METASTABILITY IN GLAUBER DYNAMICS IN THE LOW-TEMPERATURE LIMIT: BEYOND EXPONENTIAL ASYMPTOTICS

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ABSTRACT. We consider Glauber dynamics of classical spin systems of Ising type in the limit when the temperature tends to zero in finite volume. We show that information on the structure of the most profound minima and the connecting saddle points of the Hamiltonian can be translated into *sharp* estimates on the distribution of the times of *metastable* transitions between such minima as well as the low lying spectrum of the generator. In contrast with earlier results on such problems, where only the asymptotics of the exponential rates is obtained, we compute the precise pre-factors up to multiplicative errors that tend to 1 as $T \downarrow 0$. As an example we treat the nearest neighbor Ising model on the 2 and 3 dimensional square lattice. Our results improve considerably earlier estimates obtained by Neves-Schonmann [NS], Ben Arous-Cerf [BC] and Alonso-Cerf [AC]. Our results employ the methods introduced by Bovier, Eckhoff, Gayrard, and Klein in [BEGK1,BEGK2].

1. INTRODUCTION.

Controlling the transitions from metastable states to equilibrium in the stochastic dynamics of lattice spin systems at low temperatures has been and still is a subject of considerable interest in statistical mechanics. The first mathematically rigorous results can be traced back to the work of Cassandro et al. [CGOV] that initiated the so-called "path-wise approach" to metastability. For a good review of the earlier literature, see in particular [Va]. All the mathematical investigations in the subject require some 'small parameter' that effectively makes the timescales for metastable phenomena 'large'. The somewhat simplest of these limiting situations is the case when a system in a finite volume $\Lambda \subset \mathbb{Z}^d$ is studied for small values of the temperature $T = 1/\beta$. In systems with discrete spin space one is then in the situation where the dynamics can be considered as a small perturbation of a deterministic process, a situation very similar to what Freidlin and Wentzell [FW] called 'Markov chains with exponentially small transition probabilities'. Consequently, most of the work

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concerning this situation [OS1,OS2,C,CC,BC,N,NS] can be seen as extensions and improvements of the *large deviation* approach initiated by Freidlin and Wentzell. This consists essentially in identifying the most likely path (in the sense of a sequence of transitions) and proving a large deviation principle on path-space. While this approach establishes very detailed information on e.g. the typical exit paths from metastable states, the use of large deviations methods entails a rather limited precision. Results for e.g. exit times τ are therefore typically of the following type: For any $\varepsilon > 0$,

$$\mathbb{P}\left(e^{\beta(\Delta-\varepsilon)} < \tau < \varepsilon^{\beta(\Delta+\varepsilon)}\right) \uparrow 1, \text{as } \beta \uparrow \infty$$

where Δ can be computed explicitly. Similarly, one has results on eigenvalues of the generator that are of the form

$$\lim_{\beta\uparrow\infty} \beta^{-1} \ln \lambda_i(\beta) = \gamma_i$$

with explicit expressions for the γ_i (see e.g. [FW,S]). From many points of view, the precision of such results is not satisfactory, and rather than just exponential rates, one would in many situations like to have precise expressions that also provide the precise pre-factors. This is particularly important if one wants to understand the dynamics of systems with a very complex structure of metastable states, and in particular *disordered* systems. (For a rather dramatic illustration, see e.g. [BBG1,BBG2] where aging phenomena in the random energy model are studied.) Another drawback of the large deviation methods employed is that they are rather heavy handed and require a *very detailed knowledge* of the entire energy landscape, a requirement that frequently cannot be met. Sharper estimates on eigenvalues are obtained by Miclo [Mi], using a variational approach and techniques inspired by the work of Holley, Kusuoka, and Strook [HKS] that obtained estimates on the first eigenvalues only. In fact Miclo gave upper and lower bounds on eigenvalues that differ only by a constant. In two recent papers [BEGK1,BEGK2] a somewhat new approach to the problem of metastability has been initiated aiming at improving the precision of the results while reducing at the same time the amount of information necessary to analyze a given model. To achieve this goal, the attempt to construct the precise exit paths is largely abandoned, as are, to a very large extent, large deviation methods.
The general structure of this approach is as follows. In [BEGK2] the notion of a *set of metastable points* is introduced. The definition of this set employs only one type of objects, namely *Newtonian capacities* (which may also be interpreted as *escape probabilities*). If such a set of metastable points can be identified, [BEGK2] provides a general theorem that yields precise asymptotic formula for the *mean exit time* from each metastable state, shows that this time is asymptotically exponentially distributed (in a strong sense), and states that each mean exit time is the inverse of one small eigenvalue of the generator. While [BEGK2] assumes reversibility of the dynamics, in [E] is shown that similar results can be obtained in the general case. Thus, the analysis of metastability is essentially reduced to the computation

of Newtonian capacities. The great advantage of such a result is that capacities are particularly easy to estimate, due to the fact that they verify a particularly manageable *variational principle*. This fact is well known and has been exploited in the analysis of transience versus recurrence properties of Markov chains (see e.g. [DS]); however, its particular usefulness in the context of metastability seems to have been noticed only in [BEGK1] where it was used in the context of reversible discrete diffusion processes motivated from certain mean field spin systems.
In this short paper we will show that the approach is even more efficient and simple in the context of the zero temperature limit of Glauber dynamics of spin systems in finite volume. We will show that capacities in this limit can be computed virtually exactly in terms of properties of the *energy landscape*, and therefore all interesting properties of the dynamics can be inferred from a (not overly detailed) analysis of the energy landscape generated by the Hamiltonian considered. As a particular application that should illustrate the power of our approach, we apply the general results to the Ising model (in two and three dimension).

2. The general setting and the main theorem.

In this section we set up the general context to which our results will apply. It will be obvious that Glauber dynamics of finite volume spin systems at low temperatures provide particular examples. We will consider Markov processes on a finite state space Ω (the *configuration space*). To define the dynamics, we need the following further objects.

(1) A *connected graph* $\mathcal{G}$ on Ω. We denote by $E(\mathcal{G})$ the set of the edges in $\mathcal{G}$.
(2) A *Hamiltonian* $H : \Omega \to \mathbb{R}$ also called *energy*.
(3) The *Gibbs measure* $\mathbb{Q}(x) := \frac{1}{\mathcal{Z}} \exp(-\beta H(x))$, where $\mathcal{Z}$ is the normalization factor called partition function, and β is the *inverse temperature*.

We consider *transition probabilities* $P(x, y)$ such that if $\{x, y\} \in E(\mathcal{G})$, $P(x, y) > 0$, and $P(x, y) = 0$ if $x \neq y$ and $\{x, y\} \notin E(\mathcal{G})$. We assume moreover that the transition probabilities are reversible with respect to the Gibbs measure, i.e.

$$\mathbb{Q}(x)P(x, y) = \mathbb{Q}(y)P(y, x). \tag{2.1}$$

We will also make the simplifying assumption that any existing transition in the graph is reasonably strong, i.e. we assume that there exists a constant $C > 0$ such that[1]

$$P(x, y) + P(y, x) \geq C \quad \forall \ \{x, y\} \in E(\mathcal{G}), \tag{2.2}$$

[1]The constant C will typically be of the order of the inverse of the maximum coordination number of the graph $\mathcal{G}$.

by reversibility, (2.2) is equivalent to

$$P(x,y) \geq \frac{C}{1+\exp(-\beta(H(y)-H(x)))} \quad \forall\ \{x,y\} \in E(\mathcal{G}). \tag{2.3}$$

To be able to state our results we need some further notations.

(1) Given a one-dimensional subgraph ω, we write $\omega : x \to I$ if the subgraph has one end in x and the other end in I. One dimensional subgraphs have a natural parameterization $\omega_0, \dots, \omega_K$, where $K := |\omega| - 1$, $\forall k = 0, \dots, K-1$ $\{\omega_k, \omega_{k+1}\} \in E(\mathcal{G})$ and $\omega : \omega_0 \to \omega_K$.

(2) For $A \subset \Omega$, let $\widetilde{H}(A) := \max_{z\in A} H(z)$. For $x \in \Omega$ and $I \subset \Omega$, we introduce the *communication height*, $\widehat{H}(x, I)$, between x and I as

$$\widehat{H}(x,I) := \min_{\omega : x \to I} \widetilde{H}(\{\omega\}). \tag{2.4}$$

Moreover we define the set of *saddle points* for x and I by

$$\mathcal{S}_{x,I} := \left\{ z \in \Omega\ ;\ \exists\ \omega : x \to I \text{ with } z \in \omega \text{ and } H(z) = \widetilde{H}(\{\omega\}) \right\} \tag{2.5}$$

(3) For any set $A \subset \Omega$, we define its *outer boundary* ∂A as the set of all points in A from which an edge of $\mathcal{G}$ leads to its complement, A^c.

(4) Let us assume that the saddles $z \in \mathcal{S}_{x,I}$ are *isolated* and *simple*, namely, they are not connected to each other by an edge of the graph and such that for any such $z \in \mathcal{S}_{x,I}$ there exists $\omega : z \to x$ with $\widetilde{H}(\{\omega\} \setminus z) < H(z)$.
Then, there exists a surface Z with the following properties:
(a) $\mathcal{S} := \mathcal{S}_{x,I} \subset Z$
(b) $\exists \delta > 0$ such that $\forall z \in Z \setminus \mathcal{S}$, $H(z) \geq H(\mathcal{S}) + \delta$.
(c) Z is the outer boundary of a connected set D that contains x.
An example of such a surface is the outer boundary of the set

$$D_x^I := \{ z\ ;\ H(\mathcal{S}_{z,x}) < H(\mathcal{S}_{z,I}) \} \tag{2.6}$$

(5) With respect to this surface Z, for $z \in Z$, let $\check{p}_z := \sum_{x' \in D} P(z,x')$ and $\hat{p}_z := \sum_{y' \in \Omega\setminus D\setminus z} P(z,y')$. We set

$$\mathcal{C}_{x,I} := \sum_{z \in \mathcal{S}_{x,I}} \frac{\hat{p}_z \check{p}_z}{\hat{p}_z + \check{p}_z}. \tag{2.7}$$

It is immediate to see that different choices of Z give, up to errors of order $e^{-\beta\delta}$, the same value for $\mathcal{C}_{x,I}$ (as well as for $\check{p}_z$ and $\hat{p}_z$ if $z \in \mathcal{S}_{x,I}$).

(6) Let $W_x := \{y\ ;\ H(y) < H(x)\}$. For $x \in \Omega$, we set $\Gamma(x) := H(\mathcal{S}_{x,W_x}) - H(x)$. If x is not a local minimum of the Hamiltonian, $\Gamma(x) = 0$. If x is a global minimum of the Hamiltonian, we set $\Gamma(x) = \infty$.

(7) For the process X_t starting at x, we define the *hitting time* to the set $I \subset \Omega$ as $\tau_I^x := \inf\{0 < t \in \mathbb{N}\ ;\ X_t \in I\}$.

(8) We denote by $\widetilde{\mathcal{M}}$ the set of all *local minima* of H. We call a subset $\mathcal{M} \subset \widetilde{\mathcal{M}}$ a set of *metastable states*, if a point that realizes the absolute minimum of H is contained in $\mathcal{M}$ and if, for all $y \in \widetilde{\mathcal{M}} \backslash \mathcal{M}$, $\Gamma(y) < \min_{x \in \mathcal{M}} \Gamma(x)$. It is important to realize that for given H, $\mathcal{M}$ may often be chosen in different ways. The idea will be that we will observe the process only at its visits to $\mathcal{M}$. Thus, the actual choice of $\mathcal{M}$ will depend on how much information we want to retain about the detailed behavior of the process. Note that this definition implies that for all $z \notin \mathcal{M}$, $\widehat{H}(z, \mathcal{M}) \geq \widehat{H}(z, W_z)$.[2]

(9) Finally, for $x \in \mathcal{M}$, we need to define the quantity

$$N_x := \# \left\{ z \in \Omega : \left\{ H(z) = H(x) \right\} \cap \left\{ \widehat{H}(x, z) < \widehat{H}(x, \mathcal{M} \backslash x) \right\} \right\},$$

which represents the degeneracy of the minima of the Hamiltonian.

We can now formulate the main general result of this paper in the general setting. Let us consider some set $\mathcal{M}$ of metastable points. To be able to formulate concise and general results, we make some further assumptions that will be true for "generic" Hamiltonians.[3]

(h1) For any $x \neq y \in \mathcal{M}$, $\Gamma(x) \neq \Gamma(y)$.

(h2) For any $x \neq y \in \mathcal{M}$, the saddles in $\mathcal{S}_{x,y}$ are isolated and simple[4].

Theorem 2.1. *Let $\mathcal{M}$ be a set of metastable states for the Hamiltonian H satisfying the conditions (h1) and (h2) above. For $x \in \mathcal{M}$, set $\mathcal{M}_x := \{y \in \mathcal{M} \ ; \ H(y) < H(x)\} = \mathcal{M} \cap W_x$. Let $\tau(x) := \tau^x_{\mathcal{M}_x}$, $\mathcal{S} := \mathcal{S}_{x,W_x}$ and $\mathcal{C}_x := \mathcal{C}_{x,W_x}$. Then there exists $\delta > 0$, independent of β, such that for any $x \in \mathcal{M}$,*

(i)

$$\mathbb{E}\ \tau(x) = N_x \mathcal{C}_x^{-1} e^{\beta \Gamma(x)} (1 + o(e^{-\beta\delta})) \tag{2.8}$$

(ii) there exists an eigenvalue λ_x of $1 - P$ such that

$$\lambda_x = \frac{1}{\mathbb{E}\ \tau(x)} (1 + o(e^{-\beta\delta})) \tag{2.9}$$

(iii) if ϕ_x is the right-eigenvector of P corresponding to λ_x, normalized so that $\phi_x(x) = 1$, then

$$\phi_x(y) = \mathbb{P}\left(\tau^y_x < \tau^y_{\mathcal{M}_x}\right) + o(e^{-\delta\beta}) \tag{2.10}$$

[2]Given a real parameter γ, we can define the set $\mathcal{M}(\gamma)$ as the set of all local minima $x \in \widetilde{\mathcal{M}}$ such that $\Gamma(x) \geq \gamma$. Obviously, $\mathcal{M}(\gamma) \subset \mathcal{M}(\gamma')$ if $\gamma \geq \gamma'$.

[3]Note that for any Hamiltonian, one may select different sets of metastable points. The requirements (h1) and (h2) depend on the Hamiltonian as well as on the choice of $\mathcal{M}$. In the case of the Ising model treated in §5, hypothesis (h1) is true only for $\mathcal{M} = \{-\mathbf{1}, +\mathbf{1}\}$ (all minuses and all pluses), while hypothesis (h2) is true only if the magnetic field does not assume certain values. If hypothesis (h1) or (h2) fails, the pre-factor in (2.8) does not assume the simple form $N_x \mathcal{C}_x^{-1}$, but it is still possible to compute it by using our procedure.

[4]In the appendix we will explain how one can proceed to obtain comparable results in the case when this condition is not satisfied.

(iv) $\forall t > 0$

$$\mathbb{P}\left(\tau(x) > t\,\mathbb{E}\,\tau(x)\right) = e^{-t(1+o(e^{-\beta\delta}))}(1+o(e^{-\beta\delta})) \tag{2.11}$$

In Section 5, we will apply Theorem 2.1 to a well known situation, the kinetic Ising model, in the limit of vanishing temperature.
Let us anticipate our main result about the kinetic Ising model, referring to Section 5 for precise definitions and notation.

Theorem 2.2. *Consider the kinetic Ising model with Metropolis dynamics in dimension $d = 2$ or $d = 3$ in a torus $\Lambda^d(l)$ with diameter l. The magnetic field $0 < h < 1$ will be chosen (depending on the dimension) such that the genericity assumptions hold.*
Then, the two configurations $-\mathbf{1}$ (all minus spins) and $+\mathbf{1}$ (all plus spins) form a metastable set (if the magnetic field h is positive, $+\mathbf{1}$ is stable), and

- *In dimension 2, let h be such that $2/h$ is not an integer. Let $\ell_2 := \lceil \frac{2}{h} \rceil$ and $\Gamma_2 := 4\ell_2 - h\left(\ell_2^2 - \ell_2 + 1\right)$ be the diameter and the activation energy of the "critical droplet", respectively. Then,*

$$\mathbb{E}\tau(-\mathbf{1}) = \frac{3}{8}\frac{1}{\ell_2 - 1}e^{\beta\Gamma_2}(1+o(e^{-\beta\delta})) = \frac{3}{16}he^{\beta\Gamma_2}(1+O(h)+o(e^{-\beta\delta})) \tag{2.12}$$

- *In dimension 3, let h be such that $2/h$ and $(h/2\,\lceil 4/h\rceil\,(4/h+1-\lceil 4/h\rceil))$ are not integer. Let $\ell_3 := \lceil \frac{4}{h} \rceil$ and $a := \lceil h/2\,\lceil 4/h\rceil\,(4/h+1-\lceil 4/h\rceil)\rceil$ (notice that a can take the value 1 or 2). The activation energy of the "critical droplet" is*

$$\Gamma_3 := \left(6\ell_3^2 - (12-4a)\ell_3 + 4\ell_2 + 4 - 2a\right) - h\left(\ell_3^3 - (3-a)\ell_3^2 + (2-a) + \ell_2^2 - \ell_2 + 1\right).$$

Then,

$$\begin{aligned}\mathbb{E}\tau(-\mathbf{1}) &= \frac{a}{16}\frac{1}{(\ell_3-\ell_2+1)(\ell_3-\ell_2+a-1)(\ell_2-1)}e^{\beta\Gamma_3}(1+o(e^{-\beta\delta})) \\ &= \frac{a}{128}h^3e^{\beta\Gamma_3}(1+O(h)+o(e^{-\beta\delta}))\end{aligned} \tag{2.13}$$

Here as in Theorem 2.1, $\delta > 0$ is independent of β (but depends on arithmetic properties of h).

Remark. Note that in our model we flip at most one spin per time step. In continuous time dynamics the mean transition times would be lowered by a factor $1/|\Lambda|$.
The above Theorem shows how the results of Theorem 2.1 can be applied (via the analysis of the energy landscape carried out for the Ising model in [NS] and [AC,BC]) to the so-called Freidlin-Wentzell regime. Notice that the methods of [BEGK2] can be applied in a very similar way to situations where the volume grows with β to compute "exactly" the probability of first appearance of a critical droplet (a preliminary problem for the infinite-volume metastability carried out in [DeSc]).

3. Basic tools.

Theorem 2.1 relies on Theorem 1.3 in [BEGK2] that links relative capacities of metastable sets to mean exit times and to the low lying spectrum of $1-P$. The additional work needed to prove Theorem 2.1 will be to estimate capacities in terms of the Hamiltonian H, and to show that the hypotheses of Theorem 1.3 in [BEGK2] are satisfied in our setting.
Let us state Theorem 1.3 in [BEGK2] specialized to our case.[5]
In their context, a set $\mathcal{M} \in \Omega$ is called a set of *metastable points* in the sense of [BEGK2] if

$$\frac{\sup_{x\neq y\in\mathcal{M}} \mathbb{P}\left(\tau_y^x < \tau_x^x\right)}{\inf_{z\in\Omega} \mathbb{P}\left(\tau_{\mathcal{M}}^z \leq \tau_z^z\right)} \to 0 \text{ as } \beta\to\infty. \tag{3.1}$$

The set $\mathcal{M}$ is *generic* in the sense of [BEGK2] if for any $x, y \in \mathcal{M}$, and $I \subset \mathcal{M}\backslash\{x,y\}$, $\frac{\mathbb{P}\left(\tau_I^x<\tau_x^x\right)}{\mathbb{P}\left(\tau_I^y<\tau_y^y\right)}$ tends either to zero or to infinity, as $\beta\uparrow\infty$, and if the absolute minimum of the Hamiltonian is not degenerate.

Theorem 3.1. (Theorem 1.3 in [BEGK2]) *Let $\mathcal{M}$ be a generic set of metastable states in the sense of [BEGK2], and let for $x\in\mathcal{M}$, $\mathcal{M}_x$ and $\tau(x)$ be defined as in Theorem 2.1. Then, for any $x\in\mathcal{M}$, the following holds:*

(i)

$$\mathbb{E}\,\tau(x) = \frac{N_x}{\mathbb{P}\left(\tau_{\mathcal{M}_x}^x < \tau_x^x\right)}(1+o(1)) \tag{3.2}$$

(ii) for any $x\in\mathcal{M}$, there exists an eigenvalue λ_x of $1-P$ such that

$$\lambda_x = \frac{1}{\mathbb{E}\,\tau(x)}(1+o(1)), \tag{3.3}$$

moreover, the eigenvalues of $1-P$ not corresponding to any $x\in\mathcal{M}$ are in the interval $(c|\Omega|^{-1}\inf_{z\in\Omega}\mathbb{P}\left(\tau_{\mathcal{M}}^z<\tau_z^z\right),2]$ for some positive constant c.

(iii) if ϕ_x is the right-eigenvector of P corresponding to λ_x, normalized so that $\phi_x(x)=1$, then

$$\phi_x(y) = \mathbb{P}\left(\tau_x^y < \tau_{\mathcal{M}_x}^y\right) + o(1) \tag{3.4}$$

(iv) for any $x\in\mathcal{M}$, for any $t>0$,

$$\mathbb{P}\left(\tau(x) > t\,\mathbb{E}\,\tau(x)\right) = e^{-t(1+o(1))}(1+o(1)). \tag{3.5}$$

Here $o(1)$ stands for a small error that depends only on the small parameters introduced via (3.1) and the non-degeneracy condition following it.

[5] This Theorem is stated in [BEGK2] in a context where the space and the metastable set depend on the parameter β. The correspondence between the symbols in the two papers is the following: $N\to\beta$, $\Gamma_N\to\Omega$, $\mathcal{M}_N\to\mathcal{M}$, $\varepsilon_N\to\exp(-\beta\text{const.})$, $R_x\to N_x^{-1}$, $r_N\to\text{const.}$, $c_N\to\text{const.}$

Theorem 2.1 will follow from Theorem 3.1 since in the finite-volume and $\beta \to \infty$ regime, we compute $\mathbb{P}\left(\tau^x_{\mathcal{M}_x} < \tau^x_x\right)$ and show that local minima of the Hamiltonian are metastable states giving at the same time the value of the nucleation rate in the limit $\beta \to \infty$.
The key estimate is the following Lemma.

Lemma 3.2. *$\forall x, y \in \widetilde{\mathcal{M}}$ such that $\mathcal{S}_{x,y}$ is a set of isolated single points, $\forall \delta > 0$,*

$$\mathbb{P}\left(\tau^x_y < \tau^x_x\right) = \mathcal{C}_{x,y} e^{-\beta(H(\mathcal{S}_{x,y}) - H(x))}(1 + o(e^{-\beta\delta})). \tag{3.6}$$

We will explain in the appendix how our method can be extended to situations where the saddles are degenerate. In this case the pre-factor $\mathcal{C}_{x,y}$ does not have the nice form in (2.7) but can still be computed explicitly in terms of small "local variational problems".

Lemma 3.3. *Let x be a minimum for the Hamiltonian. Then, the set $\mathcal{M} := \{y \ ; \ \Gamma(y) \geq \Gamma(x)\}$ is a set of metastable state (in the sense of [BEGK2]).*

Clearly, Theorem 2.1 immediately follows from Theorem 3.1, Lemma 3.2 and Lemma 3.3. Notice that hypothesis (h1) and Lemma 3.2 ensure that the set $\mathcal{M}$ is generic in the sense of [BEGK2].

4. Proof of Lemmata 3.2 and 3.3.

In order to prove Lemmata 3.2 and 3.3, we make use of many ideas contained in [BEGK1].
The following Lemma corresponds to Theorem 6.1 in [Li].

Lemma 4.1. *(Dirichlet representation).*
Let $\mathcal{H}^x_y := \{h : \Omega \to [0,1] \ ; \ h(x) = 0, h(y) = 1\}$ and

$$\Phi(h) := \frac{1}{\mathcal{Z}} \sum_{x', x'' \in \Omega} e^{-\beta H(x')} P(x', x'')[h(x') - h(x'')]^2. \tag{4.1}$$

Then,

$$\frac{e^{-\beta H(x)}}{\mathcal{Z}} \mathbb{P}\left(\tau^x_y < \tau^x_x\right) = \frac{1}{2} \inf_{h \in \mathcal{H}^x_y} \Phi(h) \tag{4.2}$$

Proof. See [Li], Chapter II.6. □

Note that the left-hand side of (4.2) has the potential-theoretic interpretation of the *Newtonian capacity* of the point y relative to x (i.e. the electric charge induced on the grounded site x when the potential is set to 1 on the site y). The Dirichlet form is just the electric energy, and the minimizer h^* is the *equilibrium potential*, with the probabilistic interpretation $h^*(z) = \mathbb{P}\left(\tau^z_y < \tau^z_x\right)$. For an extensive treatment of potential theory in the context of discrete Markov chains, see e.g. [So].

The strength of this variational representation comes from the monotonicity of the Dirichlet form in the variables $P(x', x'')$, expressed in the next Lemma, known as Rayleigh's short-cut rule (see Lemma 2.2 in [BEGK1]):

Lemma 4.2. *Let Δ be a subgraph of $\mathcal{G}$ and let $\widetilde{\mathbb{P}}_\Delta$ denote the law of the Markov chain with transition rates, for $u \neq v$, defined by $\widetilde{P}_\Delta(u,v) := P(u,v)\mathbb{I}\{\{u,v\} \in E(\Delta)\}$. If x and y are vertices in Δ, then*

$$\mathbb{P}\left(\tau_y^x < \tau_x^x\right) \geq \widetilde{\mathbb{P}}_\Delta\left(\tau_y^x < \tau_x^x\right) \tag{4.3}$$

Proof. The proof follows from Lemma 4.1 using the monotonicity of the Dirichlet form in the transition probabilities and can be found in [BEGK1]. □

The following Lemma corresponds to Lemma 2.5 in [BEGK1] and is a well known fact (see e.g. [DS]).

Lemma 4.3. (The one dimensional case).
Let ω be a one-dimensional subgraph of $\mathcal{G}$, $K := |\omega| - 1$ and let $\{\omega_n\}_n : \{0, \dots, K\} \to \Omega$ be such that $\forall n \leq K$, $\{\omega_n, \omega_{n-1}\} \in E(\mathcal{G})$

$$\widetilde{\mathbb{P}}_\omega\left(\tau_{\omega_K}^{\omega_0} < \tau_{\omega_0}^{\omega_0}\right) = \left[\sum_{n=0}^{K-1} \frac{e^{-\beta(H(\omega_0)-H(\omega_n))}}{P(\omega_n, \omega_{n+1})}\right]^{-1} \tag{4.4}$$

Remark: Lemmata 4.2, 4.3 and (2.2) immediately give the following bound: $\forall x', I$ s.t. $\mathcal{S}_{x',I}$ is made of simple points,

$$\begin{aligned}
\mathbb{P}\left(\tau_I^{x'} < \tau_{x'}^{x'}\right) &\geq \left[\sum_{n=0}^{K-1} \frac{e^{-\beta(H(x')-H(\omega_n))}}{P(\omega_n, \omega_{n+1})}\right]^{-1} \\
&\geq C\left[\sum_{n=0}^{K-1} \left(e^{-\beta(H(x')-H(\omega_n))} + e^{-\beta(H(x')-H(\omega_{n+1}))}\right)\right]^{-1} \\
&\geq \frac{C}{2} e^{-\beta(H(\mathcal{S}_{x',I})-H(x'))}\left(1 - Ke^{-\beta\delta}\right)
\end{aligned} \tag{4.5}$$

for any choice of the subgraph $\omega : x' \to I$ having its maximum energy in $\mathcal{S}_{x',I}$. The constant C is the same as in (2.3), while δ is a suitable constant related to the energy gap among the saddle and the other points in the one-dimensional subgraph.

Proof of Lemma 3.2. Let $\Gamma := H(\mathcal{S}_{x,y}) - H(x)$.
We consider the surface $Z := \partial D_x^y$.
We set $D_x := D_x^y$, $D_y := \Omega \setminus (Z \cup D_x)$, $Z^- := \partial Z \cap D_x$ and $Z^+ := \partial Z \cap D_y$.
(1) The upper bound.
We use Lemma 4.1 with $h(x') := 0$ if $x' \in D_x$ and $h(y') := 1$ if $y' \in D_y$; we choose $h(z)$ for $z \in Z$ in an optimal way.

We have

$$\mathbb{P}\left(\tau_y^x < \tau_x^x\right) \leq \frac{\mathcal{Z}e^{\beta H(x)}}{2}\Phi(h) =$$
$$= \sum_{z\in Z} e^{-\beta(H(z)-H(x))}\left(\check{p}_z h^2(z) + \hat{p}_z(1-h(z))^2\right) + o(e^{-\beta\delta}), \tag{4.6}$$

where we used reversibility. The small error comes from the mismatch on the boundary of D_x that lies higher than the saddle hight.
The quadratic form $\check{p}h^2 + \hat{p}(1-h)^2$ has a minimum for $h = \frac{\hat{p}}{\hat{p}+\check{p}}$. Hence, we can saturate the inequality (4.6) and get

$$(\text{l.h.s. of (4.6)}) \ \leq \mathcal{C}_{x,y} e^{-\beta\Gamma}\left(1 + e^{-\beta\delta}\right). \tag{4.7}$$

(2) The lower bound.
We consider the subgraph Δ obtained by cutting all the connections to the vertices in $Z \setminus \mathcal{S}$.
We use Lemma 4.2 to bound the original process by the restricted process.
We use (4.5) to estimate the probability to reach $x' \in Z^-$ and the probability to go from $y' \in Z^+$ to y:
By the strong Markov property at time $\tau_{\mathcal{S}}^x$, we have

$$\begin{aligned}\widetilde{\mathbb{P}}_\Delta\left(\tau_y^x < \tau_x^x\right) &= \sum_{z\in\mathcal{S}} \widetilde{\mathbb{P}}_\Delta\left(\tau_z^x \leq \tau_{\mathcal{S}\cup x}^x\right)\widetilde{\mathbb{P}}_\Delta\left(\tau_y^z < \tau_x^z\right) \\ &= e^{-\beta\Gamma}\sum_{z\in\mathcal{S}} \widetilde{\mathbb{P}}_\Delta\left(\tau_x^z < \tau_{\mathcal{S}}^z\right)\widetilde{\mathbb{P}}_\Delta\left(\tau_y^z < \tau_x^z\right), \end{aligned}\tag{4.8}$$

where we used reversibility.
Now,

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_x^z < \tau_{\mathcal{S}}^z\right) = \sum_{x'\in Z^-} P\left(z, x'\right)\widetilde{\mathbb{P}}_\Delta\left(\tau_x^{x'} < \tau_{\mathcal{S}}^{x'}\right). \tag{4.9}$$

We bound the last factor using a standard renewal argument (see e.g. [BEGK1] Corollary 1.6) that yields if $z' \in D_x$ the last term is exponentially close to 1:

$$\begin{aligned}\widetilde{\mathbb{P}}_\Delta\left(\tau_{\mathcal{S}}^{x'} < \tau_x^{x'}\right) &= \frac{\widetilde{\mathbb{P}}_\Delta\left(\tau_{\mathcal{S}}^{x'} < \tau_{x\cup x'}^{x'}\right)}{\widetilde{\mathbb{P}}_\Delta\left(\tau_{x\cup\mathcal{S}}^{x'} < \tau_{x'}^{x'}\right)} \leq \frac{e^{-\beta\Gamma}\sum_{z\in\mathcal{S}}\widetilde{\mathbb{P}}_\Delta\left(\tau_{x'}^z < \tau_{x\cup\mathcal{S}}^z\right)}{\widetilde{\mathbb{P}}_\Delta\left(\tau_x^{x'} < \tau_{x'}^{x'}\right)} \\ &\leq \frac{|\mathcal{S}|e^{-\beta\Gamma}}{Ce^{-\beta(\Gamma-\delta')}\left(1-e^{-\beta\delta'}\right)} \leq e^{-\beta\delta}, \end{aligned}\tag{4.10}$$

where we used (4.5). By putting together (4.9) and (4.10) we get

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_x^z < \tau_{\mathcal{S}}^z\right) \geq \check{p}_z\left(1 - e^{-\beta\delta}\right) \tag{4.11}$$

We use the same procedure to bound the last term in (4.8):

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_y^z < \tau_x^z\right) \geq \sum_{y'\in Z^+} P\left(z, y'\right)\widetilde{\mathbb{P}}_\Delta\left(\tau_y^{y'} < \tau_x^{y'}\right). \tag{4.12}$$

Again, the same arguments leading to (4.10) show that the last term in this sum is exponentially close to 1:

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_x^{y'} < \tau_y^{y'}\right) \leq \frac{|\mathcal{S}|e^{-\beta(H(z)-H(y'))}}{e^{-\beta(H(\mathcal{S}_{y,y'})-H(y'))}\left(1-e^{-\beta\delta'}\right)} \leq e^{-\beta\delta} \tag{4.13}$$

We put together (4.12) and (4.13) and get

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_y^z < \tau_x^z\right) \geq \frac{\hat{p}_z}{\hat{p}_z + \check{p}_z}(1-e^{-\beta\delta}) \tag{4.14}$$

Going back to (4.8), we get from (4.11), (4.14)

$$\widetilde{\mathbb{P}}_\Delta\left(\tau_y^x < \tau_x^x\right) \geq \mathcal{C}_{x,y}e^{-\beta\Gamma}\left(1-e^{-\beta\delta}\right) \tag{4.15}$$

□

Proof of Lemma 3.3. For any $z \notin \mathcal{M}$ we know that by definition of $\mathcal{M}$, we have that $\Gamma(z) < \min_{x\in\mathcal{M}}\Gamma(x) \equiv \Gamma$. In view of Lemma 3.2 and the lower bound (4.5) we only need to show that this implies that $\widehat{H}(z,\mathcal{M}) - H(z) < \Gamma$. Now let $u \notin \mathcal{M}$ be the point that realizes the minimum of the energy among the states such that $\widehat{H}(z,u) < \widehat{H}(z,\mathcal{M})$. so that $\widehat{H}(u,W_u) \geq \widehat{H}(z,\mathcal{M})$. Moreover, since $u \notin \mathcal{M}$, $\widehat{H}(u,W_u) - H(u) = \Gamma(u) < \Gamma$. Hence,, $\widehat{H}(z,\mathcal{M}) - H(z) \leq \widehat{H}(u,W_u) - H(u) < \Gamma$, and we are done. □

5. The Ising case.

In this section we want to illustrate the strength of Theorem 2.1 in a well known context, namely the stochastic Ising model on the d-dimensional lattice. In this case the state space is $\Omega = \{-1,+1\}^\Lambda$, where $\Lambda = \Lambda(L)$ is a torus in $\mathbb{Z}^d$ with side-length L. For $\sigma \in \Omega$, the Hamiltonian is then given by

$$H(\sigma) \equiv H_\Lambda(\sigma) = -\frac{1}{2}\sum_{<i,j>\in\Lambda}\sigma_i\sigma_j - h\sum_{i\in\Lambda}\sigma_i, \tag{5.1}$$

where the first sum concerns all the pairs of nearest neighbor sites in Λ.
Let σ^i be the configuration that differs from σ only in the value of the spin of site i and $[a]_+$ denote the positive part of the real number a. We will consider for definiteness only the case of the Metropolis dynamics, i.e. the transition probabilities are chosen

$$P(\sigma,\sigma') = \frac{e^{-\beta[H(\sigma')-H(\sigma)]_+}}{|\Lambda|}, \text{ if } \sigma' = \sigma^i, i \in \Lambda \tag{5.2}$$

$$P(\sigma,\sigma) = 1 - \sum_{i\in\Lambda}P(\sigma,\sigma^i) \tag{5.3}$$

and all others are zero.

We will use the estimate given in Theorem 2.1 to analyze this dynamics in a finite volume Λ, under a positive magnetic field, in the limit when $\beta \uparrow \infty$.
Let $-\mathbf{1}$ and $+\mathbf{1}$ be the configurations full of minuses or full of pluses, respectively. We will show in Lemma 5.2 that $\{-\mathbf{1}, +\mathbf{1}\}$ is a set of metastable states. Apart from this characterization, we will only use the description of the energy landscape given in [NS], [AC,BC] and [N] in dimension 2, 3 or larger, respectively. We will show that the methods of Theorem 2.1 allow to improve the known estimates without requiring further analysis of the energy landscape. In dimension 2 and 3, the improvement amounts to the computation of the exact (including the pre-factor $\mathcal{C}_{-\mathbf{1},+\mathbf{1}}$) asymptotic value of the expected transition time τ_+^- needed to reach $+\mathbf{1}$ starting from $-\mathbf{1}$ (that by Theorem 3.1 is the inverse of the spectral gap of P). In higher dimension, where our knowledge of the energy landscape is not so detailed, we cannot compute the pre-factor but we show that it is a constant independent of β, while previous results only gave sub-exponential bounds.
We remark that, unlike the exponential factor $\exp(-\beta\Gamma(-\mathbf{1}))$ (that only depends on the graph structure), the pre-factor $\mathcal{C}_{-\mathbf{1},+\mathbf{1}}$ is related to the particular Glauber dynamics we choose.
We set $\ell_1 := 1$ and, for $d \geq 2$,

$$\ell_d := \lceil \frac{2(d-1)}{h} \rceil, \tag{5.4}$$

$\varepsilon_d := \ell_d - \frac{2(d-1)}{h}$ and

$$a_d := \lceil (d - 1 + \frac{h}{2}\varepsilon_d)(1 - \varepsilon_d) \rceil \in [1, d-1] \tag{5.5}$$

A d-dimensional parallelepiped with a sides of length ℓ and all the other $(d-a)$ sides with length $\ell - 1$ is called *quasi-cube* in dimension d with paremeters (ℓ, a) (called *side-length* and *shape*, respectively).
We say that h is *generic* if $0 < h < 1$, for all $2 \leq k \leq d$, $\frac{2(k-1)}{h}$ and $(k - 1 + \frac{h}{2}\varepsilon_k)(1 - \varepsilon_k)$ are not integer. The following results hold for generic h. Given a d-dimensional parallelepiped $(l_1 \times l_2 \ldots \times l_d)$ and a $(d-1)$-dimensional configuration $\eta^{d-1} \in \{-1, 1\}^{(l_2 \times l_3 \ldots \times l_d)}$, let us consider a configuration where the sites in the parallelepiped as well as the sites of the form $(l_1 + 1, i_2, \ldots, i_d)$ where $\eta^{d-1}(i_2, \ldots, i_d) = +1$ have plus spin and all other sites have minus spins. For such a configuration, as well as for all its rotations and translations, we say that η^{d-1} is *attached* to the parallelepiped.
Following [N], we introduce a set $\mathcal{B}^d(v)$ in a recursive way: let $\mathcal{B}^1(v)$ be the set of configurations where the pluses form a slab with volume v, $\mathcal{B}^d(v)$ is defined as the set of all configurations with v pluses that form a d-dimensional quasi-cube with maximal volume $v' \leq v$ with a $(d-1)$-dimensional configuration $\eta \in \mathcal{B}^{d-1}(v - v')$ attached to one of its largest faces. Heuristically, these configurations are as close as

possible to a cube. It is easy to see that the energy is constant in every set $\mathcal{B}^d(v)$; we will denote this energy by $H(\mathcal{B}^d(v))$.
We make use of the following Theorem

Theorem 5.1. (Theorem 3 in [N])
In the whole d-dimensional lattice $\mathbb{Z}^d$, $\mathcal{B}^d(v)$ is a subset of the minimizers of the Hamiltonian in the manifold with volume v.

This result can be transported to the torus $\Lambda(L)$ only for sufficiently small values of v/L^d. For large values of v, the boundary conditions affect the shape of the minimizing configurations. Let $m := \min\{v \geq 1; H(\mathcal{B}^d(v)) \leq H(-\mathbf{1})\}$. We take L so large that the configurations in $\mathcal{B}^d(v)$ are minima of the energy among the configurations with v pluses for all $v \leq m$. Clearly, such an L exists and is smaller than $m+1$, since the number of pluses in the configurations winding around the torus is at least L. Hence, all configurations in the torus with less than L pluses have a corresponding configuration in $\mathbb{Z}^d$ with the same volume and the same energy.
We define the set $\bar{\mathcal{B}}^d$ of the *candidate saddles in dimension d* in a recursive way:

(1) in one dimension it is the set of configurations consisting of a single plus spin in the sea of minuses.
(2) in dimension d it is the set of configurations in which the pluses form a quasi-cube with parameters (ℓ_d, a_d) with a $(d-1)$-dimensional candidate saddle attached on one of its squared $(d-1)$-dimensional faces.

Notice that $H(\bar{\mathcal{B}}^d) = \max_{v \leq L^d} H(\mathcal{B}^d(v))$.
Clearly, all the candidate saddles have the same volume v_d^* and are in $\mathcal{B}^d(v_d^*)$. Moreover, each $\eta \in \mathcal{B}^d(v)$ is connected to a configuration in $\mathcal{B}^d(v+1)$ and to one configuration in $\mathcal{B}^d(v-1)$.
Hence, the candidate saddles are saddles between $-\mathbf{1}$ and $+\mathbf{1}$ since from any candidate saddle there exist a path leading to $-\mathbf{1}$ and a path leading to $+\mathbf{1}$ both reaching their maximum energy in the starting point.
The following lemma was communicated to us by E. Olivieri [dHNOS].

Lemma 5.2. *The set $\mathcal{M} := \{-\mathbf{1}, +\mathbf{1}\}$ is a metastable set.*

Proof. We have to show that for some $\delta > 0$, for any $\sigma \notin \{-\mathbf{1}, +\mathbf{1}\}$, $\Gamma(\sigma) < \Gamma(-\mathbf{1})$, i.e. there exists a configuration σ' such that

(1) $H(\sigma') < H(\sigma) - \delta$
(2) $\widehat{H}(\sigma, \sigma') - H(\sigma) < \widehat{H}(-\mathbf{1}, +\mathbf{1}) - H(-\mathbf{1}) - \delta$.

For $\eta \in \Omega$, let $|\eta|$ and $\wp(\eta)$ be the number of pluses and the number of pairs of nearest neighbors with different spin (namely, the perimeter, or cardinality of the contour), respectively. It is a well known fact that the Hamiltonian of the Ising model can be written as

$$H(\eta) = \frac{1}{2} \sum_{<i,j> \in \Lambda} |\eta_i - \eta_j| - h|\eta| + H(-\mathbf{1}) = \wp(\eta) - h|\eta| + H(-\mathbf{1}) \tag{5.6}$$

Let $m := \min\{k \geq 1; \exists \eta \text{ with } |\eta| = k \text{ and } H(\eta) \leq H(-\mathbf{1})\}$. Let $\omega : -\mathbf{1} \to +\mathbf{1}$ be a monotone one-dimensional subgraph such that $\omega_k \in \mathcal{B}^d(k)$ that reaches its maximal energy in $\mathcal{S}(-\mathbf{1}, +\mathbf{1})$. Clearly, $H(\omega_m) \leq H(-\mathbf{1})$. Let $\sigma \cup \eta$ denote the configuration where $(\sigma \cup \eta)(x) := \sigma(x) \vee \eta(x)$ and $\sigma \cap \eta$ denote the configuration where $(\sigma \cap \eta)(x) := \sigma(x) \wedge \eta(x)$.
A simple computation shows that

$$\wp(\sigma) + \wp(\eta) \geq \wp(\sigma \cup \eta) + \wp(\sigma \cap \eta). \tag{5.7}$$

Indeed, let us assume without loss of generality that $\sigma_i \geq \max\{\sigma_j, \eta_i, \eta_j\}$; then

$$|\sigma_i - \sigma_j| + |\eta_i - \eta_j| \geq |(\sigma \cup \eta)_i - (\sigma \cup \eta)_j| + |(\sigma \cap \eta)_i - (\sigma \cap \eta)_j|, \tag{5.8}$$

where the equality clearly holds if $\eta_j \leq \sigma_j$ or $\eta_j \leq \eta_i$, while for $\eta_j > \max\{\sigma_j, \eta_i\}$,

$$\begin{aligned} &|\sigma_i - \sigma_j| + |\eta_i - \eta_j| = \sigma_i + \eta_j - \sigma_j - \eta_i = \\ &|\sigma_i - \eta_j| + |\eta_i - \sigma_j| + 2(\eta_j - \max\{\sigma_j, \eta_i\}) = \\ &|(\sigma \cup \eta)_i - (\sigma \cup \eta)_j| + |(\sigma \cap \eta)_i - (\sigma \cap \eta)_j| + 2(\eta_j - \max\{\sigma_j, \eta_i\}). \end{aligned} \tag{5.9}$$

Since σ is neither $+\mathbf{1}$ nor $-\mathbf{1}$, there exists at least one pair of nearest neighbour sites i, j such that $\sigma(i) = -1$ and $\sigma(j) = +1$. By translation invariance we may assume that the first site with a plus spin in the sequence ω_k is i and the second is j. Thus in the first step, $\sigma \cap \omega_1 \neq -\mathbf{1}$ and $H(\sigma \cup \omega_1) - H(\sigma) < H(\omega_1) - H(-\mathbf{1})$, while in the second step $\sigma \cup \omega_2 = \sigma \cup \omega_1$, so that $|\sigma \cap \omega_k| < k$ for all $k \geq 2$. We choose $\sigma' = \sigma \cup \omega_m$.
In order to prove point 2. we notice that for $k \leq m$,

$$\begin{aligned} H(\sigma \cup \omega_k) - H(\sigma) &= \wp(\sigma \cup \omega_k) - \wp(\sigma) - h(|\sigma \cup \omega_k| - |\sigma|) \\ &\leq \wp(\omega_k) - \wp(\sigma \cap \omega_k) - h(|\omega_k| - |\sigma \cap \omega_k|) \\ &= H(\omega_k) - H(\sigma \cap \omega_k) < H(\omega_k) - H(-\mathbf{1}), \end{aligned} \tag{5.10}$$

since by definition, $|\sigma \cap \omega_k| < m$.
For $k = m$, from (5.10) we get point 1. since

$$H(\sigma \cup \omega_m) - H(\sigma) < H(\omega_m) - H(-\mathbf{1}) \leq 0 \tag{5.11}$$

By putting together (5.11) and (5.10), we see that the energy of the configuration σ' is lower than the energy of σ and that the maximal energy in the one-dimensional subgraph $\sigma \cup \omega_k : \sigma \to \sigma'$ is lower than $\widehat{H}(-\mathbf{1}, +\mathbf{1})$. □

In the next Theorem, we use the results of [NS] and [BC] (Theorem 6.18, 7.17) to describe the energy landscape.

Theorem 5.3. (from [NS] and [BC]). *In dimension* 2 *and* 3,

(1) The set of saddles between $-\mathbf{1}$ *and* $+\mathbf{1}$ *coincides with the set of candidate saddles.*
(2) The saddles are isolated.
(3) If h *is generic, the saddles are simple.*

Conjecture 5.4. *Theorem 5.3 holds in any dimension.*

We define D_+ as the set of all states that are larger than a candidate saddle (namely of the form $\sigma \cup \eta \neq \sigma$ for some candidate saddle σ). By the same procedure of the proof of Lemma 5.2, we can easily see that all configurations in D_+ have the saddle with $+\mathbf{1}$ below the saddle with $-\mathbf{1}$. We set $Z := \partial D_+$ and $D_- := \Omega \setminus (D_+ \cup Z)$. Clearly, if Conjecture 5.4 holds (as in dimension 2 and 3) Z fulfills the conditions (a), (b) and (c) (see pag. 4) and the computation of $\mathcal{C}_{-\mathbf{1},+\mathbf{1}}$ with respect to this surface gives the pre-factor of the expected transition time from $-\mathbf{1}$ to $+\mathbf{1}$. In the following Lemmata, we will compute this quantity.

Lemma 5.5. *The number of distinct tiles with the shape of a d-dimensional quasi-cube with parameters (l, a) contained in a box with the shape of a d-dimensional quasi-cube with parameters (L, b), where $L \geq l$ is:*

$$N^d_{l,a}(L,b) = \sum_{k=[a+b-d]_+}^{\min\{a,b\}} \binom{k}{b}\binom{a-k}{d-b} (L-l+1)^{d-a-b+2k} (L-l)^{a-k} (L-l+2)^{b-k} \tag{5.12}$$

The number of distinct tiles with the shape of a d-dimensional quasi-cube with parameters (l, a) contained in a torus with side-length $L \geq l$ is:

$$\widetilde{N}^d_{l,a}(L,b) = \binom{a}{d} L^d \tag{5.13}$$

Proof. The proof is rather straightforward: let k be the number of long sides of the tile that are parallel to long sides of the box. The number of long sides of the tile that are parallel to short sides of the box is $a-k$; the number of short sides of the tile that are parallel to long sides of the box is $b-k$; the number of short sides of the tile that are parallel to short sides of the box is $d-a-b+k$. Obviously, $[a+b-d]_+ \leq k \leq \min\{a,b\}$. There are $\binom{k}{b}$ ways to arrange k long sides of the tile parallel to the b long sides of the box and $\binom{a-k}{d-b}$ ways to arrange the remaining $a-k$ long sides of the tile parallel to the $d-b$ short sides of the box. The last three factors in (5.12) come from the possible translations of the tile in the box.
Similarly, we can prove (5.13) □

Let $N^d := N^d_{\ell_d, a_d+1}(\ell_{d+1}, a_{d+1})$ for $d \geq 3$ and $N^2 := \ell_2$.

Lemma 5.6. *The number of candidate saddles in dimension d contained in a d-dimensional quasi-cube $\Lambda_{l,b}$ with parameters (l, b), where $l \geq \ell_d$ is*

$$\mathcal{N}^d(l,b) = N^d_{\ell_d, a_d+1}(l,b) 2^{d-2} \prod_{k=2}^{d} (a_k+1) N^k. \tag{5.14}$$

All the candidate saddles have $\check{p} = |\Lambda_{l,b}|^{-1}$, while $\hat{p}$ can take the value $|\Lambda_{l,b}|^{-1}$ or $2|\Lambda_{l,b}|^{-1}$. The fraction of candidate saddles with $\hat{p} = |\Lambda_{l,b}|^{-1}$ is $\frac{2}{\ell_2}$, independently of d, b and l.

Proof. Let $\mathcal{N}^d := \mathcal{N}^d(\ell_d, a_d + 1)$.
The key observation is that the pluses of a candidate saddle are contained in exactly one quasi-cube with parameters $(\ell_d, a_d + 1)$.
By Lemma 5.5,

$$\mathcal{N}^d(l, b) = N^d_{\ell_d, a_d+1}(l, b)\mathcal{N}^d. \tag{5.15}$$

Given a quasi-cube with parameters (ℓ_d, a_d+1), there are $2(a_d+1)$ possible choices for the incomplete face and $\mathcal{N}^{d-1}(\ell_d)$ ways to arrange the $(d-1)$-dimensional candidate droplet on this face.
Hence,

$$\begin{aligned} \mathcal{N}^d &= 2(a_d + 1)\mathcal{N}^{d-1}(\ell_d, a_d) = 2(a_d + 1)N^{d-1}_{\ell_{d-1}, a_{d-1}+1}(\ell_d, a_d)\mathcal{N}^{d-1} \\ &= 2(a_d + 1)N^{d-1}\mathcal{N}^{d-1}. \end{aligned} \tag{5.16}$$

For $d = 2$, a_2 can only take the value 1. Since $\mathcal{N}_1 = 1$, by (5.15), (5.16), we get

$$\mathcal{N}^2(l, b) = 4N^2_{\ell_2,2}(l, b)N^1_{1,1}(\ell_2, b). = 4\ell_2 \left(l - \ell_2 + 1\right)^b \left(l - \ell_2\right)^{2-b} \tag{5.17}$$

By induction on d, we get (5.14).
The computation of the number $m_d(l, b)$ of candidate saddles with $\hat{p} = |\Lambda_{l,b}|^{-1}$ is very similar: In dimension two, $m_2(\ell_2, 1) = 8$ i.e. the number of configurations made of a quasi-square plus a protuberance at one end of one of the longest sides. All other candidate saddles have $\hat{p} = 2|\Lambda_{l,b}|^{-1}$, since there are two neighbors of the protuberance that can be occupied. All candidate saddles have $\check{p} = |\Lambda_{l,b}|^{-1}$, since we can void the protuberance and reach a configuration in D_-. In general, for $d > 1$, the only sites with d plus-neighbors are in an incomplete face of the tile with parameters $(\ell_d, a_d + 1)$ that contains the critical droplet. Hence, $m_d(\ell_d, b)$ is equal to the number of $(d-1)$-dimensional tiles with parameters $(\ell_{d-1}, a_{d-1} + 1)$ on one of the largest faces of the d-dimensional critical quasi-cube times $m_{d-1}(\ell_{d-1}, a_{d-1} + 1)$ namely, $m_d(\ell_d, a_d) = 2(a_d+1)N_{d-1}m_{d-1}(\ell_{d-1}, a_{d-1}+1)$. On the other hand, $m_d(l, b) = N^{\ell_d, a_d+1}(l, b)m_d(\ell_d, a_d + 1)$. Thus, the ratio $m_d(l, b)/\mathcal{N}^d(l, b)$ does not depend on d, b or on l and is equal to $2/\ell_2$. □

Lemma 5.7. *The number of candidate saddles in dimension d contained in a d-dimensional torus of side-length $l \geq \ell_d$ is*

$$\widetilde{\mathcal{N}}^d(l) = \binom{a_d + 1}{d} l^d 2^{d-1} \prod_{k=2}^{d} (a_k + 1)N_{k-1} \tag{5.18}$$

In particular, for $d = 2$,

$$\widetilde{\mathcal{N}}^2(l) = 4l^2\ell_2 = \frac{8}{h}(1 + O(h))l^2, \tag{5.19}$$

for $d = 3$,

$$\widetilde{\mathcal{N}}^3(l) = \frac{24}{a_3} l^3 \ell_2 \left(\ell_3 - \ell_2 + 1\right)^{a_3} \left(\ell_3 - \ell_2\right)^{2-a_3} = \frac{192}{a_3} \frac{1}{h^3} (1 + O(h))\, l^3, \tag{5.20}$$

All the candidate saddles have $\check{p} = l^{-d}$, while $\hat{p}$ can take the value l^{-d} or $2l^{-d}$. The fraction of candidate saddles with $\hat{p} = l^{-d}$ is $\frac{2}{\ell_2}$, independently of d and l.

Proof. The proof is very similar to that of Lemma 5.6.
By Lemma 5.5, we get

$$\widetilde{\mathcal{N}}^d(l) = \widetilde{N}^d_{\ell_d, a_d+1}(l) \mathcal{N}^d = \binom{a_d + 1}{d} l^d \mathcal{N}^d \tag{5.21}$$

and, from Lemma 5.6, we get the thesis.
In particular, the result for $d = 2$ comes from $\mathcal{N}^2 = 4\ell_2$, $a_2 = 1$. The approximation comes from $\ell_2 = 2/h(1 + O(h))$.
For $d = 3$, from (5.17) and (5.21), we have

$$\widetilde{\mathcal{N}}^3(l) = l^3 8 \binom{a_3 + 1}{3} (a_3 + 1) l_2 \left(\ell_3 - \ell_2 + 1\right)^{a_3} \left(\ell_3 - \ell_2\right)^{2-a_3} \tag{5.22}$$

since, for $a_3 \in (1, 2)$, $\binom{a_3+1}{3}(a_3 + 1) = 6/a_3$, we get (5.20).
By using the approximation $\ell_3 - \ell_2 + 1 = (\ell_3 - \ell_2)\,(1 + O(h)) = \ell_2(1 + O(h))\frac{2}{h}\,(1 + O(h))$ we get the estimate in (5.20).
The computation of the fraction of saddles with $\check{p} = l^{-d}$ is the same as for Lemma 5.6. □

Let

$$\begin{aligned} \Gamma_d := \quad 2 \textstyle\sum_{k=2}^{d} \quad & \big(2a_k \ell_k^{a_k - 1} (\ell_k - 1)^{d - a_k} + 2(d - a_k) \ell_k^{a_k} (\ell_k - 1)^{d - a_k - 1} \\ & - h \left(\ell_k^{a_k} (\ell_k - 1)^{d - a_k}\right) \big) + 2 - h \end{aligned} \tag{5.23}$$

be the activation energy of the candidate saddle in dimension d.

Theorem 5.8. *For the Ising model on a (sufficiently large) $d-$dimensional torus $\Lambda(l)$, in dimension $d > 3$, there exists a constant c_d such that $\forall \delta > 0$,*

$$\mathbb{E}\tau_+^- = c_d e^{\beta \Gamma_d} (1 + o(e^{-\beta\delta})) \tag{5.24}$$

If h is generic and Conjecture 5.4 holds, then the pre-factor c_d is equal to

$$\frac{3}{2} \frac{\ell_2}{\ell_2 - 1} \frac{1}{\widetilde{\mathcal{N}}^d(l)} l^d = \frac{3}{2} \frac{\ell_2}{\ell_2 - 1} \frac{1}{\binom{a_d+1}{d} \mathcal{N}^d} \tag{5.25}$$

Proof of Theorems 2.2 and 5.8: The results of Theorem 2.2 are straightforward consequences of Theorem 2.1, Lemma 5.3, Lemma 5.2, and Lemma 5.7. In higher dimension, the corresponding result comes from Theorem 2.1 and Lemma 5.2. If Conjecture 5.4 holds, as in dimension 2 and 3, Lemma 5.7 gives (5.25). □

In conclusion, let us notice that the form of the quantities $\mathbb{P}\left(\tau_y^x < \tau_x^x\right)$ in the case of the Metropolis dynamics may offer an interpretation in terms of "free energy of the set of saddle points". Indeed, every point in Z gives a contribution to the pre-factor $\mathcal{C}_{x,y}$ that does not depend on β and can be bounded by a constant c. With the arguments in the proof of Lemma 3.2, we get

$$\mathbb{P}\left(\tau_y^x < \tau_x^x\right) \sim c\mathcal{N}e^{-\beta\Gamma} = c\exp\left(-\beta(\Gamma - T\log\mathcal{N})\right), \tag{5.26}$$

where $\mathcal{N}$ is the number of saddles between x and y and $T = \beta^{-1}$. The logarithm of $\mathcal{N}$ can be interpreted as an entropy. This interpretation could be related to the results by Schonmann and Shlosman (see [ScSh]) on the connections between Wulff droplets and the metastable relaxation of kinetic Ising model.

6. Appendix.

In this appendix we briefly explain how our general approach can be generalized to situations when the saddles are more complicated than the isolated single points assumed in Section 2. The point we want to make is that in such a case it is still possible to localize the problem to the understanding of the neighborhood of the saddle points and to thus reduce the analysis of the capacities to a 'local' variational problem. We will be very brief; a more detailed presentation will be given in forthcoming papers. Let us consider a situation when in the computation of a transition from x to y we encounter a set of saddles $\mathcal{S}_{x,y}$ that can be decomposed into a collection of disconnected subsets $\mathcal{S}^{(k)}$, $k = 1, \dots, L$. By definition, it must be true that each of the sets $\mathcal{S}^{(k)}$ is connected to two subsets $\mathcal{R}^{(k)}$ and $\mathcal{N}^{(k)}$ of D_x^y and D_y^x, respectively. Let us define

$$C(k) := \sum_{i\in\mathcal{N}^{(k)}} e^{-\beta(H(x)-H(i))}\widetilde{\mathbb{P}}\left(\tau^i_{\mathcal{R}^{(k)}} < \tau^i_{\mathcal{N}^{(k)}}\right) \tag{6.1}$$

where $\widetilde{\mathbb{P}}$ is the law of the chain where all the edges exiting from the sets $S^{(k)}$ not leading to $\mathcal{N}^{(k)}$ or $\mathcal{R}^{(k)}$ are cut. Note that it is not difficult to see that

$$C^{(k)} = \inf_{h\in\mathcal{H}^{\mathcal{R}}_{\mathcal{N}}} \widetilde{\Phi}(h) \tag{6.2}$$

Repeating the steps of the proof of Lemma 4.2, one obtains then that

Lemma 6.1. *In the situation described above we have that*

$$\mathbb{P}\left(\tau_y^x < \tau_x^x\right) = \sum_{k=1}^{L} C^{(k)}\left(1 + o(e^{-\beta\delta})\right) \tag{6.3}$$

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