text{ is a union of at most } \lambda(\beta) \text{ quasi-squares with} \\ \text{no particle inside } \bigcup_i [\bar{\Lambda}_i(t), \Delta - \alpha] \text{ except for those} \\ \text{in the quasi-squares, one for each local box } \bar{\Lambda}_i(t) \end{array} \right\}, \\
\mathcal{X}_E &= \{\eta \in \mathcal{X}_{\Delta+} : \eta \text{ has no quasi-square}\},
\end{aligned}$$

where $[\bar{\Lambda}_i(t), \Delta - \alpha]$ are the boxes of volume $e^{(\Delta - \alpha)\beta}$ with the same center as $\bar{\Lambda}_i(t)$. \spadesuit

Define the set

$$\mathcal{R}' := \left\{ \eta \in \mathcal{X}_\beta : \begin{array}{l} \text{all clusters of } \eta \text{ have volume at most } \ell_c(\ell_c - 1) + 2 \\ \text{except for at most one cluster with volume less than } \frac{1}{8}\lambda(\beta) \end{array} \right\}, \quad (2.8)$$

where $\lambda(\beta)$ satisfies (1.18). For $C^* > 0$ large enough, our theorem about the tube of typical trajectories will hold up to time T^* defined as

$$T^* = e^{C^*\beta} \wedge \min\{t \geq 0 : X(t) \notin \mathcal{R}'\}. \quad (2.9)$$

In [1, Definition 2.3] we introduced a subset of configurations $\mathcal{X}^* \subset \mathcal{X}_\beta$ satisfying certain regularity properties. We referred to this subset as the *typical environment*. In [1, Proposition 2.6] we showed that if our system is started from the restricted ensemble $\mu_{\mathcal{R}}$, then with probability SES it escapes from \mathcal{X}^* within time T^* . Thus, effectively our system is confined to \mathcal{X}^* , which is needed for certain arguments later on.

3 Lower bound

In this section we prove the lower bound for the time $\tau_{\mathcal{R}^c}$ stated in Theorem 1.1 for any $\Delta < \Theta < \Gamma - (2\Delta - U)$.

Consider the partition of Λ_β into boxes Λ_i of side $2\ell_c$, with $i = 1, \dots, \frac{|\Lambda_\beta|}{4\ell_c^2}$, and set $T_- = e^{(\Gamma - \Theta - \delta)\beta}$. If the system exits from \mathcal{R} within time T_- , then within that time there exists a box Λ_i having a non-empty intersection with one free particle and $\ell_c(\ell_c - 1) + 1$ other particles. Given a fixed box Λ_i and a configuration η , we define η_i^{in} as the configuration given by free particles and clusters of η with a non-empty intersection with Λ_i . Note that the support of η_i^{in} may not be completely contained in Λ_i . Indeed, clusters of η may intersect Λ_i , but not be contained inside. Moreover, we define η_i^{out} as the configuration such that $\eta = \eta_i^{\text{out}} + \eta_i^{\text{in}}$, i.e., $\eta(x) = \eta_i^{\text{out}}(x) \vee \eta_i^{\text{in}}(x)$ for any $x \in \Lambda_\beta$ and $\eta_i^{\text{out}}(x) = 0$ for any $x \in \Lambda_\beta$ such that $\eta_i^{\text{in}}(x) = 1$. Note that η_i^{out} and η_i^{in} have disjoint support. Define $A_i := \{\eta \in \mathcal{R} : \eta_i^{\text{in}} \text{ has one free particle and } \ell_c(\ell_c - 1) + 1 \text{ other particles}\}$ and $B_i := \{\eta \in \mathcal{R} : \eta_i^{\text{in}} \text{ is a critical configuration for the local model}\}$. By using the invariance of $\mu_{\mathcal{R}}$, and considering the embedded discrete-time process we have constructed with a Poisson process of rate $4\ell_c^2$, we have

$$P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{R}^c} \leq T_-) \leq \text{SES} + 2 \sum_{i=1}^{\frac{|\Lambda_\beta|}{4\ell_c^2}} \sum_{t=1}^{4\ell_c^2 e^{\frac{\delta}{2}\beta} T_-} \mu_{\mathcal{R}}(A_i) \leq \text{SES} + 2 \sum_{i=1}^{\frac{|\Lambda_\beta|}{4\ell_c^2}} \sum_{t=1}^{4\ell_c^2 e^{\frac{\delta}{2}\beta} T_-} \mu_{\mathcal{R}}(B_i),$$

where the second inequality holds because any configuration in A_i has energy at least that of the configurations in B_i . Indeed, note that the configurations in the two sets have the same total number of particles, and those in A_i have at least one free particle, which is the number of free particles in the configurations in B_i . By the isoperimetric inequality, the configurations with one free particle and $\ell_c(\ell_c - 1) + 1$ other particles that have minimal energy are those in B_i , and so the claim follows. For fixed i , due to the decomposition of each $\eta = \eta_i^{\text{out}} + \eta_i^{\text{in}}$, we have $H(\eta) + \Delta|\eta| = H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}| + H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|$. Moreover, we denote by B_i^{in} the set of configurations η_i^{in} compatible with the event B_i , and by $\eta_i^{\text{out}} \sim \eta_i^{\text{in}}$ a configuration η_i^{out} compatible with a given η_i^{in} . Let η^0 be the configuration that is equal to zero everywhere. Since $|B_i^{\text{in}}|$ can be bounded by the number of possible configurations inside a box of side length at most $3\ell_c^2$, we can write

$$\mu_{\mathcal{R}}(B_i) = \frac{\sum_{\eta_i^{\text{in}} \in B_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|]} \sum_{\eta_i^{\text{out}} \sim \eta_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]}}{\sum_{\eta_i^{\text{in}} \in \mathcal{R}} e^{-\beta[H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|]} \sum_{\eta_i^{\text{out}} \sim \eta_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]}} \leq |B_i^{\text{in}}| e^{-\Gamma\beta} \leq e^{-(\Gamma - \frac{\delta}{4})\beta},$$

where we use that the energy of the configurations in B_i^{in} is constant and equal to Γ and that the denominator is bounded from below by $\sum_{\eta_i^{\text{out}} \sim \eta^0} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]}$. Thus, we deduce that

$$P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{R}^c} \leq e^{(\Gamma - \Theta - \delta)\beta}) \leq \text{SES} + 2e^{-\frac{\delta}{4}\beta},$$

and the desired lower bound follows.

4 Upper bound and tube: moderate volume

In this section we prove the upper bound for the time $\tau_{\mathcal{R}^c}$ in Theorem 1.1 and identify the nucleation pattern stated in Theorem 1.2, both in the case of moderate volume, i.e., $\Delta < \Theta \leq \theta$.

For Theorem 1.1 it is enough to provide an upper bound on the exit time from \mathcal{R} , i.e., we will prove that

$$P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{R}^c} > e^{(\Gamma - \Theta + \delta)\beta}) = \text{SES}. \quad (4.1)$$

The proof of (4.1) is divided into two steps, which will be addressed in Sections 4.1 and 4.2, respectively. In the first step, we prove a recurrence property to the set $\mathcal{X}_E \cup \mathcal{R}^c$ within time $e^{(\theta + \delta)\beta}$ (Section 4.1). In particular, by introducing the usual shift operator ϑ_s , $s \geq 0$, defined by $\vartheta_s(X) = X(s + \cdot)$, for $\delta > 0$ and a stopping time τ , we will show that

$$P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{X}_E \cup \mathcal{R}^c} \circ \vartheta_{\tau} \geq T_{\theta} e^{\delta\beta}, \tau + \tau_{\mathcal{X}_E \cup \mathcal{R}^c} \circ \vartheta_{\tau} \leq T^*) = \text{SES}. \quad (4.2)$$

In the second step, we build a nucleation event for the exit from the set \mathcal{R} starting from \mathcal{X}_E within time $e^{(\Gamma - \Theta)\beta} e^{\delta\beta}$ (Section 4.2). In particular, for any $\eta \in \mathcal{X}_E$ we prove that

$$P_{\eta}(\tau_{\mathcal{R}^c} \leq T_{\theta} e^{\frac{\delta}{3}\beta}) \geq e^{(\Theta - \Gamma)\beta} e^{\theta\beta} e^{-\frac{\delta}{3}\beta}. \quad (4.3)$$

This is enough to prove the desired upper bound for the time $\tau_{\mathcal{R}^c}$. Indeed, by dividing the time interval $[0, e^{(\Gamma - \Theta)\beta} e^{\delta\beta}]$ into $e^{(\Gamma - \Theta - \theta)\beta} e^{\frac{2}{3}\delta\beta}$ intervals of length $T_{\theta} e^{\frac{\delta}{3}\beta}$ and using (4.2) and (4.3) together with the strong Markov property at the time $\tau_{\mathcal{R}^c}$, we get

$$P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{R}^c} > e^{(\Gamma - \Theta)\beta} e^{\delta\beta}) \leq \left(1 - e^{(\Theta - \Gamma)\beta} e^{\theta\beta} e^{-\frac{\delta}{3}\beta}\right)^{e^{(\Gamma - \Theta - \theta)\beta} e^{\frac{2}{3}\delta\beta}} = \text{SES}.$$

The proof of Theorem 1.2 will be given in Sections 4.3–4.5. We first rule out the possibility of an exit from \mathcal{R} by coalescence in Section 4.3. We subsequently construct the subcritical and the supercritical tube of typical trajectories in Sections 4.4 and 4.5 respectively, which give us the complete geometrical description of the tube of typical paths stated in Theorem 1.2 for $\Delta < \Theta \leq \theta$.

4.1 Recurrence to vacuum

Here we show recurrence to the set $\mathcal{X}_E \cup \mathcal{R}^c$ within time $T_\theta e^{\delta\beta}$, where $T_\theta = e^{\theta\beta}$, namely, we prove (4.2). To this end, divide the time interval $[0, T_\theta e^{\delta\beta}]$ into $e^{\frac{3}{4}\delta\beta}$ intervals I_j of length $T_\theta e^{\frac{\delta}{4}\beta}$. We have

$$\begin{aligned} \sup_{\eta \in \mathcal{X}^*} P_\eta(\tau_{\mathcal{X}_E \cup \mathcal{R}^c} \wedge \tau_{\mathcal{X}_\beta \setminus \mathcal{X}^*} > T_\theta e^{\delta\beta}) &\leq \prod_{1 \leq j < e^{\frac{3}{4}\delta\beta}} \sup_{\eta \in \mathcal{X}^*} P_\eta(\tau_{\mathcal{X}_E \cup \mathcal{R}^c}, \tau_{\mathcal{X}_\beta \setminus \mathcal{X}^*} \notin I_j) \\ &= \left(1 - \inf_{\eta \in \mathcal{X}^*} P_\eta(\tau_{\mathcal{X}_E \cup \mathcal{R}^c} \wedge \tau_{\mathcal{X}_\beta \setminus \mathcal{X}^*} \leq T_\theta e^{\frac{\delta}{4}\beta})\right)^{e^{\frac{3}{4}\delta\beta}}, \end{aligned}$$

where we use the strong Markov property for the stopping time $\tau_{\mathcal{X}_E \cup \mathcal{R}^c}$. By [1, Remark 2.5 and Proposition 2.6], it suffices to prove that

$$\inf_{\eta \in \mathcal{X}^*} P_\eta(\tau_{\mathcal{X}_E \cup \mathcal{R}^c} \wedge \tau_{\mathcal{X}_\beta \setminus \mathcal{X}^*} \leq T_\theta e^{\frac{\delta}{4}\beta}) \geq e^{-\frac{\delta}{4}\beta}. \quad (4.4)$$

By the typical return time theorem ([1, Theorem 1.5]), we know that the dynamics reaches the set $\mathcal{X}_{\Delta+}$ with probability $1 - \text{SES}$ within time $e^{(\Delta+\alpha+\delta)\beta}$ without exiting the environment \mathcal{X}^* . If the configuration $X(\tau_{\mathcal{X}_{\Delta+}})$ contains a supercritical quasi square, namely, a $\ell_1 \times \ell_2$ quasi-square with $\ell_1 \geq \ell_c$, then the dynamics is already in \mathcal{R}^c and therefore (4.4) directly follows. Otherwise, all the quasi-squares in $X(\tau_{\mathcal{X}_{\Delta+}})$ are subcritical. By the typical update time theorem ([1, Theorem 1.6]), we know that with probability $1 - \text{SES}$ the projected dynamics remains in $\pi(X(\tau_{\mathcal{X}_{\Delta+}}))$ through successive visits in $\mathcal{X}_{\Delta+}$ within time $e^{(r(\ell_1, \ell_2)+\delta)\beta} \leq T_\theta e^{\delta\beta}$. Therefore, by the typical transition theorem ([1, Theorem 1.8]), we know that with probability at least $1 - e^{-\delta\beta}$ the smallest quasi-square either decays into a smaller quasi-square or a *coalescence occurs at time t* , i.e., there exist two sleeping particles in different local boxes at time t^- that are in the same local box at time t . In the first case, the volume of the droplets decreases. In the second case, two local boxes become too close to each other at time t^- , so that there is a non negligible probability that a coalescence between clusters appears. Thus, the number of droplets decreases. By iterating this argument for a non-exponential number of times, since the dynamics is in \mathcal{X}^* and hence the number of clusters is at most $\lambda(\beta)$, from [1, Theorem 1.5] we obtain that the dynamics reaches the set $\mathcal{X}_E \cup \mathcal{R}^c$ within time $T_\theta e^{\delta\beta}$ with probability at least $e^{-\frac{\delta}{4}\beta}$, which proves (4.4).

4.2 Exit from the set of subcritical configurations

Here we provide the proof of (4.3). To this end, we estimate from below the probability that the following event for the exit from \mathcal{R} occurs. Let x be a fixed site in Λ_β , and let \mathcal{G}_x be the event corresponding to the creation of a 2×2 square droplet containing x that afterwards grows up to the exit from \mathcal{R} , visiting all the quasi-squares inbetween within time $T_\theta e^{\frac{\delta}{3}\beta}$, without the creation of other clusters. To prove (4.3), it is enough to show that, for any $\eta \in \mathcal{X}_E$ and any $x \in \Lambda_\beta$,

$$P_\eta(\mathcal{G}_x) \geq e^{-\Gamma\beta} e^{\theta\beta} e^{-\frac{\delta}{3}\beta}. \quad (4.5)$$

Indeed, since these nucleation events towards the exit from \mathcal{R} around a given site x are disjoint events, if we choose for example x as the first site in lexicographic order of the initial 2×2 droplet, then we get

$$P_\eta(\tau_{\mathcal{R}^c} \leq T_\theta e^{\frac{\delta}{3}\beta}) \geq \sum_{x \in \Lambda_\beta} P_\eta(\mathcal{G}_x) = e^{(\Theta - \Gamma)\beta} e^{\theta\beta} e^{-\frac{\delta}{3}\beta}.$$

Thus, it remains to prove (4.5).

To this end, for any $\bar{\delta} > 0$ divide the time interval $[0, T_\theta e^{\frac{\delta}{3}\beta}]$ into $e^{(\theta - \Delta - \alpha)\beta} e^{(\frac{\delta}{3} - \bar{\delta})\beta}$ intervals I_j of length $e^{(\Delta + \alpha + \bar{\delta})\beta}$. We can estimate from below the probability that the first 2×2 droplet containing a given site $x \in \Lambda_\beta$ appears during the time interval I_j as in the proof of [1, Proposition 3.1]. Since the creations of droplets in each time interval I_j are disjoint, by summing over $j < e^{(\theta - \Delta - \alpha)\beta} e^{(\frac{\delta}{3} - \bar{\delta})\beta}$ and using [1, (4.2)-(4.3)], we get that the probability of the event constructed is at least

$$\sum_{j < e^{(\theta - \Delta - \alpha)\beta} e^{(\frac{\delta}{3} - \bar{\delta})\beta}} e^{-3[\Delta - U + O(\alpha, d, \bar{\delta})]\beta} e^{-[U + O(\bar{\delta}, d)]\beta} \geq e^{\theta\beta} e^{-(4\Delta - 2U)\beta} e^{\frac{\delta}{3}\beta} e^{-O(\alpha, d, \bar{\delta})\beta}.$$

Starting from a 2×2 droplet, the nucleation event proceeds as follows. First, let the droplet grow into a 2×3 droplet and so on, until the path reaches a $(\ell_c - 1) \times \ell_c$ quasi-square, which is the last quasi-square visited by the path before exiting from \mathcal{R} . The lower bound for this nucleation event is controlled by the atypical transition theorem [1, Theorem 1.9]. In particular, using the strong Markov property at the times corresponding to each return time in $\mathcal{X}_{\Delta+}$, we get

$$\begin{aligned} P_\eta(\mathcal{G}_x) &\geq e^{\theta\beta} e^{-(4\Delta - 2U)\beta} e^{\frac{\delta}{3}\beta} \prod_{\ell_1=2}^{\ell_c-1} \prod_{\ell_2=\ell_1}^{\ell_1+1} e^{-[(2\Delta - U) - r(\ell_1, \ell_2)]\beta} e^{-O(\alpha, d, \bar{\delta})\beta} \\ &= e^{\theta\beta} e^{-(4\Delta - 2U)\beta} e^{\frac{\delta}{3}\beta} \prod_{\ell_1=2}^{\ell_c-1} e^{-2[(2\Delta - U) - (\ell_1 - 2)(2U - \Delta) - 2U]\beta} e^{-O(\alpha, d, \bar{\delta})\beta} \\ &= e^{\theta\beta} e^{-(4\Delta - 2U)\beta} e^{-2 \sum_{\ell_1=2}^{\ell_c-1} [(2\Delta - U) - (\ell_1 - 2)(2U - \Delta) - 2U]\beta} e^{\frac{\delta}{3}\beta} e^{-O(\alpha, d, \bar{\delta})\beta} \\ &\geq e^{-\Gamma\beta} e^{\theta\beta} e^{-\frac{\delta}{3}\beta}, \end{aligned}$$

where in the last step we use the fact that, after fixing any $\delta > 0$, we can choose $d, \alpha, \bar{\delta} > 0$ small enough such that $\frac{2}{3}\delta > |O(\alpha, d, \bar{\delta})|$. This is possible because $O(\alpha, d, \bar{\delta})$ is a linear function of α, d and $\bar{\delta}$.

4.3 Exclude escape via coalescence

In order to prove Theorem 1.2 for $\Theta \leq \theta$, we first need to exclude the escape from \mathcal{R} by coalescence.

We say that *the exit from \mathcal{R} is via coalescence* if there are two sleeping particles in different clusters at time $\tau_{\mathcal{R}^c}^-$ that are in the same supercritical cluster, with volume larger than $\ell_c(\ell_c - 1) + 2$, at time $\tau_{\mathcal{R}^c}$. We prove that

$$P_{\mu_{\mathcal{R}}} \left(\tau_{\mathcal{R}^c} \leq e^{(\Gamma - \Theta + \delta)\beta} \text{ and the exit is via coalescence} \right) \leq e^{-(\Delta - U)\beta} e^{3\delta\beta}. \quad (4.6)$$

Consider the partition of Λ_β into boxes Λ_i of sidelength $2\ell_c$, with $i = 1, \dots, \frac{|\Lambda_\beta|}{4\ell_c^2}$, and set $T_+ = e^{(\Gamma - \Theta + \delta)\beta}$. If the exit from \mathcal{R} within T_+ is via coalescence, then within that time there

exists a box Λ_i having a non-empty intersection with $k \geq 2$ different clusters, say, C_i^1, \dots, C_i^k , of $X(\tau_{\mathcal{R}^c}^-)$, with size less than $\ell_c(\ell_c - 1) + 2$ but such that $|C_i^1| + \dots + |C_i^k| > \ell_c(\ell_c - 1) + 2$. First, consider the case $k = 2$. Given a fixed box Λ_i and a configuration η , we define η_i^{in} and η_i^{out} as in Section 3. Moreover, we define $A_i := \{\eta \in \mathcal{R} : \eta_i^{\text{in}} \supseteq C_i^1 \cup C_i^2\}$, with C_i^1 and C_i^2 two disjoint subcritical clusters of η such that $|C_i^1| + |C_i^2| > \ell_c(\ell_c - 1) + 2$. By using the invariance of $\mu_{\mathcal{R}}$, and considering the embedded discrete-time process, we have constructed a Poisson process with rate $4\ell_c^2$ and

$$\begin{aligned} P_{\mu_{\mathcal{R}}}(\tau_{\mathcal{R}^c} \leq e^{(\Gamma - \Theta + \delta)\beta} \text{ and the exit is via coalescence}) \\ \leq \text{SES} + \sum_{i=1}^{\frac{|\Lambda_\beta|}{4\ell_c^2}} \sum_{t=1}^{4\ell_c^2 e^{\delta\beta} T_+} \mu_{\mathcal{R}}(A_i) \leq \text{SES} + e^{(\Gamma + 2\delta)\beta} \sup_i \mu_{\mathcal{R}}(A_i). \end{aligned}$$

For fixed i , due to the decomposition $\eta = \eta_i^{\text{out}} + \eta_i^{\text{in}}$, we have $H(\eta) + \Delta|\eta| = H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}| + H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|$. Denote by A_i^{in} the set of configurations η_i^{in} compatible with the event A_i , and by $\eta_i^{\text{out}} \sim \eta_i^{\text{in}}$ a configuration η_i^{out} compatible with a given η_i^{in} . Let η^0 be the configuration that is equal to zero everywhere. Since $|A_i^{\text{in}}|$ can be bounded by the number of possible configurations inside a box of side length at most $3\ell_c^2$, we can write

$$\begin{aligned} \mu_{\mathcal{R}}(A_i) &= \frac{\sum_{\eta_i^{\text{in}} \in A_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|]} \sum_{\eta_i^{\text{out}} \sim \eta_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]} \\ &\quad \sum_{\eta_i^{\text{in}} \in \mathcal{R}} e^{-\beta[H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{out}}|]} \sum_{\eta_i^{\text{out}} \sim \eta_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]} \\ &\leq |A_i^{\text{in}}| \sup_{\eta_i^{\text{in}} \in A_i^{\text{in}}} e^{-\beta[H(\eta_i^{\text{in}}) + \Delta|\eta_i^{\text{in}}|]} \leq |A_i^{\text{in}}| e^{-(\Gamma + \Delta - U)\beta} \leq e^{-(\Gamma + \Delta - U - \delta)\beta}, \end{aligned}$$

where we use that the denominator is bounded from below by $\sum_{\eta_i^{\text{out}} \sim \eta^0} e^{-\beta[H(\eta_i^{\text{out}}) + \Delta|\eta_i^{\text{out}}|]}$. Moreover, $H(\eta_i^{\text{in}}) \geq \Gamma + \Delta - U$ for any $\eta_i^{\text{in}} \in A_i^{\text{in}}$. Indeed, since C_i^2 is a subcritical cluster, we get

$$H(\eta_i^{\text{in}}) \geq H(C_i^1) + H(C_i^2) \geq H(C_i^1) + H(\bar{C}_i^2)$$

for a suitable choice of \bar{C}_i^2 such that $\bar{C}_i^2 \subset \Lambda_i \cap C_i^2$ and $|C_i^1| + |\bar{C}_i^2| = \ell_c(\ell_c - 1) + 3$. To get the claim, it remains to show that $H(C_i^1) + H(\bar{C}_i^2) \geq \Gamma + \Delta - U$. To this end, using [4, Corollary 6.18], we know that the perimeter of a cluster with volume n is bounded from below by $4\sqrt{n}$. Assume that $|C_i^1| = n_1$ and $|\bar{C}_i^2| = n_2$, with $2 \leq n_1, n_2 \leq \ell_c(\ell_c - 1) + 1$ and $n_1 + n_2 = \ell_c(\ell_c - 1) + 3$. Thus, we deduce that the total perimeter of the two disjoint clusters is at least $4(\sqrt{n_1} + \sqrt{n_2})$. Since $\ell_c > 2$, by direct computation we deduce that the minimum value of the perimeter is achieved for either $n_1 = 2$ and $n_2 = \ell_c(\ell_c - 1) + 1$ or $n_1 = \ell_c(\ell_c - 1) + 1$ and $n_2 = 2$. For the isoperimetric inequality applied to each cluster, we know that the minimal perimeter is achieved when one cluster is a dimer and the other cluster is a $(\ell_c - 1) \times \ell_c$ quasi-square with a protuberance. Thus, the total energy of the two clusters is at least

$$(\Gamma - \Delta) + (2\Delta - U) = \Gamma + (\Delta - U),$$

which concludes the proof of (4.6) for $k = 2$.

The general case $k \geq 3$ can be treated in a similar way by a simple induction argument. Finally, by (4.6) we deduce that the exit from \mathcal{R} via coalescence has a probability exponentially small to occur within time T_+ , so that by using the lower bound T_- obtained in Section 3 we deduce that the exit via coalescence is typically excluded.

4.4 Subcritical tube of typical trajectories

Here we describe the uphill motion of the dynamics. From the typical transition theorem for subcritical quasi-squares ([1, Theorem 1.8]), we know that a $\ell_1 \times \ell_2$ quasi-square, with $2 \leq \ell_1 < \ell_c$, decays into a $(\ell_2 - 1) \times \ell_1$ quasi-square, while a 2×2 square dissolves, up to time T^* defined in (2.9). To construct the subcritical part of the tube of typical trajectories, we use the argument carried out in [12] exploiting the reversibility of the dynamics. In particular, the first part of the typical tube of exiting trajectories is the time-reversal of a typical evolution of a shrinking subcritical quasi-square. Thus, with probability exponentially close to 1 the system nucleates a wandering cluster that visits the full increasing sequence of quasi-squares up to the $\ell_c \times \ell_c$ square. Note that the path described above is fully covered by the dynamics in a time at most T^* . Indeed, during the last transition from the $(\ell_c - 1) \times \ell_c$ quasi-square to the $\ell_c \times \ell_c$ square, the system remains in \mathcal{R}' but exits for the first time from \mathcal{R} , and the time needed to escape from \mathcal{R} is shorter than T^* by Theorem 1.1, provided C^* is large enough, where we recall (2.9) for the definition of T^* and C^* .

4.5 Supercritical tube of typical trajectories

Here we describe the downhill motion of the dynamics. Using the subcritical part of the typical trajectories described in Section 4.4, we know that with probability exponentially close to 1 the dynamics nucleates a wandering cluster that visits all the quasi-squares up to the $\ell_c \times \ell_c$ square. Afterwards, by the typical transition theorem for supercritical quasi-squares ([1, Theorem 1.8]), we know that the wandering cluster grows in the same way up to time T^* . By Theorem 1.1 and the construction of the tube of typical trajectories given above, the time T^* coincides with the appearance time of a single large cluster of volume $\frac{1}{8}\lambda(\beta)$ with probability tending to 1. Thus, our description of the supercritical part of the tube of typical trajectories holds up to the formation of a $\sqrt{\lambda(\beta)/8} \times \sqrt{\lambda(\beta)/8}$ square. Finally, note that the time used to reach this square after the exit of \mathcal{R} is of order $e^{(b-\Theta)\beta}$, where b is the largest depth of the valleys visited afterwards, which is exponentially smaller than $e^{(\Gamma-\Theta)\beta}$, i.e., than the order used to reach \mathcal{R}^c (see Theorem 1.1).

5 Upper bound and tube: large volume

In this section we prove the upper bound for the time $\tau_{\mathcal{R}^c}$ in Theorem 1.1 and identify the nucleation pattern stated in Theorem 1.2, in the case of large volume, i.e., $\theta < \Theta < \Gamma - (2\Delta - U)$. In Section 5.1 we first construct a toy model for our droplet dynamics on moderately large boxes and identify the exit time from \mathcal{R} for this model. In Section 5.2 we use the latter, together with the near-independence of the dynamics in different boxes of moderate volume, to estimate the nucleation time and identify the nucleation pattern.

5.1 Independence of moderately large boxes: a toy model

In [1] we showed that the process, seen at the return times in $\mathcal{X}_{\Delta+}$ after seeing an active particle in the local boxes, is close, up to coalescence and exit from \mathcal{R} , to a Markov chain ξ on the subset of QS with dimensions (ℓ_1, ℓ_2) such that $(\ell_1, \ell_2) = (0, 0)$ or $2 \leq \ell_1 \leq \ell_2 \leq \ell_1 + 1 \leq \ell_c$. These dimensions in QS are either those of the smallest quasi-square at the return times in $\mathcal{X}_{\Delta+}$, or

$(0, 0)$ in case there is no sleeping particle anymore. Letting $s = (\ell_1, \ell_2)$, we set

$$s + 1 = \begin{cases} (\ell_2, \ell_1 + 1), & \text{if } 2 \leq \ell_1 \leq \ell_2 \leq \ell_1 + 1 \leq \ell_c, \\ (2, 2), & \text{if } s = (0, 0), \end{cases}$$

and

$$s - 1 = \begin{cases} (\ell_2 - 1, \ell_1), & \text{if } 2 < \ell_2 \leq \ell_1 + 1 \leq \ell_c, \\ (0, 0), & \text{if } s = (2, 2). \end{cases}$$

Thus, ξ is a birth-death process with transition probability

$$p(s, s + 1) = \begin{cases} e^{-(r(0,0)-\Delta)\beta}, & \text{if } s = (0, 0), \\ e^{-(\Delta-U)\beta}, & \text{if } s \neq (0, 0), \end{cases}$$

where $r(0, 0) = 4\Delta - 2U - \theta$ is the resistance of a configuration in \mathcal{X}_E , and

$$p(s, s - 1) = e^{-(r(s)-\Delta)\beta}, \quad \text{if } s \neq (0, 0).$$

Taking into account coalescence events, we provided an upper bound for the exit time from \mathcal{R} in case $\Theta \leq \theta$, by relating it to an estimate of the hitting time in $s = (\ell_c, \ell_c)$ for ξ . In case $\Theta > \theta$ we can relate back to a toy model that can be described as a birth-death process ζ of such chains ξ , independently from each other.

Toy model ζ . With each arrival in $(0, 0)$ of a chain ξ on a subset of QS we associate the death of the chain itself. Rather than considering transitions from $(0, 0)$ to $(2, 2)$ with probability $e^{-(r(0,0)-\Delta)\beta} = e^{\theta\beta}e^{(4\Delta-2U)\beta}e^{\Delta\beta}$ as in the case $\Theta = \theta$, at each step of the process ζ we add a Poisson number of new chains ξ with mean $b(\beta) = e^{\Theta\beta}e^{-(4\Delta-2U)\beta}e^{\Delta\beta}$. We associate a birth event with each arrival of these chains. For $\zeta_k = (\xi_i)_{1 \leq i \leq n} \in \cup_{j \geq 0} \text{QS}^j$, the next configuration ζ_{k+1} of the process ζ is constructed as follows:

- (i) For any $\xi = s \neq (0, 0)$, we choose a new $\xi'_i \in \{s-1, s, s+1\}$ according to $p(s, \cdot)$ independently of everything else.
- (ii) From the list $(\xi'_i)_{1 \leq i \leq n}$, we delete all the $(0, 0)$, so that we eventually obtain a shorter list.
- (iii) At the end of the reduced list, we add a Poisson number of $(2, 2)$ with mean $b(\beta)$.

Starting from a list of dimensions $(\ell_{1,i}, \ell_{2,i})_{1 \leq i \leq n}$ with $2 \leq \ell_1 \leq \ell_2 \leq \ell_1 + 1 \leq \ell_c$ for any $1 \leq i < n$, each chain ξ typically dies and has a small probability to reach (ℓ_c, ℓ_c) before. We are interested in the process ζ that is absorbed in every configuration for which there exists a chain ξ that has reached (ℓ_c, ℓ_c) for. Each chain ξ of the process ζ either dies or is absorbed within time $e^{(\theta-\Delta)\beta}e^{\delta\beta}$ with probability $1 - \text{SES}$. Furthermore, the probability of reaching (ℓ_c, ℓ_c) within time $e^{(\theta-\Delta)\beta}e^{\delta\beta}$ is at least $e^{-(\Gamma-(4\Delta-2U))\beta}$. Indeed,

$$\begin{aligned} & P_{(2,2)}(\tau_{(\ell_c, \ell_c)} < \tau_{(0,0)}, \tau_{(\ell_c, \ell_c)} < e^{(\theta-\Delta+\delta)\beta}) \\ &= P_{(2,2)}(\tau_{(\ell_c, \ell_c)} < \tau_{(0,0)}, \tau_{(0,0)} \wedge \tau_{(\ell_c, \ell_c)} < e^{(\theta-\Delta+\delta)\beta}) \\ &= P_{(2,2)}(\tau_{(\ell_c, \ell_c)} < \tau_{(0,0)}) - P_{(2,2)}(\tau_{(\ell_c, \ell_c)} < \tau_{(0,0)}, \tau_{(0,0)} \wedge \tau_{(\ell_c, \ell_c)} \geq e^{(\theta-\Delta+\delta)\beta}) \\ &\geq e^{-(\Gamma-(4\Delta-2U))\beta} - \text{SES}. \end{aligned} \tag{5.1}$$

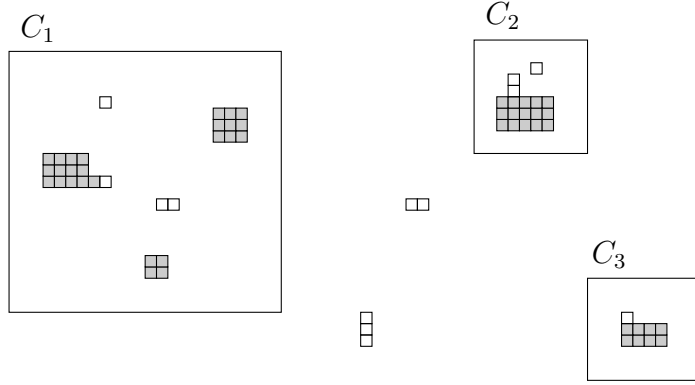


Figure 4: Construction of the clouds $(C_i)_{1 \leq i \leq 3}$ at time $t = 0$. Note that $\text{dist}(C_{i_1}, C_{i_2}) = \sqrt{T_\theta e^{-\kappa\beta}}$, with $\kappa > 0$ small enough, for $1 \leq i_1, i_2 \leq 3$ and $i_1 \neq i_2$.

Within k steps of ζ , with probability $1 - \text{SES}$ we have that at least $kb(\beta)e^{-\frac{\delta}{4}\beta}$ new chains ξ are born. Thus, for $k \gg e^{(\theta-\Delta)\beta}$, the probability that no such chains ξ manages to reach (ℓ_c, ℓ_c) before dying is at most

$$\left(1 - e^{(\Gamma-(4\Delta-2U))\beta}\right)^{kb(\beta)e^{-(\delta/4)\beta}} = \text{SES} \quad \text{if} \quad k \gg e^{(\Gamma-\Theta-\Delta)\beta}.$$

Thus, the exit time from the set \mathcal{R} has the order claimed in Theorem 1.1 for this toy model, thanks to [1, Theorem 1.8]. By excluding the escape from \mathcal{R} via coalescence as in Section 4.3, and by arguing as in Sections 4.4-4.5, together with the independence of the chains ξ , we deduce that Theorem 1.2 holds for the toy model ζ . To resume, the three key properties of the toy model, which imply Theorems 1.1 and 1.2, are the following:

- (1) The evolutions of the chains ξ_i are independent.
- (2) The probability that a chain ξ_i reaches (ℓ_c, ℓ_c) before dying within time $e^{(\theta-\Delta)\beta}e^{\delta\beta}$ is at least $e^{-(\Gamma-(4\Delta-2U))\beta}e^{\delta\beta}$ for any $\delta > 0$.
- (3) At each step a Poisson number with mean $b(\beta)$ of new boxes appears.

In Section 5.2 we will show that for our model we can define a birth-death process that is *close* to the toy model, i.e., up to negligible events properties (1)-(3) still hold. This will imply Theorems 1.1 and 1.2 in the case $\theta < \Theta < \Gamma - (2\Delta - U)$.

5.2 Near-independence of moderately large boxes in the original model

At time $t = 0$, we declare as sleeping all the particles that belong to a quasi-square (ℓ_1, ℓ_2) with $\ell_1 \geq 2$. We define $A(0)$ as the set of sites in Λ_β that are occupied by a sleeping particle, and put

$$\bar{S}(0) = \{B(a, r_0) \mid a \in A(0)\}, \quad r_0 = e^{\frac{1}{2}(\theta-\kappa)\beta}, \quad \kappa > 0.$$

At time $t = 0$, we define the set of *clouds* $(C_i)_{1 \leq i \leq N(0)}$ as $g_{r_0}(\bar{S}(0))$, i.e., the collection of rectangles at distance at least r_0 from each other. (See Fig. 4.) Let Ξ_i be the restriction of the process X to the cloud C_i . We couple Ξ_i with Ξ_i^{pb} , which is a Kawasaki dynamics on C_i with periodic boundary conditions and initial condition $\Xi_i(0)$. To construct this coupling we assign

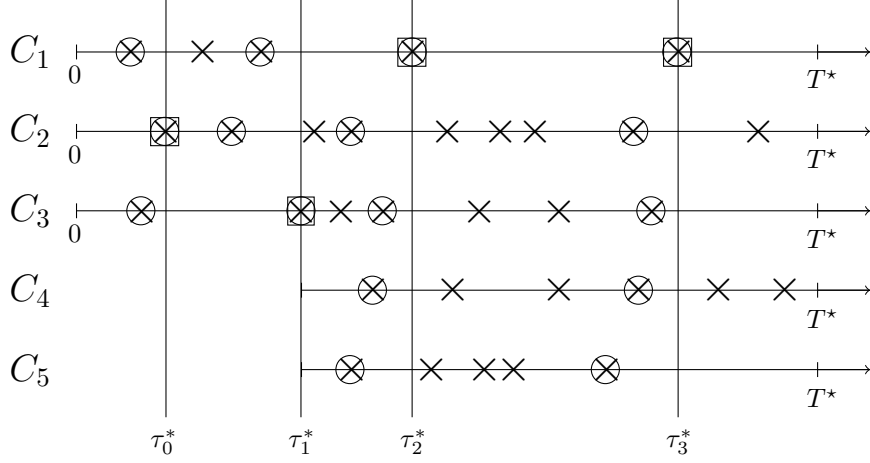


Figure 5: We depict the construction of the times $(\tau_{j,i}^*)_{0 \leq j \leq 3}$ for $i = 1, \dots, N(j)$, where $N(0) = N(1) = 3$ and $N(2) = N(3) = N(4) = 5$. In particular, each line corresponds to the time horizon for a cloud up to time T^* and each cross represents a return time $\bar{\tau}_{j,i}$, where we highlight with a circle the times $\tau_{j,i}^*$ and with a square the times τ_j^* .

colours to some particles, as follows. We paint *black* the particles of the process Ξ_i that visit $\Lambda_\beta \setminus C_i$ or share a cluster with a black particle. We paint *white* the particles of the process Ξ_i^{pb} that visit the internal boundary of C_i or share a cluster with a white particle. All the other particles have no colour, both in Ξ_i and Ξ_i^{pb} . Let $B(t)$ and $W(t)$ be the sets of sites in C_i that were visited by a black and a white particle, respectively, within time t . [7, Theorem 2 and Corollary 1.2] provide a control on the growth of these two sets. Indeed, for any $t \geq e^{\Delta\beta}$ and $\delta > 0$, with probability $1 - \text{SES}$ the two zones remain contained within a distance $te^{\Delta\beta}e^{\delta\beta}$ from the boundary of C_i . We use the natural coupling that ensures equality of Ξ_i and Ξ_i^{pb} in $C_i \setminus (B(t) \cup W(t))$ for any $t \geq 0$. With any Ξ_i^{pb} we associate the sequence $(\bar{\tau}_{k,i})_{k \geq 0}$ of return times in $\mathcal{X}_{\Delta+}$ after seeing an active particle in the local boxes (see [1, Eq. (1.22)-(1.23)]). We define the stopping times

$$\tau_0^* = \max_{1 \leq i \leq N(0)} \bar{\tau}_{0,i}$$

and

$$\tau_{0,i}^* = \max_{k \geq 0} \{\bar{\tau}_{k,i} \leq \tau_0^*\},$$

i.e., the last time before τ_0^* when Ξ_i^{pb} recurs in $\mathcal{X}_{\Delta+}$.

At time $t = \tau_{j-1}^*$, $j \in \mathbb{N}$, we similarly construct the set of clouds $(C_i)_{1 \leq i \leq N(j)}$, where we now replace r_0 by $r_j = e^{-\frac{1}{2} \frac{\kappa}{2j} \beta} r_{j-1}$. We then define the stopping times

$$\tau_j^* = \max_{1 \leq i \leq N(j)} \min_{k \geq 0} \{\bar{\tau}_{k,i} : \bar{\tau}_{k,i} > \tau_{j-1}^*\}, \quad j \in \mathbb{N},$$

i.e., the first time after time τ_{j-1}^* when all the Ξ_i^{pb} have recurred in $\mathcal{X}_{\Delta+}$, where we consider the configuration at time τ_{j-1}^* as initial condition. (See Fig. 5.) Note that $\tau_{j,i}^* > \tau_{j-1}^*$ for any j, i . We then define the process

$$Z_j = (\Xi_i(\tau_{j,i}^*))_{1 \leq i \leq N(j)}, \quad 0 \leq j \leq J^*,$$

where

$$J^* = \max_{j \geq 0} \{\tau_j^* \leq T^*\}.$$

It is important that we monitor the droplet dynamics at times $(\tau_{j,i}^*)_{j \in \mathbb{N}_0, 1 \leq i \leq N(j)}$ rather than at times $(\bar{\tau}_{j,i})_{j \in \mathbb{N}_0, 1 \leq i \leq N(j)}$, because for the former all the clouds *recur almost simultaneously*, i.e., within a time interval of length $T_{\Delta+}$. This fact is needed to obtain the near independence of the droplet dynamics in these boxes. In the same way we view ζ as a birth-death process of independent Markov chains ξ , and view Z as a birth-death process of *essentially* independent histories of configurations Ξ . To identify a history Ξ along the configurations $Z_0 = (\Xi_i(\tau_{0,i}^*))_{1 \leq i \leq N(0)}$, $Z_1 = (\Xi_i(\tau_{1,i}^*))_{1 \leq i \leq N(1)}, \dots$, we have to

- (i) decide which is the successor Ξ'_j in $Z_{k+1} = (\Xi'_j)_{1 \leq j \leq N(k+1)}$ of Ξ_i in $Z_k = (\Xi_i)_{1 \leq i \leq N(k)}$ for any $k \geq 0$, if such a successor exists;
- (ii) identify the death events of an history Ξ , i.e., the absence of a successor Ξ'_j in Z_{k+1} of Ξ_i in Z_k ;
- (iii) associate with the appearance of each Ξ'_j in Z_{k+1} without predecessor Ξ_i in Z_k a birth event.

To this end, in each configuration Ξ in Z_k we consider one of the clusters containing at least one sleeping particle outside the black and the white zones (where the clusters coincide with the quasi-squares of Ξ_i^{pb}), and we choose the one with the smallest dimensions. In this cluster we consider the particle that is asleep for a longer time (or one of these, if they are more than one). As long as this particle is still sleeping in one of the Ξ'_j in Z_k , we identify Ξ'_j as the successor of Ξ_i . Otherwise, we say that Ξ_i has no successor, which corresponds to a death of a history Ξ . We then associate with each Ξ'_j without predecessor the start of a new history Ξ .

Remark 5.1 The choice that $(r_k)_{k \geq 0}$ is a decreasing sequence allows us to control the appearance of clusters outside or at the boundary of the clouds at the previous step without having an increasing number of clusters along a history Ξ . (It may however happen that the number of clusters decreases together with a birth event: this occurs whenever the clusters in the same cloud become clusters in different clouds at the next time step.) Then the number of clusters can increase along a history Ξ , but up to coalescence and with a negligible probability compared to that of growing a row on the smallest quasi-square.

Remark 5.2 From [1, Theorem 1.5], up to an event of probability SES, there are no more than $e^{(\alpha+\delta)\beta}$ return times in $\mathcal{X}_{\Delta+}$ of Ξ_i^{pb} between two successive configurations of the same history Ξ for any $\delta > 0$. This, together with [1, Theorems 1.6, 1.8 and 1.9], implies that, unless a coalescence occurs, the smallest quasi-square (ℓ_1, ℓ_2) along a history Ξ

- (i) typically resists for a time of order $e^{(r(\ell_1, \ell_2) - \Delta)\beta}$ if $\ell_1 \geq 2$;
- (ii) typically either decays in a quasi-square $(\ell_2 - 1, \ell_1)$ if $\ell_2 > 2$ or dies if $(\ell_1, \ell_2) = (2, 2)$;
- (iii) grows into a quasi-square $(\ell_2, \ell_1 + 1)$ with a probability of order $e^{((2\Delta - U) - \Delta)\beta}$.

This shows that each history typically dies or exits from \mathcal{R} within a time of order $e^{(\theta - \Delta)\beta}$ with probability $1 - \text{SES}$.

The proposition below is the core result of this section and ensures that the key properties of the toy model ζ also hold for our model Z .

Proposition 5.3 *Up to an event of probability SES:*

- (1) *The evolutions of the histories Ξ_i are independent.*
- (2) *The probability that a history Ξ_i reaches (ℓ_c, ℓ_c) before dying within time $e^{(\theta-\Delta)\beta}e^{\delta\beta}$ is at least $e^{-(\Gamma-(4\Delta-2U))\beta}e^{\delta\beta}$ for any $\delta > 0$.*
- (3) *At each step a Poisson number with mean $b(\beta)$ of new boxes appears.*

Proof. Property (1) is immediate from [7, Theorem 3]. Indeed, at each step $0 \leq j \leq J^*$, uniformly in $1 \leq i_1, i_2 \leq N(j)$, the distance between the clouds C_{i_1} and C_{i_2} is at least $r_j \gg e^{\frac{\Delta}{2}\beta}e^{\delta\beta}$ for any $\delta > 0$, which implies that the condition in [7, Eq. (1.23)] is satisfied. Property (2) readily follows from Remark 5.2 after arguing as in (5.1). Property (3) follows from the fact that the number of new clouds that are created at each step dominates a Poisson random variable with mean $b(\beta) = e^{\Theta\beta}e^{-(4\Delta-2U)\beta}e^{\Delta\beta}$. This is related to creation of new local boxes and can be obtained after arguing as in the proof of [1, Lemma 4.1]. \blacksquare

By Proposition 5.3, it is immediate that, for any $\delta > 0$,

$$P_{\mu_{\mathcal{R}}} \left(\tau_{\mathcal{R}^c} > \frac{e^{\Gamma\beta}}{|\Lambda_\beta|} e^{\delta\beta} \right) \leq \left(1 - e^{-(\Gamma-(4\Delta-2U))\beta} e^{-\delta\beta} \right)^{e^{(\Gamma-(3\Delta-2U))\beta} e^{-\frac{\delta}{4}\beta}} = \text{SES}.$$

This, together with the argument developed in Section 3, implies Theorem 1.1. Once we provide the upper bound for the exit time from \mathcal{R} , we can use the same argument as in Section 4.3 to exclude the escape via coalescence in the case of large volumes, so that in this case Theorem 1.2 follows from the near-independence of the histories Ξ_i and from the arguments in Sections 4.4 and 4.5.

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