Critical configurations of the hard-core model on square grid graphs

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Abstract

We consider the hard-core model on a finite square grid graph with stochastic Glauber dynamics parametrized by the inverse temperature β. We investigate how the transition between its two maximum-occupancy configurations takes place in the low-temperature regime $\beta \to \infty$ in the case of periodic boundary conditions. The hard-core constraints and the grid symmetry make the structure of the critical configurations for this transition, also known as essential saddles, very rich and complex. We provide a comprehensive geometrical characterization of these configurations that together constitute a bottleneck for the Glauber dynamics in the low-temperature limit. In particular, we develop a novel isoperimetric inequality for hard-core configurations with a fixed number of particles and show how the essential saddles are characterized not only by the number of particles but also their geometry.

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1 Introduction

We consider a stochastic model, known in the literature as *hard-core lattice gas model* [10, 35], where particles have a non-negligible radius and therefore cannot overlap. Assuming a finite volume, the hard-core constraints are modeled with a finite undirected graph Λ. More specifically, particles can reside on the sites of Λ and edges connect the pairs of sites in Λ that cannot be occupied simultaneously. In other words, any hard-core configuration is an independent set of Λ. In this paper, we take Λ as a square grid graph with periodic boundary conditions. The resulting hard-core particle configurations are then those whose occupied sites have all the corresponding four neighboring sites empty, see Fig. 1 for an example of such configurations.

This interacting particle system evolves according to a stochastic dynamics that is fully characterized by the *Hamiltonian* or *energy function* in (2.3) and is parametrized by the *inverse temperature* β. In particular, the appearance and disappearance of particles are modeled via a Glauber-type update Markov chain $\{X_t\}_{t\in\mathbb{N}}$ with Metropolis transition probabilities induced by the Hamiltonian, see (2.4) later for more details. The stochastic process is reversible with respect to the corresponding Gibbs measure μ_β, cf. (2.2), which is then its equilibrium distribution. Specifically, for any independent set I on the graph Λ, the hard-core configuration with particles precisely on the vertices in I has stationary probability proportional to $e^{\beta|I|}$. Taking $\beta = 0$, this process can thus be used to sample uniformly independent sets of Λ.

Considering a regime with large β, on the other hand, the same Markov chain can also be seen as a randomized scheme with local updates to find maximum independent sets, which is an NP-hard problem [45]. Indeed, in the low-temperature regime (i.e., $\beta \to \infty$), the most likely states in view of μ_β for this interacting particle system are those with a maximum number of particles. These configurations correspond to the maximum independent sets of Λ and we will refer to them as *stable states*. On the square grid graph Λ of even length, there are two such stable states, corresponding to the two chessboard-like patterns.

When β grows large, however, it takes a very long time for the system to move from one stable state to the other, since such a transition involves visiting intermediate configurations that are very unlikely in terms of μ_β. Such transitions become thus rare events and, as a consequence, the stochastic process also takes a very long time to converge to stationarity, exhibiting so-called *slow/torpid mixing* [31, 54]. It is natural to expect such slow mixing of hard-core dynamics for a large β, since fast mixing in this regime would imply that the NP-hard problem of finding maximum independent sets could be solved or approximated efficiently.

Several papers [19, 31–33, 36, 39, 42, 44, 53] studied the slow mixing of the hard-core model by identifying how the mixing times of the Glauber dynamics scale on other graphs, depending on the type of graph, the size, the boundary conditions or the maximum vertex degree. The common main idea behind this line of work has been to identify as precisely as possible the subset of configurations that constitutes a bottleneck for the dynamics to transition from one stable state to another. Some of these approaches also heavily rely on geometric features exhibited by the configurations in this bottleneck part of the state space, like the so-called *fault lines* in [53] and *fat contours* in [36].

In this paper, we look at a complementary aspect of the hard-core model in the low-temperature regime, focusing on the hitting times between its stable states and the "bottleneck configurations" visited along these trajectories. The asymptotic behavior of the first hitting time between the maximum-occupancy configurations of this model in the low-temperature regime $\beta \to \infty$ has already been studied in [47]. Denoting by $\tau^{\mathbf{e}}_{\mathbf{o}}$ the first hitting time of Markov chain $\{X_t\}_{t\in\mathbb{N}}$ corresponding to hard-core dynamics on a grid graph Λ, in [47] the authors showed that there exists a constant $\Gamma(\Lambda) > 0$ such that for every $\epsilon > 0$,

$$\lim_{\beta\to\infty} \mathbb{P}_\beta \left(e^{\beta(\Gamma(\Lambda)-\epsilon)} < \tau^{\mathbf{e}}_{\mathbf{o}} < e^{\beta(\Gamma(\Lambda)+\epsilon)} \right) = 1 \tag{1.1}$$

and

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}\tau^{\mathbf{e}}_{\mathbf{o}} = \Gamma(\Lambda). \tag{1.2}$$

In particular, the authors showed in the same article how this constant $\Gamma(\Lambda)$, which characterizes the order of magnitude of the first hitting time between the two stable configurations, depends on the grid sizes and boundary conditions by means of an extension of the setting in [43].

However, instead of directly using the general strategy proposed in [43], which allows to jointly derive the asymptotic behavior of the transition time as $\beta \to \infty$ together with a characterization of the critical configurations, the authors of [47] adopted a novel combinatorial method to estimate the energy barrier between the two stable states of the model, which is disentangled with respect to the description of the critical configurations. Consequently, the geometrical description of the critical configurations had yet to be addressed.

The main motivation of this paper is to fill this knowledge gap. Indeed, the geometrical characterization of the critical configurations, also known as *essential saddles*, is a relevant goal both from a probabilistic and a physical point of view since it provides insightful details of the dynamical behavior of the system. This represents a crucial point in describing the trajectories that the system follows with high probability during the transition from one stable state to the other. We remark that in several models analyzed in the context of Freidlin-Wentzell Markov chains evolving under Glauber dynamics, the *essential gate*, i.e., the set of the critical configurations, was unique [1] but, in general, there may exist many minimal sets that are crossed with high probability during the phase transition, either distinct or overlapping (see e.g. [5, 6] for this description in the case of the conservative Kawasaki dynamics). Interestingly, this is what happens also for our model despite evolving under the non-conservative Glauber dynamics. This peculiar feature relies on the hard-core constraints and on the intrinsic symmetry of the system due to the existence of two stable states. This is also the case of Glauber dynamics for the Ising and Potts models when there is no external magnetic field (see, e.g., [12]). In statistical physics, the study of such transition between stable states is usually referred to as *tunneling*. When the particle system does not have an intrinsic symmetry or the symmetry of the system is broken, e.g., by an external magnetic field, the situation drastically changes. For interacting particle systems with a single stable state, the main object of investigation then becomes their *metastability*, i.e., the transition from the metastable state(s) to the stable one. Generally speaking, interacting particle systems that exhibit tunneling behavior have a much larger and complex set of essential saddles. This is precisely the case for the hard-core model on a square grid graph Λ, with the additional complication that the only admissible configurations are its independent sets.

In order to geometrically characterize the critical configurations, we associate with each cluster of particles its *contour*, that is, a union of edges on the dual graph of Λ. The equivalent representation of a configuration using its Peierls contour is a powerful tool that has been extensively used in the literature to study the phase transition of the hard-core model, identify sharper bounds for the critical temperature β_c, and to obtain high-fugacity expansion of macroscopic quantities of the model; we refer the interested reader to, e.g., [18, 38].

As part of our proof strategy, we provide some results regarding the model-dependent isoperimetric inequality for the hard-core model on grid graphs. In particular, we show that for a fixed area, the unique clusters that minimize the perimeter have a *rhomboidal* shape. However, the energy landscape is much more complex as the periodic boundary conditions give rise to other types of clusters with minimal perimeter for a given area, such as the configurations having a column containing a fixed number of particles.

We remark that our analysis yields a comprehensive geometrical description of the configurations in the bottleneck part of the state space, together with an overview of the exact structure of the bottleneck subset itself. However, pairing this analysis with precise counting arguments is beyond the scope of the present paper. Hence, we do not explore the energy-entropy tradeoff of the hard-core model or shine more light on its phase transition.

In order to link geometrical properties of hard-core configurations with the properties of the stochastic process $\{X_t\}_{t\in\mathbb{N}}$, in this paper we adopt the framework of the *pathwise approach*, introduced in the context of metastability by [24], later developed in [50, 51], and summarized in the monograph [52]. A modern version of this approach can be found in [26, 27, 43, 47]. The pathwise approach

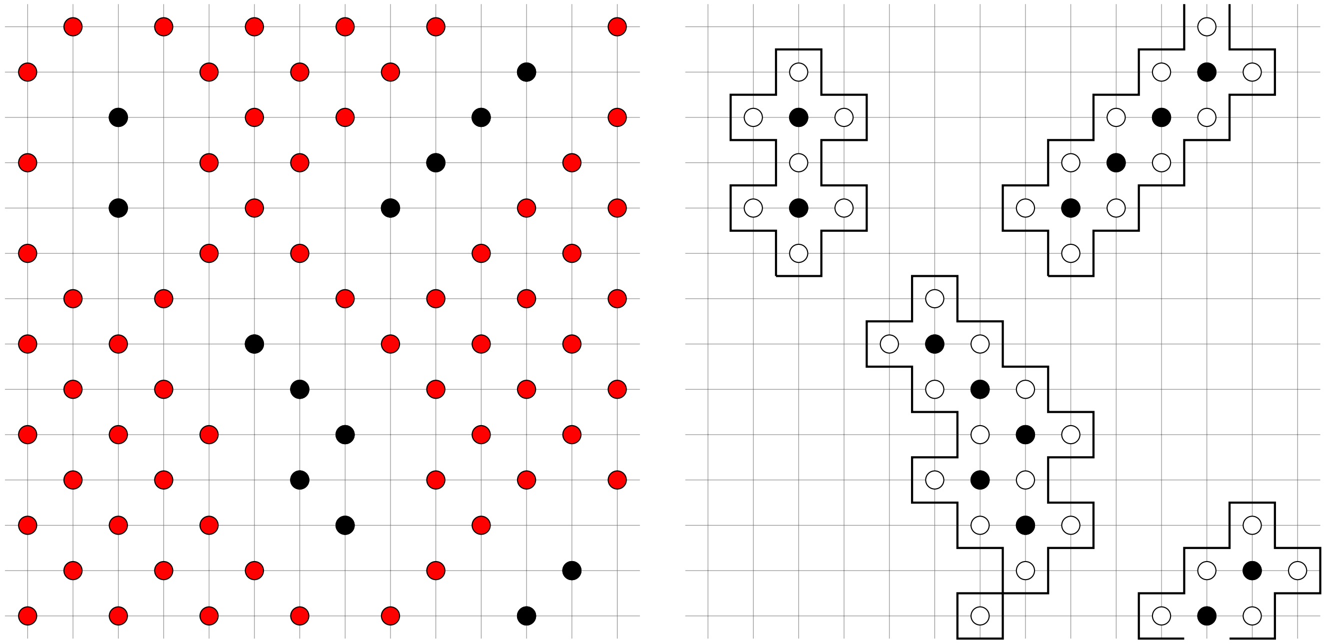

Figure 1: Example of a hard-core configuration on the 14×14 square grid with periodic boundary conditions. On the left, the occupied sites in $V_{\mathbf{o}}$ (resp. in $V_{\mathbf{e}}$) are highlighted in black (resp. in red). On the right, we depict the same configuration using a different visual convention, in which we highlight the odd clusters that the configuration has by drawing only the empty sites in $V_{\mathbf{e}}$ (in white), the occupied sites in $V_{\mathbf{o}}$ (in black), and a black line around each odd cluster representing its contour.

has been widely adopted for studying the low-temperature behavior of finite-volume models with single-spin-flip Glauber dynamics, e.g. [1, 2, 11–14, 25, 49, 55, 56], with Kawasaki dynamics, e.g. [4–7, 37, 46], and with parallel dynamics, e.g. [28–30]. The more involved infinite-volume limit at low temperature was studied via this approach in [3, 34, 37]. A different method to study the limiting behavior of interacting particle systems is the so-called *potential-theoretic approach*, initiated in [22] and later summarized in the monograph [23] (see, for instance, [20, 21, 48] for the application of this approach to specific models both in finite and infinite volume). Since these two approaches rely on different definitions of metastable states, they are not completely equivalent. The situation is particularly delicate for infinite-volume systems, irreversible systems, and degenerate systems, as discussed in [15, 26, 27]. More recent approaches are developed in [8, 9, 16, 17, 40, 41].

The paper is organized as follows. In Section 2, we provide a detailed model description and state our main result regarding the geometric features of the critical configurations, Theorem 2.1. The rest of the paper is then devoted to the proof of this result. First, Section 3 provides some preliminary definitions and auxiliary results, and then finally the proof of the main theorem is given in Section 4. For the sake of clarity, the proofs of some auxiliary lemmas are deferred to a later section, namely Section 5. Lastly, Section 6 concludes the paper and discusses some future work.

2 Model description and main results

We consider the stochastic evolution of the hard-core model on finite two-dimensional square lattices. More precisely, given an integer $L \geq 2$ we consider the $L \times L$ square grid graph $\Lambda = (V, E)$ with periodic boundary conditions, which we will refer to as $L \times L$ *toric grid graph*. We denote by E the edge set of the grid graph Λ and by V the collection of its $N = L^2$ sites. We identify each site $v \in \Lambda$

by its coordinates (v_1, v_2), that is, we take $V := \{0, \dots, L-1\} \times \{0, \dots, L-1\}$ as set of sites. In the rest of the paper, we will assume that L is an even integer, which guarantees that Λ is a bipartite graph, and that $L \geq 6$, to avoid pathological trivial cases.

A particle configuration on Λ is described by associating a variable $\sigma(v) \in \{0, 1\}$ with each site $v \in \Lambda$, indicating the absence (0) or the presence (1) of a particle on that site. Let $\mathcal{X} \subset \{0, 1\}^N$ be the collection of *hard-core configurations on* Λ, i.e.,

$$\mathcal{X} := \{\sigma \in \{0, 1\}^N \mid \sigma(v)\sigma(w) = 0, \ \forall (v, w) \in E\}, \tag{2.1}$$

i.e., the particle configurations on Λ with no particles residing on neighboring sites.

A site of Λ is called *even* (respectively *odd*) if the sum of its two coordinates is even (respectively odd) and we denote by $V_{\mathbf{e}}$ and $V_{\mathbf{o}}$ the collection of even sites and that of odd sites of Λ. Clearly $|V_{\mathbf{e}}| = |V_{\mathbf{o}}| = L^2/2$. We denote by $\mathbf{e}$ ($\mathbf{o}$, respectively) the particle configuration on Λ with particles at each site in $V_{\mathbf{e}}$ ($V_{\mathbf{o}}$, respectively), i.e.,

$$\mathbf{e}(v) := \begin{cases} 1 & \text{if } v \in V_{\mathbf{e}}, \\ 0 & \text{if } v \in V_{\mathbf{o}}, \end{cases} \quad \text{and} \quad \mathbf{o}(v) := \begin{cases} 0 & \text{if } v \in V_{\mathbf{e}}, \\ 1 & \text{if } v \in V_{\mathbf{o}}. \end{cases}$$

Both $\mathbf{e}$ and $\mathbf{o}$ are hard-core configurations due to the assumption that L is even.

Fig. 1 shows an example of a hard-core configuration. Throughout the paper, all figures are drawn using the following conventions. They all depict hard-core configurations on a 14×14 grid with periodic boundary conditions. The occupied (empty) sites in $V_{\mathbf{o}}$ ($V_{\mathbf{e}}$, respectively) are shown in black (white), and we draw a black line around each odd cluster representing its contour. We tacitly assume that all the even (odd) sites outside the odd region are occupied (empty, respectively) but they are not displayed to avoid cluttering the figures. See Section 3.1 for more precise definitions of odd clusters and odd regions.

Consider the Gibbs measure on $\mathcal{X}$ given by

$$\mu_\beta(\sigma) := \frac{e^{-\beta H(\sigma)}}{Z_{\beta,\Lambda}}, \qquad \sigma \in \mathcal{X}, \tag{2.2}$$

where H is the Hamiltonian $H : \mathcal{X} \to \mathbb{R}$ that is taken to be proportional to the number of present particles, namely

$$H(\sigma) := -\sum_{v \in V} \sigma(v), \tag{2.3}$$

with $Z_{\beta,\Lambda} := \sum_{\sigma \in \mathcal{X}} e^{-\beta H(\sigma)}$ being the normalizing constant. The two hard-core configurations on the $L \times L$ toric grid graph Λ introduced above have energy equal to

$$H(\mathbf{e}) = H(\mathbf{o}) = -\frac{L^2}{2},$$

which is the minimum value the Hamiltonian can take on $\mathcal{X}$ [47].

We assume the interacting particle system described evolves according to stochastic Glauber-type dynamics described by a single-step update Markov chain $\{X_t^\beta\}_{t \in \mathbb{N}}$ on $\mathcal{X}$ with transition probabilities between any pair of configurations $\sigma, \sigma' \in \mathcal{X}$ given by

$$P_\beta(\sigma, \sigma') := \begin{cases} q(\sigma, \sigma') e^{-\beta[H(\sigma') - H(\sigma)]^+}, & \text{if } \sigma \neq \sigma', \\ 1 - \sum_{\eta \neq \sigma} P_\beta(\sigma, \eta), & \text{if } \sigma = \sigma', \end{cases} \tag{2.4}$$

where $[\cdot]^+ = \max\{\cdot, 0\}$ and q is the *connectivity matrix* that allows only single-step updates, i.e., for every $\sigma, \sigma' \in \mathcal{X}$ we set

$$q(\sigma, \sigma') := \begin{cases} \frac{1}{N}, & \text{if } |\{v \in V : \sigma(v) \neq \sigma'(v)\}| = 1, \\ 0, & \text{if } |\{v \in V : \sigma(v) \neq \sigma'(v)\}| > 1. \\ 1 - \sum_{\eta \neq \sigma} q(\sigma, \eta), & \text{if } \sigma = \sigma'. \end{cases} \tag{2.5}$$

The resulting dynamics P_β is reversible with respect to the Gibbs measure μ_β given in (2.2). The triplet $(\mathcal{X}, H, q)$ is usually referred to as *energy landscape* and (2.4) as *Metropolis transition probabilities*.

The connectivity matrix q given in (2.5) is irreducible, i.e., for any pair of configurations $\sigma, \sigma' \in \mathcal{X}$, $\sigma \neq \sigma'$, there exists a finite sequence ω of configurations $\omega_1, \dots, \omega_n \in \mathcal{X}$ such that $\omega_1 = \sigma$, $\omega_n = \sigma'$ and $q(\omega_i, \omega_{i+1}) > 0$, for $i = 1, \dots, n-1$. We will refer to such a sequence as a *path* from σ to σ' and denote it by $\omega : \sigma \to \sigma'$. Given a path $\omega = (\omega_1, \dots, \omega_n)$, we define its *height* Φ_ω as

$$\Phi_\omega := \max_{i=1,\dots,n} H(\omega_i). \tag{2.6}$$

The *communication energy* between two configurations $\sigma, \sigma' \in \mathcal{X}$ is the minimum value that has to be reached by the energy in every path $\omega : \sigma \to \sigma'$, i.e.,

$$\Phi(\sigma, \sigma') := \min_{\omega:\sigma\to\sigma'} \Phi_\omega = \min_{\omega:\sigma\to\sigma'} \max_{\eta\in\omega} H(\eta). \tag{2.7}$$

Let $\mathcal{X}^s \subset \mathcal{X}$ denote the set of global minima of the Hamiltonian H on $\mathcal{X}$, to which we will refer to as *stable states*. In [47] it has been proved that for the hard-core model on a finite $L \times L$ square grid graph the following statements hold:

(i) There are exactly two stable states

$$\mathcal{X}^s = \{\mathbf{e}, \mathbf{o}\}; \tag{2.8}$$

(ii) The communication energy between the two stable states is equal to

$$\Phi(\mathbf{e}, \mathbf{o}) - H(\mathbf{e}) = L + 1; \tag{2.9}$$

(iii) The corresponding energy landscape has no deep wells, i.e.,

$$\max_{\sigma\in\mathcal{X}} [\Phi(\sigma, \{\mathbf{e}, \mathbf{o}\}) - H(\sigma)] \leq L < \Phi(\mathbf{e}, \mathbf{o}) - H(\mathbf{e}). \tag{2.10}$$

Together, these facts imply that the value of the constant appearing in the asymptotic statements (1.1) and (1.2) for the first hitting time $\tau^{\mathbf{e}}_{\mathbf{o}}$ is $\Gamma(\Lambda) = L + 1$.

2.1 Essential saddle characterization

Our results give insight into the way the transitions between $\mathbf{e}$ and $\mathbf{o}$ most likely occur in the low-temperature regime. This is usually described by identifying the optimal paths, saddles, and essential saddles that we define as follows.

- $\mathcal{S}(\mathbf{e}, \mathbf{o})$ is the *communication level set* between $\mathbf{e}$ and $\mathbf{o}$ defined by

  $$\mathcal{S}(\mathbf{e}, \mathbf{o}) := \{\sigma \in \mathcal{X} \mid \exists\, \omega \in (\mathbf{e} \to \mathbf{o})_{\mathrm{opt}},\ :\ \sigma \in \omega \text{ and } H(\sigma) = \Phi_\omega = \Phi(\mathbf{e}, \mathbf{o})\},$$

  where $(\mathbf{e} \to \mathbf{o})_{\mathrm{opt}}$ is the set of *optimal paths* from $\mathbf{e}$ to $\mathbf{o}$ realizing the minimax in $\Phi(\mathbf{e}, \mathbf{o})$, i.e.,

  $$(\mathbf{e} \to \mathbf{o})_{\mathrm{opt}} := \{\omega : \mathbf{e} \to \mathbf{o} \mid \Phi_\omega = \Phi(\mathbf{e}, \mathbf{o})\}.$$

- The configurations in $\mathcal{S}(\mathbf{e},\mathbf{o})$ are called *saddles*. Given an optimal path $\omega \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$, we define the set of its saddles $S(\omega)$ as $S(\omega) := \{\sigma \in \omega \mid H(\sigma) = \Phi_\omega = \Phi(\mathbf{e},\mathbf{o})\}$. A saddle $\sigma \in \mathcal{S}(\mathbf{e},\mathbf{o})$ is called *essential* if either

  (i) $\exists \omega \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$ such that $S(\omega) = \{\sigma\}$, or

  (ii) $\exists \omega \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$ such that $\sigma \in S(\omega)$ and $S(\omega') \not\subseteq S(\omega) \setminus \{\sigma\} \quad \forall \omega' \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$.

  A saddle $\sigma \in \mathcal{S}(\mathbf{e},\mathbf{o})$ that is not essential is called *unessential saddle* or *dead-end*, i.e., for any $\omega \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$ such that $\omega \cap \{\sigma\} \neq \emptyset$ we have that $S(\omega) \setminus \{\sigma\} \neq \emptyset$ and there exists $\omega' \in (\mathbf{e} \to \mathbf{o})_{\text{opt}}$ such that $S(\omega') \subseteq S(\omega) \setminus \{\sigma\}$.

- The *essential gate* $\mathcal{G}(\mathbf{e},\mathbf{o}) \subset \mathcal{X}$ is the collection of essential saddles for the transition $\mathbf{e} \to \mathbf{o}$.

The aim of the present paper is to accurately identify the set $\mathcal{G}(\mathbf{e},\mathbf{o})$ of essential saddles for the transition from $\mathbf{e}$ to $\mathbf{o}$ for the Metropolis dynamics of the hard-core model on a $L \times L$ grid with periodic boundary conditions.

The set $\mathcal{G}(\mathbf{e},\mathbf{o})$ will be described as the union of six disjoint sets, each characterized by configurations with specific geometrical features. Although we refer the reader to Section 4 for a precise definition of these sets (cf. Definitions 4.2–4.6), we provide here some intuitive descriptions of the geometrical features of the configurations in these sets. We denote by

- $\mathcal{C}_{ir}(\mathbf{e},\mathbf{o})$, $\mathcal{C}_{gr}(\mathbf{e},\mathbf{o})$, and $\mathcal{C}_{cr}(\mathbf{e},\mathbf{o})$ the collections of configurations with a unique cluster of particles in odd sites of rhomboidal shape with exactly two adjacent even empty sites as in Fig. 2 and Fig. 3 (left). Roughly speaking, $\mathcal{C}_{ir}(\mathbf{e},\mathbf{o})$ contains the configurations with $(\frac{L}{2}-1)^2$ occupied odd particles and L^2+2 empty even sites; $\mathcal{C}_{gr}(\mathbf{e},\mathbf{o})$ (resp. $\mathcal{C}_{cr}(\mathbf{e},\mathbf{o})$) contains the configurations obtained from $\mathcal{C}_{ir}(\mathbf{e},\mathbf{o})$ (resp. $\mathcal{C}_{gr}(\mathbf{e},\mathbf{o})$) by removing some occupied even sites attached to the rhombus and growing along one (resp. the longest) side by adding some particles in the nearest odd sites of the rhombus.

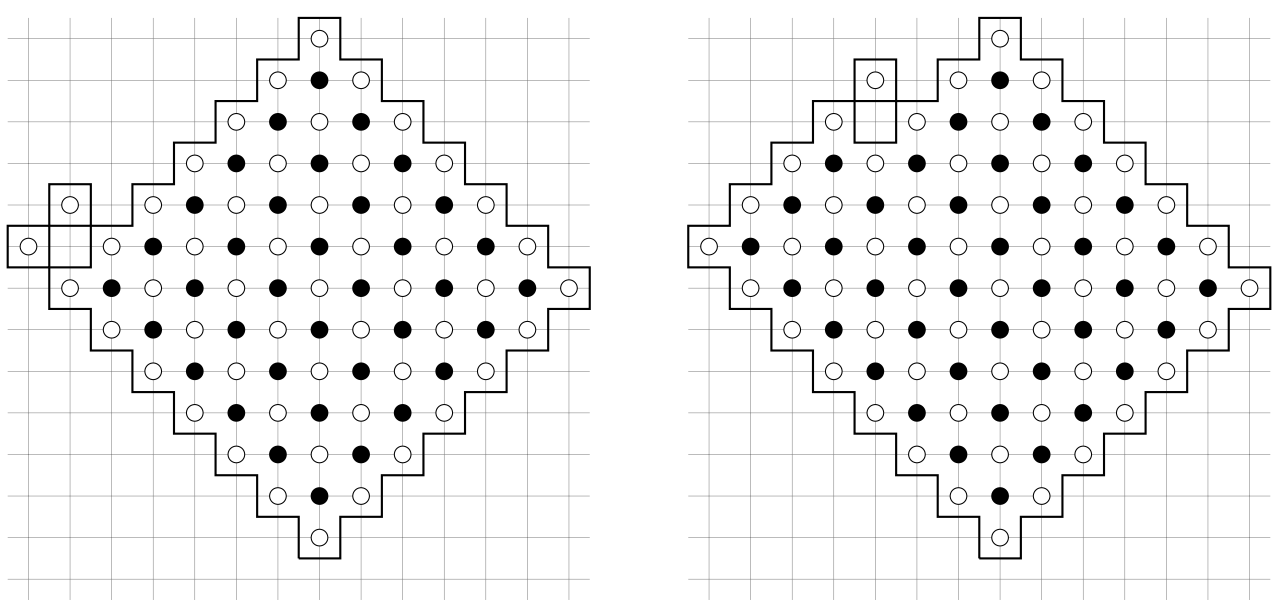

Figure 2: An example of a configuration in $\mathcal{C}_{ir}(\mathbf{e},\mathbf{o})$ (on the left) and one in $\mathcal{C}_{gr}(\mathbf{e},\mathbf{o})$ (on the right).

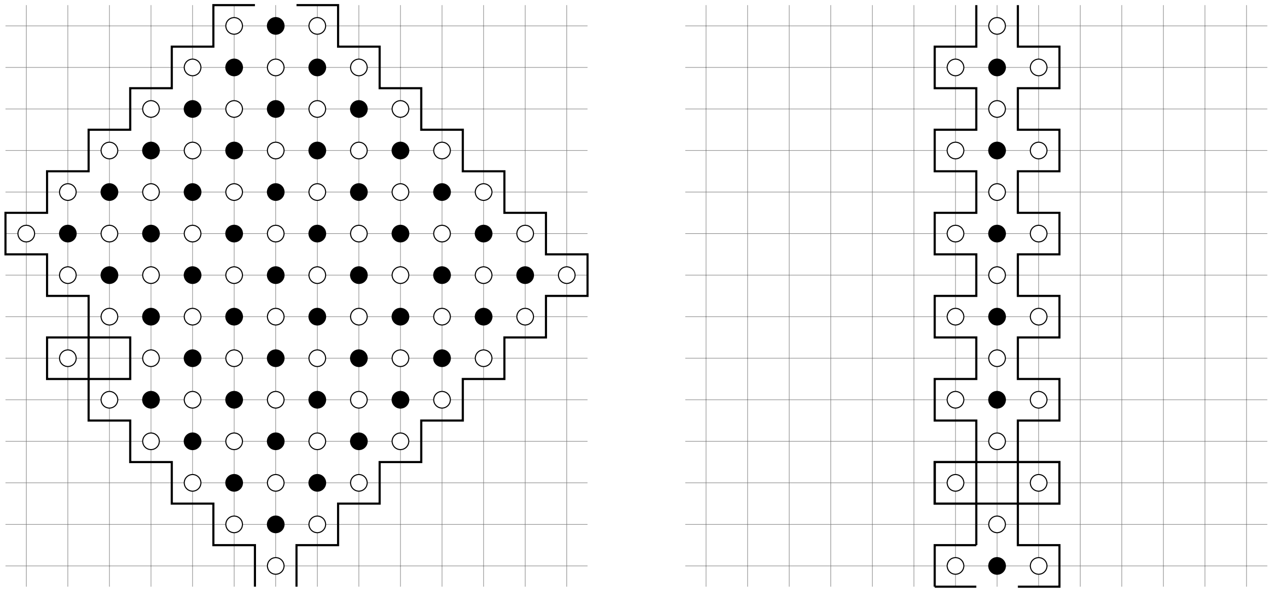

Figure 3: An example of a configuration in $\mathcal{C}_{cr}(\mathbf{e},\mathbf{o})$ (on the left) and one in $\mathcal{C}_{sb}(\mathbf{e},\mathbf{o})$ (on the right).

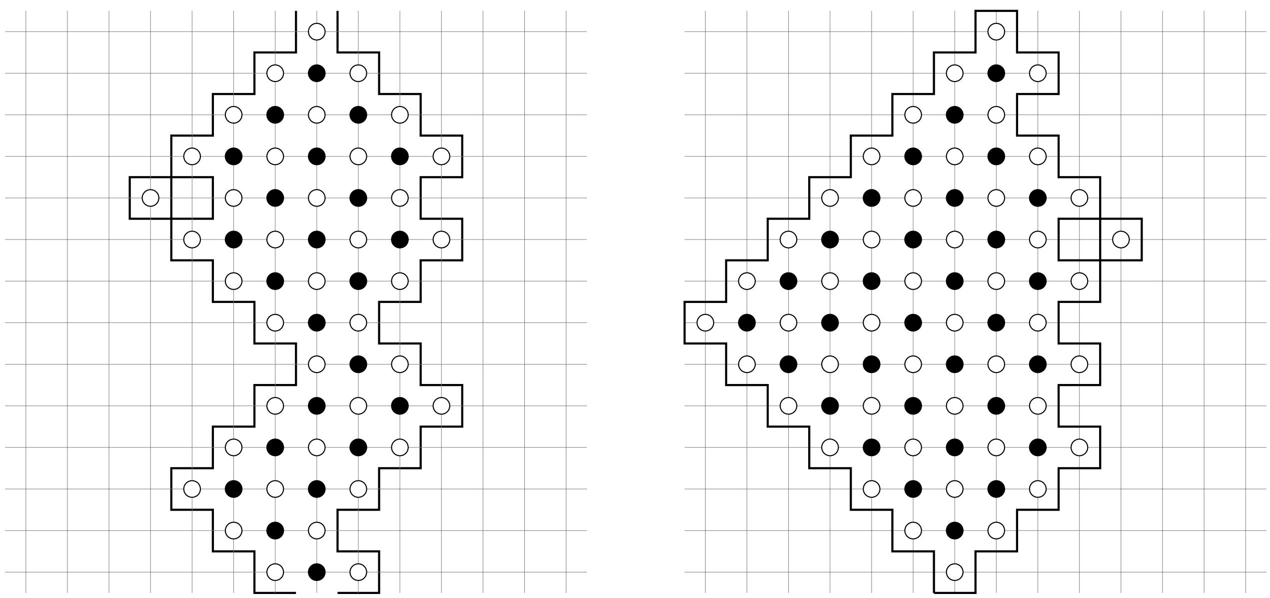

Figure 4: An example of a configuration in $\mathcal{C}_{mb}(\mathbf{e},\mathbf{o})$ (on the left) and one in $\mathcal{C}_{ib}(\mathbf{e},\mathbf{o})$ (on the right).

- $\mathcal{C}_{sb}(\mathbf{e},\mathbf{o})$, $\mathcal{C}_{mb}(\mathbf{e},\mathbf{o})$, and $\mathcal{C}_{ib}(\mathbf{e},\mathbf{o})$ the collections of configurations with a unique cluster of particles at odd sites with at most two additional empty even sites as in Fig. 3 (right) and in Fig. 4. In particular, $\mathcal{C}_{sb}(\mathbf{e},\mathbf{o})$ contains the configurations with $\frac{L}{2}-1$ particles arranged in an odd column with two other empty even sites; $\mathcal{C}_{mb}(\mathbf{e},\mathbf{o})$ contains the configurations obtained from $\mathcal{C}_{sb}(\mathbf{e},\mathbf{o})$ such that there is at least one column or row with $\frac{L}{2}$ particles arranged in odd sites. $\mathcal{C}_{ib}(\mathbf{e},\mathbf{o})$ contains the configurations obtained from $\mathcal{C}_{sb}(\mathbf{e},\mathbf{o})$ without having column or row with $\frac{L}{2}$ particles.