RENORMALIZATION–GROUP AT CRITICALITY AND COMPLETE ANALYTICITY OF CONSTRAINED MODELS: A NUMERICAL STUDY.

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Abstract

We study the majority rule transformation applied to the Gibbs measure for the 2–D Ising model at the critical point. The aim is to show that the renormalized hamiltonian is well defined in the sense that the renormalized measure is Gibbsian. We analyze the validity of Dobrushin–Shlosman Uniqueness (DSU) finite–size condition for the "constrained models" corresponding to different configurations of the "image" system. It is known that DSU implies, in our 2–D case, complete analyticity from which, as it has been recently shown by Haller and Kennedy, Gibbsianness follows. We introduce a Monte Carlo algorithm to compute an upper bound to Vasserstein distance (appearing in DSU) between finite volume Gibbs measures with different boundary conditions. We get strong numerical evidence that indeed DSU condition is verified for a large enough volume V for all constrained models.

Keywords: Majority–rule; Renormalization–group; non–Gibbsianness; Finite–size conditions; Complete analyticity; Ising model.

1. Introduction.

In the recent few years many efforts have been devoted to the problem of a correct definition, on rigorous grounds, of various real–space renormalization–group maps.

The main question is whether or not a measure

$$\nu = T_b \mu \tag{1.1}$$

arising from the application of a renormalization group transformation (RGT) T_b, defined "on scale b", to the Gibbs measure μ is Gibbsian. In other words we ask ourselves whether or not ν is the Gibbs measure corresponding to a finite–norm translationally invariant potential so that the "renormalized hamiltonian" is well defined.

To be concrete let us suppose that $\mu = \mu_{\beta,h}$ is the Gibbs measure describing 2–D Ising model at inverse temperature β and external magnetic field $h \neq 0$. Moreover we assume that our RGT can be expressed as:

$$\nu(\sigma') = \sum_{\sigma} T_b(\sigma', \sigma) \mu_{\beta,h}(\sigma) \tag{1.2}$$

where $T_b(\sigma', \sigma)$ is a normalized non–negative kernel. The system described in terms of the σ variables by the original measure μ is called "object system". The σ''s are the "block variables" of the "image system" described by the renormalized measure ν.

We can think of the transformation T_b as directly acting at infinite volume or we can consider a finite volume version and subsequently try to perform the thermodynamic limit. We refer to the basic reference [EFS] for a clear and complete description of the general set–up of renormalization maps from the point of view of rigorous statistical mechanics.

The above mentioned pathological behaviour (non–Gibbsiannes of ν) can be a consequence of the violation of a necessary condition for Gibbsiannes called *quasi–locality* (see [Ko], [EFS]). It is a continuity property of the finite volume conditional probabilities of ν which, roughly speaking, says that they are almost independent of very far away conditioning spins.

In [Ko] it is shown that a sort of converse statement holds true; namely: quasilocality + nonnulness (uniform positivity of conditional probabilities) of a stochastic field implies Gibbsianness but only in the sense of the existence of a finite norm but in general not translationally invariant potential associated to ν. The construction of the potential in Kozlov's proof is somehow artificial: it involves reordering of a semi–convergent sum. To get a translationally invariant finite norm potential one needs some additional stronger assumptions on how weakly the conditional probabilities of ν depend on far away conditioning spins. We refer to [BMO] for a more detailed discussion on this point.

In some situations (see, for instance [C], [HK]) it is possible to use much stronger methods, based on cluster expansion, to compute renormalized potentials, showing finiteness of their norm.

In many interesting examples (see [E1], [EFS], [EFK]) violation of quasi–locality and consequently non–Gibbsiannes of the renormalized measure ν is a direct consequence of the appearance of a first order phase transition for the original (object) system described by μ conditioned to some particular configuration of the image system. More precisely given a block configuration σ' let us consider the probability measure on the original spin variables given by:

$$\mu_{\sigma'}(\sigma) \;=\; \frac{T_b(\sigma',\sigma)\mu(\sigma)}{\sum_\eta T_b(\sigma',\eta)\mu(\eta)}$$

It defines the "constrained" model corresponding to σ' (which here plays the role of an external parameter).

For some particular σ' it may happen that the corresponding measure $\mu_{\sigma'}(\sigma)$ exhibits long range order. See also [GP], [I] where this mechanism was first pointed out.

One can ask himself about "robustness" of the pathology of non–Gibbsianness. There are examples (see [MO4]) in which, even though the measure $\nu = T_b\mu_{\beta,h}$ is not Gibbsian, one has that with the same β, h, by choosing $b' > b$ sufficiently large, the measure $\nu' = T_{b'}\mu_{\beta,h}$ is Gibbsian. Alternatively one can think to iterate the map and, even though after the first step the resulting renormalized measure is not Gibbsian, it may happen, after a sufficiently large number of iterations that one gets back to the set of Gibbsian measures. This is often related to the fact that, given suitable values of the parameters β, h (near the coexistence line $h = 0, \beta > \beta_c$), on a suitable scale b some constrained model can undergo a phase transition (somehow related to the phase transition of the object system); whereas given the same h, β, for sufficiently large scale b any constrained model is in the one–phase region.

Another notion of robustness of the pathology (see [LV], [MO5]) refers to see whether or not it survives after application of a decimation transformation (see [EFS]); this can be relevant since decimation transformation does not change the thermodynamic functions or the long range correlations.

Finally we want to say that weaker notions of Gibbsiannes of a renormalized measure ν can also be considered. The usual notion of Gibbsiannes requires a control of quasi–locality of ν *uniform* in σ'. It may happen hat the particular σ' responsible for the pathology is highly non–typical w.r.t. ν. It appears plausible to ask for quasi–locality only for ν–almost all configurations σ' (see [D2], [FP], [Ma]). We refer to [E2] for a nice up–to–date review of all the above problematic.

Now we want to notice that in many examples it happens that even though the object system is well inside the one–phase region, nonetheless for some particular block configuration σ' the corresponding constrained model undergoes a first order phase transition. Conversely there are many indications that if the constrained models are in the weak coupling regime then Gibbsianness of the renormalized measure follows. Recently Haller and Kennedy gave very interesting new rigorous results in this direction. They proved, under very general hypotheses, that if *all* constrained models are uniformly completely analytical (see [DS2], [DS3]) then the renormalized measure is Gibbsian with a finite norm potential which can be computed via a convergent cluster expansion.

Let us give now the example of the Block–Averaging Transformation (BAT). Suppose to partition $\mathbb{Z}^2$ into squared blocks B_i of side 2. In this case the new measure ν is obtained by assigning to each block B_i an integer value $m_i \in \{-4,-2,0,+2,+4\}$ and by computing the probability, w.r.t. the original Gibbs measure $\mu_{\beta,h}$ of the event: $\sum_{x\in B_i}\sigma_x = m_i$. Then in this case we have:

$$T_b(m,\sigma) \;=\begin{cases} 1 & \text{if } \displaystyle\sum_{x\in B_i}\sigma_x = m_i \;\; \forall i \\ 0 & \text{otherwise} \end{cases} .$$

In this case a constrained model is a "multicanonical" Ising model namely an Ising model subject to the constraint of having, for every i, magnetization m_i in the block B_i. It has been shown in [EFK] that for BAT transformation the constrained model corresponding to $m_i = 0 \;\forall\; i$, undergoes a first order phase transition at low enough temperature and that this implies violation of quasi–locality and then non–Gibbsianness of the renormalized measure ν. Notice that for any constrained model with given $\{m_i\}$ the value of the external magnetic field h is totally irrelevant. On the other hand, for h very large one can prove, by standard methods, absence of phase transition for the original model in the strongest possible sense: complete analyticity in the strong Dobrushin–Shlosman sense holds true in this case. This, as it has been shown in [EFS] gives an example of non–Gibbsiannes of a measure ν arising from the application of a renormalization map to a measure μ corresponding to the very weak coupling region. We remark that, as it has been shown in [EFS], this non–Gibbsiannes is robust w.r.t. the choice of the scale b (or w.r.t iteration) whereas for large h it can be eliminated by applying one decimation transformation (see [MO5]).

Other interesting examples have been found (see [EFK], [E1], [E2]).

We want to stress that, in general, it is not sufficient to control that one single constrained model is in the one–phase region to imply Gibbsianness of the renormalized measure. In [CG] and in [BMO] for the BAT transformation it was suggested that the fact that the constrained model with $m_i = 0$ was in the high temperature phase could be sufficient to imply the existence of a finite norm renormalized potential. Recently A. van Enter showed with an example that this believe is not sufficiently justified and some extra arguments related to the specific nature of BAT transformation are needed to imply Gibbsiannes from absence of phase transitions for $\{m_i = 0\}$ constrained model (see [E1], [E2]).

Thus, in general, the moral is that what is relevant for Gibbsiannes of ν are the (intermediate) constrained models; we repeat that it can be sufficient that even only one constrained model undergoes a phase transition with long–range order (despite of the possible very weak coupling regime of the object system) to imply non–Gibbsiannes of ν; whereas, in general, absence of phase transition in a very strong sense is needed *for all constrained models* to imply Gibbsiannes of ν in the strong, cluster expansion, sense as it has been shown in [HK].

In the present paper we will analyze a particular RGT: the majority rule transformation applied to the 2D critical Ising model. It will be precisely defined in next Section 2. This transformation, in the same situation of criticality, has been studied by Tom Kennedy in [K2]. The author establishes some rigorous results reducing absence of phase transition for some particularly relevant constrained models to the verification of some suitable "finite size conditions" introduced in [K1]. It is an "almost computer assisted proof" of absence of phase transition for these constrained models.

In the present paper we inquire for the validity, in principle for every possible constrained model, of a finite size condition: the Dobrushin–Shlosman uniqueness condition (DSU, see Section 2 below) which implies (as it will be explained in Section 2) complete analyticity and then, using the results of [HK], Gibbsianness of ν.

Strictly speaking the proof of [HK] does not directly apply to our case since it requires the condition that the kernel $T(\sigma', \sigma)$ is strictly positive for every σ', σ. Probably this is only a technical restriction that can be removed ([K3]). In any case in [HK] the authors claim that for the majority rule they are able to obtain an equivalent system with $T(\sigma', \sigma) > 0$ by first summing out some spins in the original system.

Our results and their strength are, in a sense, complementary to the ones of [K2]. Our study will be numerical but, similarly to [K2] not only in the sense of "traditional" Monte Carlo simulations. Rather, for each constrained model, we will try to measure by a computer a quantity appearing in DSU such that if we could rigorously prove that it is strictly less than one then we could deduce from some theorems strong properties typical of the one–phase region, for arbitrarily large and even infinite systems.

In [K2] some constrained models were analyzed in terms of a finite size condition easier to be satisfied than DSU, for which the author could also have provided a computation based on interval arithmetics suited for a computer assisted proof. This finite size condition of reference [K1] is not sufficient to imply complete analyticity. In the present paper, as we said before, we try to verify for every constrained model DSU condition; but, as it will appear clear in Section 5 we can, with nowadays machines, only perform a Monte Carlo calculation. For many reasons we cannot, at the moment, hope to improve our calculations to get a complete control and possibly a computer assisted proof. We will explain in Section 6, devoted to the conclusions, in what sense our results can be considered satisfactory.

The DSU condition involves the calculation of the so–called Vasserstein distance between two Gibbs measures in a finite volume with boundary conditions differing only in one conditioning site. In a recent paper ([BMO]) the authors, in the context of BAT transformation, for one particularly relevant constrained model ($\{m_i\} = 0 \ \forall \ i$) tried to verify the same DSU condition but they were only able to provide a (numerical) lower bound for the concerned Vasserstein distance. The reason was that a lower bound (see (2.16)) in terms of total variation distance can be found involving thermal averages; thus this lower bound is well adapted to be studied by Monte Carlo methods but, on the other hand, it is only able to give some indications on the validity of the true condition and this since it appears reasonable to expect that it is a good lower estimate; strictly speaking it is only useful to *disprove* the condition.

In the present paper we present a Monte Carlo algorithm, inspired by the "surgery method" introduced by Dobrushin and Shlosman (see [DS1], [DS2]) that we call *dynamical surgery*. It provides an upper bound to the Vasserstein distance and so it goes into the correct direction to *prove* DSU condition.

Our numerical results strongly suggest that indeed DSU condition is satisfied in our present situation for all constrained models and this, as we said before implies Gibbsiannes of renormalized measure.

The paper is organized as follows: in Section 2 we define in detail our majority rule transformation and the constrained models. In Section 3 by using "conventional" Monte Carlo methods we provide rough estimates of the critical temperatures of some particularly relevant constrained models. In Section 4 we introduce our algorithm. In Section 5 we give our main numerical results. In Section 6 we give the conclusions. In Appendix A we present the computation of the best joint representation of two measures which is used in our algorithm.

2. The majority rule transformation and the constrained models.

We will consider the usual (ferromagnetic nearest neighbors interaction) 2D Ising model, with zero external field, on a finite square with even side: $\Lambda := \{1, ..., 2L\}^2 \subset \mathbb{Z}^2$ with $L \in \mathbb{N}^*$. We denote by $\sigma \in \Omega_\Lambda := \{-1, +1\}^\Lambda$ a configuration of the system in Λ and by $\tau \in \{-1, +1\}^{\partial\Lambda^+}$ a boundary condition, namely a configuration in $\partial\Lambda^+$ defined by

$$\partial\Lambda^+ := \{i \in \mathbb{Z}^2 \setminus \Lambda : \exists j \in \Lambda : \ i \text{ and } j \text{ are nearest neighbors}\} \ . \tag{2.1}$$

By $\sigma_i \in \{-1, +1\}$ and $\tau_j \in \{-1, +1\}$ we denote the spin variables on the site $i \in \Lambda$ and $j \in \partial\Lambda^+$. It is also convenient to think of τ as an extended configuration in $\{-1, +1\}^{\mathbb{Z}^2 \setminus \Lambda}$.

The energy associated to $\sigma \in \Omega_\Lambda$ with τ boundary condition outside Λ and zero external magnetic field is given by

$$H^\tau_\Lambda(\sigma) := -\sum_{\substack{<i,j> \\ i,j \in \Lambda}} \sigma_i \sigma_j - \sum_{\substack{<i,j> \\ i \in \Lambda, j \in \partial\Lambda^+}} \sigma_i \tau_j \quad \forall \sigma \in \Omega_\Lambda \ , \tag{2.2}$$

where the first sum runs over all pairs of nearest neighbors sites in Λ, while the second sum runs over all pairs $< i, j >$ of nearest neighbors sites such that $i \in \Lambda$ and $j \in \partial\Lambda^+$. The Gibbs measure describing the equilibrium properties of the system at the inverse temperature β is denoted by $\mu^\tau_{\beta,\Lambda}(\sigma)$ $\forall \sigma \in \Omega_\Lambda$ and is given by

$$\mu^\tau_{\beta,\Lambda}(\sigma) := \frac{e^{-\beta H^\tau_\Lambda(\sigma)}}{\sum_{\eta \in \Omega_\Lambda} e^{-\beta H^\tau_\Lambda(\eta)}} \quad \forall \sigma \in \Omega_\Lambda \ . \tag{2.3}$$

In the following four steps we give the precise definition of the "Majority Rule" (on scale 2) transformation.

1. $\forall x, y \in \mathbb{Z}$ let $B_{(x,y)}$ denote the 2×2 block whose center has coordinates: $\left(2x - \frac{1}{2}, 2y - \frac{1}{2}\right)$; the collection of all blocks $B_{(x,y)}$ $\forall x, y \in \mathbb{Z}$ gives rise to a partition of the lattice $\mathbb{Z}^2$. If we restrict ourselves to pairs $(x, y) \in \{1, ..., L\}^2$ we get a partition of our box Λ. Given $\sigma \in \Omega_\Lambda$ we denote by $\sigma^1_{(x,y)}, ..., \sigma^4_{(x,y)}$ the four spins corresponding to the four sites of the block $B_{(x,y)}$ and we define $m_{(x,y)} := \sum_{i=1}^4 \sigma^i_{(x,y)}$; we suppose the four spins $\sigma^i_{(x,y)}$ $\forall i = 1, ..., 4$ ordered in lexicographic way.
2. We define the new lattice Λ' by collecting the centers of all $B_{(x,y)}$ blocks and by rescaling the lattice spacing by a factor two; the site of Λ', which is the center of the block $B_{(x,y)}$, will be simply denoted by the pair (x, y).

3. On each site $(x,y) \in \Lambda'$ we define the *renormalized spin* $\sigma'_{(x,y)} \in \{-1,+1\}$ and we consider the space $\Omega'_{\Lambda'} := \{-1,+1\}^{\Lambda'}$. We define the kernel $K : (\sigma,\sigma') \in \Omega_\Lambda \times \Omega'_{\Lambda'} \to K(\sigma,\sigma') \in \{0,1\}$ as follows

$$K(\sigma,\sigma') := \begin{cases} 0 \text{ if } \exists\, (x,y) \in \Lambda' :\ m_{(x,y)} \neq 0 \text{ and } m_{(x,y)} \cdot \sigma'_{(x,y)} < 0 \\ 0 \text{ if } \exists\, (x,y) \in \Lambda' :\ m_{(x,y)} = 0 \text{ and } \sigma^1_{(x,y)} \cdot \sigma'_{(x,y)} < 0 \\ 1 \text{ otherwise} \end{cases} \quad . \tag{2.4}$$

4. The *Majority Rule Transformation* is the transformation which maps the "object" model $(\Lambda, \Omega_\Lambda, \mu^\tau_{\beta,\Lambda}(\sigma))$ onto the "image" model $(\Lambda', \Omega'_{\Lambda'}, \mu'^\tau_{\beta,\Lambda'}(\sigma'))$, where

$$\mu'^\tau_{\beta,\Lambda'}(\sigma') := \frac{\sum_{\sigma\in\Omega_\Lambda} K(\sigma,\sigma')\mu^\tau_{\beta,\Lambda}(\sigma)}{\sum_{\eta'\in\Omega'_{\Lambda'}} \sum_{\sigma\in\Omega_\Lambda} K(\sigma,\eta')\mu^\tau_{\beta,\Lambda}(\sigma)} \quad \forall\sigma' \in \Omega'_{\Lambda'} \ . \tag{2.5}$$

Notice that we could have used the notation $\Omega_{\Lambda'}$ in place of $\Omega'_{\Lambda'}$ since here, for the majority rule transformation, contrary to other transformations like BAT, the single renormalized spin variable still takes values in $\{-1,+1\}$.

This transformation is well known in physics literature and it has been widely used to investigate the properties of many spin models (see, e. g., [NL] and references therein).

A very important role in our discussion will be played by the "constrained models": given $\sigma' \in \Omega'_{\Lambda'}$ we call *constrained model corresponding to* σ', and we denote it by $\mathcal{I}^\tau_{\beta,\sigma'}$, the model $(\Lambda, \Omega_\Lambda, \mu^\tau_{\beta,\Lambda,\sigma'}(\sigma))$, where

$$\mu^\tau_{\beta,\Lambda,\sigma'}(\sigma) := \frac{K(\sigma,\sigma')\mu^\tau_{\beta,\Lambda}(\sigma)}{\sum_{\eta\in\Omega_\Lambda} K(\eta,\sigma')\mu^\tau_{\beta,\Lambda}(\eta)} \tag{2.6}$$

is a probability measure on Ω_Λ. Due to the fact that $K(\sigma,\sigma') \in \{0,1\}$ we have that, $\forall\sigma \in \Omega_\Lambda$ and $\forall\sigma' \in \Omega'_{\Lambda'}$ the constrained model $\mathcal{I}^\tau_{\beta,\sigma'}$ can be seen as the model

$$\left(\Lambda, \Omega_{\Lambda,\sigma'}, \mu^\tau_{\beta,\Lambda,\sigma'}(\sigma) = \frac{e^{-\beta H^\tau_\Lambda(\sigma)}}{\sum_{\eta\in\Omega_{\Lambda,\sigma'}} e^{-\beta H^\tau_\Lambda(\eta)}}\right) , \tag{2.7}$$

where we have introduced the *constrained configuration space*

$$\Omega_{\Lambda,\sigma'} := \{\sigma \in \Omega_\Lambda :\ \forall (x,y) \in \Lambda' :$$

$$(m_{(x,y)} \neq 0 \text{ and } m_{(x,y)} \cdot \sigma'_{(x,y)} > 0) \text{ or } (m_{(x,y)} = 0 \text{ and } \sigma^1_{(x,y)} \cdot \sigma'_{(x,y)} > 0)\} \ . \tag{2.8}$$

In other words we can say that the constrained model $\mathcal{I}^{\tau}_{\beta,\sigma'}$ is a model defined on the original lattice Λ, with the same hamiltonian $H^{\tau}_{\Lambda}(\sigma)$ as the object model, but with configuration space $\Omega_{\Lambda,\sigma'}$.

The microscopic states of the constrained models can be characterized by means of a suitable *block–variable*. In the original Ising model there are $2^4 = 16$ allowed configurations in each block $B_{(x,y)}$. We partition these block–configurations into two disjoint classes C_+ and C_- as follows:

- block–configurations belonging to class C_+

$$\begin{bmatrix} - & + \\ + & + \end{bmatrix} \begin{bmatrix} + & - \\ - & + \end{bmatrix} \begin{bmatrix} + & - \\ + & - \end{bmatrix} \begin{bmatrix} + & - \\ + & + \end{bmatrix} \begin{bmatrix} + & + \\ - & - \end{bmatrix} \begin{bmatrix} + & + \\ - & + \end{bmatrix} \begin{bmatrix} + & + \\ + & - \end{bmatrix} \begin{bmatrix} + & + \\ + & + \end{bmatrix} \tag{2.9}$$

- block–configurations belonging to class C_-

$$\begin{bmatrix} - & - \\ - & - \end{bmatrix} \begin{bmatrix} - & - \\ - & + \end{bmatrix} \begin{bmatrix} - & - \\ + & - \end{bmatrix} \begin{bmatrix} - & - \\ + & + \end{bmatrix} \begin{bmatrix} - & + \\ - & - \end{bmatrix} \begin{bmatrix} - & + \\ - & + \end{bmatrix} \begin{bmatrix} - & + \\ + & - \end{bmatrix} \begin{bmatrix} + & - \\ - & - \end{bmatrix} \tag{2.10}$$

For any constrained model $\mathcal{I}^{\tau}_{\beta,\sigma'}$ we allow, in the block $B_{(x,y)}$, only the configurations in the class $C_{\mathrm{sign}\,\sigma'_{(x,y)}}$; in order to classify these block–configurations we introduce the block–variable $S_{(x,y)} \in \{1,2,...,8\}$: to the values $S_{(x,y)} = 1,...,8$ correspond, respectively, the eight block–configurations in (2.9) if $\sigma'_{(x,y)} = +1$, the eight block–configurations in (2.10) if $\sigma'_{(x,y)} = -1$.

Warning.
Here, and in what follows, we use the (non–conventional) expression *block–variable* referring to the variable $S_{(x,y)}$ taking values in the set $\{1,2,...,8\}$; the spin variables $\sigma'_{(x,y)}$, defined on the renormalized lattice Λ' and taking values in $\{-1,+1\}$, will be sometimes called *renormalized variables.*

Obviously, given any constrained model $\mathcal{I}^{\tau}_{\beta,\sigma'}$, one and only one configuration $S \in \widetilde{\Omega}_{\Lambda'} := \{1,2,...,8\}^{\Lambda'}$ can be associated to any $\sigma \in \Omega_{\Lambda,\sigma'}$, and viceversa. Hence, each state of the model $\mathcal{I}^{\tau}_{\beta,\sigma'}$ can be represented by a collection $S \in \widetilde{\Omega}_{\Lambda'}$ of block–variables $S_{(x,y)}$, but we recall that the "meaning" (in terms of the original spin variables) of each block–variable $S_{(x,y)}$ depends on the sign of $\sigma'_{(x,y)}$.

Due to the bijection between $\Omega_{\Lambda,\sigma'}$ and $\widetilde{\Omega}_{\Lambda'}$ the hamiltonian $H^{\tau}_{\Lambda}(\sigma)$ of the model $\mathcal{I}^{\tau}_{\beta,\sigma'}$ can be thought, for any $\sigma \in \Omega_{\Lambda,\sigma'}$, as a function $H^{\mathcal{T}}_{\Lambda',\sigma',\tau'}(S)$ of the block–variables configuration $S \in \widetilde{\Omega}_{\Lambda'}$; here by τ' we mean a configuration of the renormalized variables in $\partial\Lambda'^{+}$, that is $\tau' \in \Omega'_{\partial\Lambda'^{+}} := \{-1,+1\}^{\partial\Lambda'^{+}}$, where

$$\partial\Lambda'^{+} := \{(x,y) \in \mathbb{Z}^2 : 0 \leq x, y \leq L+1,\ x \neq y,\ (x,y) \notin \Lambda'\} \ ; \tag{2.11}$$

by $\mathcal{T} \in \widetilde{\Omega}_{\partial\Lambda'^{+}} := \{1, ..., 8\}^{\partial\Lambda'^{+}}$ we mean the boundary condition expressed in terms of the block–variables in the set $\partial\Lambda'^{+}$. Notice that given the original τ and τ' in general $\mathcal{T}$ is not uniquely determined.

We remark that a block–variable in $B_{(x,y)}$, for $(x,y) \in \Lambda' \cup \partial\Lambda'^{+}$, is completely "meaningless" if the correspondent renormalized variable has not been specified. Finally, one can say that the constrained model (2.7) is equivalent to the model defined on the lattice Λ', with configuration space $\widetilde{\Omega}_{\Lambda'}$ and equilibrium measure given by

$$\mu^{\mathcal{T}}_{\beta,\Lambda',\sigma',\tau'}(S) := \frac{e^{-\beta H^{\mathcal{T}}_{\Lambda',\sigma',\tau'}(S)}}{\sum_{\Upsilon \in \widetilde{\Omega}_{\Lambda'}} e^{-\beta H^{\mathcal{T}}_{\Lambda',\sigma',\tau'}(\Upsilon)}} \quad \forall S \in \widetilde{\Omega}_{\Lambda'} \ . \tag{2.12}$$

Now, we want to study the above defined constrained models by means of the *finite size Dobrushin–Shlosman uniqueness condition* (DSU); to introduce DSU we need some definitions.

Let us consider two measures μ_1 and μ_2 on a finite set Y; let $\rho(\cdot,\cdot)$ be a metrics on Y and denote by $\mathcal{K}(\mu_1,\mu_2)$ the set of joint representations of μ_1 and μ_2, namely the set of all measures μ on the Cartesian product $Y \times Y$ such that

$$\sum_{y \in B, y' \in Y} \mu(y,y') = \mu_1(B) \quad \text{and} \quad \sum_{y \in Y, y' \in B} \mu(y,y') = \mu_2(B) \quad \forall B \subset Y \ .$$

We set:

$$Var(\mu_1,\mu_2) := \frac{1}{2} \sum_{y \in Y} |\mu_1(y) - \mu_2(y)| \tag{2.13}$$

and, given a metrics ρ on Y

$$\mathcal{D}_\rho(\mu_1,\mu_2) := \inf_{\mu \in \mathcal{K}(\mu_1,\mu_2)} \sum_{y,y' \in Y} \rho(y,y') \cdot \mu(y,y') \ ; \tag{2.14}$$

$Var(\mu_1,\mu_2)$ and $\mathcal{D}_\rho(\mu_1,\mu_2)$ are respectively called *total variation distance* and *Vasserstein distance with respect to* ρ between the two measures μ_1 and μ_2.

Let us consider a spin system on $\mathbb{Z}^d$ with single spin space $\mathcal{S}$ and range–one interaction (generalization to arbitrary finite range is trivial); we denote by η_i the spin variable associated to the site $i \in \mathbb{Z}^d$.

For any finite set $V \subset \mathbb{Z}^d$ we denote by ∂V^+ the set of points outside V whose spins interact with the spins inside V and by $\eta_V \in \mathcal{S}^V$ a spin configuration on V. Given the boundary condition $\xi \in \mathcal{S}^{V^c}$, we denote by μ_V^ξ the Gibbs measure in V with boundary conditions ξ outside V. Given a metrics ρ on $\mathcal{S}$ we associate to it a metrics ρ_V on $\mathcal{S}^V$ defined as follows

$$\rho_V(\eta_V, \eta'_V) := \sum_{i \in V} \rho(\eta_i, \eta'_i) \quad \forall \eta_V, \eta'_V \in \mathcal{S}^V \quad .$$

We say that condition $DSU_\rho(V, \delta)$ (the Dobrushin–Shlosman Uniqueness condition in V with respect to the metrics ρ and uniqueness parameter δ) is satisfied if and only if $\exists$ a finite set $V \subset \mathbb{Z}^d$ and $\exists \delta > 0$ such that: $\forall j \in \partial V^+ \ \exists \alpha_j > 0$ such that for any couple of boundary conditions $\xi, \xi' \in \mathcal{S}^{V^c}$ with $\xi_i = \xi'_i \ \forall i \neq j$ one has

$$\mathcal{D}_{\rho_V}(\mu_V^\xi, \mu_V^{\xi'}) \leq \alpha_j \rho(\xi_j, \xi'_j) \quad ,$$

and

$$\sum_{j \in \partial V^+} \alpha_j \leq \delta |V| \quad .$$

Let us consider the metrics on the single site variable given by:

$$\widetilde{\rho}(\eta, \eta') := \begin{cases} 1 & \text{iff } \eta \neq \eta' \\ 0 & \text{otherwise} \end{cases} \quad ; \tag{2.15}$$

in this case condition $DSU_{\tilde{\rho}}(V, \delta)$ will be simply denoted by $DSU(V, \delta)$.

We observe that, in this case

$$\mathcal{D}_{\rho_V}(\mu_V^\xi, \mu_V^{\xi'}) \geq \sum_{i \in V} \mathcal{D}_{\tilde{\rho}}(\mu_i^\xi, \mu_i^{\xi'}) = \sum_{i \in V} Var(\mu_i^\xi, \mu_i^{\xi'}) \tag{2.16}$$

as it easily follows from (2.14) and Proposition A1 in the Appendix.

In order to describe Dobrushin–Shlosman's results based on $DSU_\rho(V, \delta)$ condition we need some more definitions. We are going to introduce two kinds of mixing conditions, of a priori different strength, for Gibbs measures in a finite volume Λ. The first ones are weak mixing (WM) conditions saying that the influence of a local change in conditioning spins decays exponentially fast with the distance from the boundary $\partial\Lambda$; the second kind, the one of strong mixing (SM) conditions, corresponds to the case where the influence of a change of a conditioning spin x decays exponentially fast with the distance from x. We refer to [MO1], [MO2] for a critical discussion of these different notions. It has been shown with some examples (see [Sh]) that it may happen that WM is satisfied whereas the corresponding SM is not. Since we are speaking of finite volume mixing condition we have to make explicit in the notation the constants referring to the concerned exponential decay. Of course a particularly interesting case is when we have these mixing conditions in a class of arbitrarily large volumes Λ with uniform constants. We refer again to [MO1], [MO2] for a discussion of these point. It turns out that a crucial aspect is the class of volumes that we are considering. In particular in the Dobrushin–Shlosman theory of complete analyticity (see [DS2], [DS3]) arbitrary shapes were considered whereas in the approach developed in [O], [OP], [MO2] only sufficiently regular domains were involved.

We say that a Gibbs measure μ_Λ^τ on Ω_Λ satisfies a *strong mixing* condition with constants C, γ if for every subset $\Delta \subset \Lambda$:

$$\sup_{\tau, \tau^{(y)} \in \Omega_{\Lambda^c}} Var(\mu_{\Lambda,\Delta}^\tau \;\; \mu_{\Lambda,\Delta}^{\tau^{(y)}}) \leq C e^{-\gamma \mathrm{dist}(\Delta, y)} \tag{2.17}$$

where $\tau_x^{(y)} = \tau_x$ for $x \neq y$ and $\mu_{\Lambda,\Delta}^\tau$ is the μ_Λ^τ–probability distribution of the spins in Δ. We denote this condition by $SM(\Lambda, C, \gamma)$.

We say that a Gibbs measure μ_Λ^τ satisfies a *weak mixing* condition with constants C, γ if for every subset $\Delta \subset \Lambda$

$$\sup_{\tau, \tau' \in \Omega_{\Lambda^c}} Var(\mu_{\Lambda,\Delta}^\tau, \mu_{\Lambda,\Delta}^{\tau'}) \leq C \sum_{x \in \Delta,\, y \in \partial \Lambda^+} \exp(-\gamma |x-y|) \;\; ; \tag{2.18}$$

we denote this condition by $WM(\Lambda, C, \gamma)$.

Theorem DS (see [DS1])

Let $DSU(V, \delta)$ be satisfied for some V and $\delta < 1$; then $\exists \;\; C > 0, \gamma > 0$ such that condition $WM(\Lambda, C, \gamma)$ holds *for every* Λ.

Theorem MOS (see [MOS])

Let the dimension of the lattice be $d = 2$. If there exist positive constants C and γ such that the Gibbs measure μ_Λ^τ satisfies the weak mixing condition $WM(\Lambda, C, \gamma)$ for any finite $\Lambda \subset \mathbb{Z}$, then there exist positive constants C' and γ' such that the Gibbs measure μ_Λ^τ satisfies the strong mixing condition $SM(\Lambda, C', \gamma')$ for any sufficiently regular domain Λ and in particular for any square Λ_L with arbitrary side L.

Here "sufficiently regular" means "multiple of a sufficiently large square" (see [MO1]).

Remark

Actually the conclusion of the above theorem remains true even if we assume the weak mixing *not* for *all* finite subsets of $\mathbb{Z}$ but *only* for all subsets of a square Λ_{L_o} provided that

L_o is large enough (depending of course on the constants C and γ and on the range of the interaction).

Then our strategy to show Gibbsianness of the renormalized measure arising from the application of the Majority Rule transformation is based on the following chain of implications.

We try to verify $DSU(V, \delta)$ for some given V and $\delta < 1$ for any constrained model. Then if we could apply Theorem DS we would get $WM(\Lambda, C, \gamma)$ $\forall\Lambda$ with the same constants C, γ for all Λ and for all constrained model. Subsequently, if we could apply Theorem MOS (by exploiting two–dimensionality), we would get $SM(\Lambda, C', \gamma')$ for all sufficiently regular domains Λ with the same constants C', γ' for all these Λ and for all constrained model. This would directly imply the validity of the conclusions of Theorem 1.1 in [HK]; indeed it immediately follows from the proof of Theorem 1.1 in [HK] that the authors could have obtained exactly the same result by only assuming their strong mixing hypothesis, (that they express in an equivalent form, valid for Ising–like systems, as exponential decay of two–points spin–spin truncated correlations) uniformly in the constrained model and in the boundary conditions *only for all sufficiently regular* (in the above specified sense) domains instead of *for all* domains.

Strictly speaking Theorems DS and MOS apply to translationally invariant situations and our constrained models are not, in general, translationally invariant. However it is easy to convince oneself that both Theorems extend in a straightforward way to the non–translationally invariant case provided we assume spatial uniformity of the bounds appearing in the hypotheses. In other words we have that it is sufficient to assume the validity, for a given constrained model, of $DSU(V, \delta)$ for some V and some $\delta < 1$ *uniformly* in the location of V to imply SM (for arbitrary sufficiently regular volumes with uniform constants) for the same model. But if we are able to show that $DSU(V, \delta)$ is verified for a given V and $\delta < 1$ *for all* constrained models (namely for all $\sigma' \in \Omega_{V'}$) this implies, at the same time, (using extended versions of Theorem DS and MOS) the validity of SM (for arbitrary sufficiently regular volumes with uniform constant) for all constrained models and then, via Theorem 1.1 in [HK], Gibbsianness of the renormalized measure.

Now we start applying the above strategy. We first introduce some specific definitions. Let us consider a squared volume $V' \subset \Lambda'$ with side l and the corresponding subset V, with side $2l$, of the original lattice Λ. Let us consider the metrics on the single block–variable space $\{1, ..., 8\}$ defined by

$$\widetilde{\rho}(\alpha, \alpha') := \begin{cases} 1 & \text{iff } \alpha \neq \alpha' \\ 0 & \text{otherwise} \end{cases} \quad \forall \alpha, \alpha' \in \{1, ..., 8\} \ . \tag{2.19}$$

and the metrics on $\widetilde{\Omega}_{V'}$ given by

$$\rho_{V'}(S,S') := \sum_{(x,y)\in V'} \widetilde{\rho}(S_{(x,y)},S'_{(x,y)}) \quad \forall S,S' \in \widetilde{\Omega}_{V'} \ . \tag{2.20}$$

Now, given $\sigma' \in \Omega'_{V'}$ and $\tau' \in \Omega'_{\partial V'^+}$, we denote by $[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}$ a pair of boundary conditions $\mathcal{T}_1$, $\mathcal{T}_2 \in \widetilde{\Omega}_{\partial V'^+}$ such that $\mathcal{T}_{1_{(x',y')}} = \mathcal{T}_{2_{(x',y')}}$ $\forall (x',y') \in \partial V'^+ \setminus \{(x,y)\}$ and we define

$$\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'} := \mathcal{D}_{\rho_{V'}}(\mu^{\mathcal{T}_1}_{\beta,V',\sigma',\tau'},\mu^{\mathcal{T}_2}_{\beta,V',\sigma',\tau'})\frac{|\partial V'^+|}{|V'|} = \mathcal{D}_{\rho_{V'}}(\mu^{\mathcal{T}_1}_{\beta,V',\sigma',\tau'},\mu^{\mathcal{T}_2}_{\beta,V',\sigma',\tau'})\frac{4}{l} \ , \tag{2.21}$$

where $\mathcal{D}_{\rho_{V'}}(\mu^{\mathcal{T}_1}_{\beta,V',\sigma',\tau'},\mu^{\mathcal{T}_2}_{\beta,V',\sigma',\tau'})$ is the Vasserstein distance between two equilibrium measures for the constrained model corresponding to σ',τ' which have been obtained by modifying the boundary conditions just in one site in $\partial V'^+$. We set:

$$\mathcal{E}_{\beta,V',\sigma'} := \sup_{(x,y)\in\partial V'^+} \ \sup_{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}} \mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'} \ ; \tag{2.22}$$

heuristically we can say that $\mathcal{E}_{\beta,V',\sigma'}$ measures how much the equilibrium of the constrained model is modified if one changes the boundary condition in one site, uniformly in the site and in the boundary conditions; it can be called *uniqueness parameter* (in the sense of DSU condition) in V' for the constrained model characterized by σ' at inverse temperature β

It is a trivial consequence of the definitions that if $\mathcal{E}_{\beta,V',\sigma'} < 1$ then the Dobrushin–Shlosman uniqueness condition $DSU(V',\delta)$ is satisfied for some $\delta < 1$ for the constrained model corresponding to σ',τ'. The main aim of this paper is to build up a Monte Carlo algorithm in order to estimate $\mathcal{E}_{\beta,V',\sigma'}$ and to show that at $\beta = \beta_c := \frac{1}{2}\log(1+\sqrt{2})$ (the critical inverse temperature of the standard 2D Ising model) there exists a volume V' such that for all possible constrained models $\mathcal{E}_{\beta,V',\sigma'} < 1$, namely:

$$\mathcal{E}_{\beta,V'} := \sup_{\sigma'\in\Omega'_{V'}} \mathcal{E}_{\beta,V',\sigma'} \ < 1 \ . \tag{2.23}$$

3. Rough estimate of critical temperatures.

In the following sections we will see that two constrained models (the *chessboard* and the *striped* model, see definition below) are particularly "dangerous", that is they satisfy DSU condition for volumes larger than those needed by the other constrained models.

The *chessboard* and the *striped* models are the constrained models corresponding, respectively, to the two configurations $\mathcal{C}, \mathcal{S} \in \Omega'$ defined as follows

$$\mathcal{C}_{(x,y)} := \begin{cases} 1 & \text{if } x+y \text{ is even} \\ -1 & \text{otherwise} \end{cases} \qquad \mathcal{S}_{(x,y)} := \begin{cases} 1 & \text{if } y \text{ is even} \\ -1 & \text{otherwise} \end{cases} \quad ; \tag{3.1}$$

these two configurations are respectively depicted in Fig.1b and Fig.1c.

We study the equilibrium properties of the chessboard and the striped model by means of a standard Monte Carlo procedure based on a suitable Heat Bath dynamics. This dynamics is generally used to compute mean values (with respect to the equilibrium Gibbs measure) of some observables as time averages; this mean value will be denoted by $< \cdot >$.

This "conventional Monte Carlo" analysis is preliminar to the main numerical results of this paper. Here we are not interested in a large scale simulation nor in a precise estimate of critical points and exponents; we just want to have a strong evidence of the fact that the critical inverse temperature of the two dangerous models is, in both cases, much greater than β_c.

By making use of the notation introduced in Section 2 (relatively to the constrained models $\mathcal{I}^{\tau}_{\beta,\sigma'}$) we describe, now, the discrete time Heat Bath dynamics used in our Monte Carlo study. It is given by the Markov chain defined below:

1. We consider the constrained model corresponding to $\sigma' \in \Omega'_{\Lambda'}$ and we assume periodic boundary conditions; we denote it by $\mathcal{I}_{\beta,\sigma'}$ and its hamiltonian by $H_{\Lambda',\sigma'}(S)$ with $S \in \widetilde{\Omega}_{\Lambda'}$.
2. At each step we perform a complete updating of all $S_{(x,y)}$ block–variables following the lexicographic order; in the remaining of this section this will be called a Monte Carlo *sweep*.
3. For any $(x,y) \in \Lambda'$ the new value $S'_{(x,y)}$ of the block–variable $S_{(x,y)}$ is chosen at random according to the Gibbs measure in $B_{(x,y)}$ with boundary condition $S^c_{(x,y)} := S|_{(\Lambda' \cup \partial\Lambda'_+) \setminus B_{(x,y)}}$. Hence, if we denote by $H_{\sigma'}(S'_{(x,y)}|S^c_{(x,y)})$ the contribution of the block $B_{(x,y)}$ to the energy of the system, the transition probability is given by

$$P_{\beta,\sigma'}(S_{(x,y)} \to S'_{(x,y)}) := \frac{\exp[-\beta H_{\sigma'}(S'_{(x,y)}|S^c_{(x,y)})]}{\sum_{S''_{(x,y)}=1}^{8} \exp[-\beta H_{\sigma'}(S''_{(x,y)}|S^c_{(x,y)})]} \quad . \tag{3.2}$$

We remark that in our notation there is'nt any explicit dependence of the boundary conditions ($\mathcal{T}$–τ'), because they are supposed to be periodic.

In order to estabilish for which value of the inverse temperature β the two models $\mathcal{I}_{\beta,\mathcal{C}}$ and $\mathcal{I}_{\beta,\mathcal{S}}$ are critical, we have computed the specific heat defined in terms of the equilibrium energy fluctuations:

$$C_{\Lambda,\sigma'} := \frac{\beta^2}{4L^2}(< H^2_{\Lambda',\sigma'} > - < H_{\Lambda',\sigma'} >^2) \quad \forall\sigma' = \mathcal{C},\mathcal{S} \ . \tag{3.3}$$

Both models have been studied in the case $L = 64$, which means that we have considered the two models defined on square lattice containing 128^2 original sites; we have considered smaller values of L, as well, in order to check the finite size behaviour. In the case of model $\mathcal{I}_{\beta,\mathcal{C}}$ we have performed 10^5 full sweeps of our Monte Carlo algorithm for each value of β, while in the case of model $\mathcal{I}_{\beta,\mathcal{S}}$ 1.5×10^5 sweeps have been performed.

In Fig.2 and in Fig.3 we have plotted the specific heat as a function of the inverse temperature β in the case of models $\mathcal{I}_{\beta,\mathcal{C}}$ and $\mathcal{I}_{\beta,\mathcal{S}}$ respectively; these results have been obtained by analyzing the Monte Carlo data by means of the "jackknife" procedure. From the pictures it is clear that both inverse critical temperatures, $\beta_c^{\mathcal{C}}$ and $\beta_c^{\mathcal{S}}$, are significantly greater than the Ising inverse critical temperature β_c. Our rough estimates are the following ones:

$$\beta_c^{\mathcal{C}} = 1.60 \pm 0.05 \quad \beta_c^{\mathcal{S}} \geq 2.2 \ . \tag{3.4}$$

4. The algorithm.

Let us consider the volume V' introduced in Section 2, $\sigma' \in \Omega'_{V'}$, $\tau' \in \Omega'_{\partial V'+}$, a pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(\bar{x},\bar{y})}$, the two equilibrium measures $\mu^{\mathcal{T}_1}_{\beta,\Lambda',\sigma',\tau'}$ and $\mu^{\mathcal{T}_2}_{\beta,\Lambda',\sigma',\tau'}$. Let us denote by $\mathcal{K}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$ the set of joint representations of $\mu^{\mathcal{T}_1}_{\beta,\Lambda',\sigma',\tau'}$ and $\mu^{\mathcal{T}_2}_{\beta,\Lambda',\sigma',\tau'}$; we want to give a numerical estimate of the quantity $\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$ defined in (2.21).

A similar problem has been studied in [BMO]: in that paper, by means of a standard Heat Bath dynamics, a lower bound to $\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$ has been calculated; now, we build up a Monte Carlo algorithm in order to obtain a numerical estimate of an upper bound to the same quantity.

First of all we heuristically describe the idea on which the algorithm is based. In order to exactly calculate the Vasserstein distance one should know a joint probability measure $Q^*(\cdot,\cdot) \in \mathcal{K}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$ on the space $\widetilde{\Omega}_{V'} \times \widetilde{\Omega}_{V'}$ such that

$$\mathcal{D}_{\rho_{V'}}(\mu^{\mathcal{T}_1}_{\beta,V',\sigma',\tau'}, \mu^{\mathcal{T}_2}_{\beta,V',\sigma',\tau'}) = \sum_{S^{(1)},S^{(2)}\in\widetilde{\Omega}_{V'}} Q^*(S^{(1)},S^{(2)})\rho_{V'}(S^{(1)},S^{(2)}) \ , \tag{4.1}$$

that is a joint probability measure "optimizing" the sum in (2.14); this is a very hard task. On the other hand it is possible to calculate the Vasserstein distance between two equilibrium measures, relative to two different local boundary conditions, of a single block–variable; indeed, in this case, from the definitions given in Section 2, it turns out that the distance between two configurations is $\widetilde{\rho}(\alpha,\alpha') = 1 - \delta_{\alpha,\alpha'}$ $\forall \alpha,\alpha' \in \{1,...,8\}$ (see (2.19)) and so the Vasserstein distance coincides with the total variation distance (see [D1], page 472). In this case it is also possible to calculate the "optimizing" joint distribution measure. Hence the idea is to build up a dynamics describing the evolution of two coupled systems, with different boundary conditions, such that at each step a single block–variable is updated according to the "local optimizing" joint distribution law.

Now we give the detailed definition of the dynamics.

1. Given $\sigma' \in \Omega'_{V'}$, $\tau' \in \Omega'_{\partial V'+}$ and a pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(\bar{x},\bar{y})}$, we want to describe the evolution of the pair of copies of the constrained model corresponding to $\sigma' \in \Omega'_{V'}$ and $\tau' \in \{-1,+1\}^{\partial V'^+}$ with boundary conditions respectively given by $\mathcal{T}_1$ and $\mathcal{T}_2$.

2. We consider the Markov Chain $X_t := (S^{(1)}(t), S^{(2)}(t))$ $\forall t \in \mathbb{N}$ where $S^{(1)}(t)$ and $S^{(2)}(t)$ are the configurations of the two copies of the system at the time t. The two processes $S^{(1)}(t)$ and $S^{(2)}(t)$ are called *marginal chains*, while X_t is called *joint chain*.

3. At each instant t one and only one site $(x,y) \in V'$ is taken into account; all sites $(x,y) \in V'$ are visited in lexicographic order, hence in an interval of time $\Delta t = |V'|$ all

sites $(x,y)\in V'$ are considered: this is called a *sweep* (or, sometimes, *full sweep*) of the dynamics.

4. Let us consider the site (x,y) which is updated at the time t; we introduce the following notation: $q^{\mathcal{T}_i}[S^{(i)}_{(x,y)}|S^{(i)}_{V'\setminus\{(x,y)\}}(t-1)]$ with $i=1,2$ is the equilibrium Gibbs probability measure for the block–variable in (x,y) conditioned to the values of the block–variables in $V'\setminus\{(x,y)\}$ at time $t-1$; we denote by $\mathcal{K}_{(x,y)}(t)$ the set of joint representations of

$$q^{\mathcal{T}_1}[S^{(1)}_{(x,y)}|S^{(1)}_{V'\setminus\{(x,y)\}}(t-1)] \text{ and } q^{\mathcal{T}_2}[S^{(2)}_{(x,y)}|S^{(2)}_{V'\setminus\{(x,y)\}}(t-1)] \tag{4.2}$$

and, finally, by

$$q^{*\ \mathcal{T}_1,\mathcal{T}_2}[S^{(1)}_{(x,y)},S^{(2)}_{(x,y)}|S^{(1)}_{V'\setminus\{(x,y)\}}(t-1)),S^{(2)}_{V'\setminus\{(x,y)\}}(t-1)] \tag{4.3}$$

the joint representation in $\mathcal{K}_{(x,y)}(t)$ such that

$$\mathcal{D}_{\widetilde{\rho}}\Big(q^{\mathcal{T}_1}[S^{(1)}_{(x,y)}|S^{(1)}_{V'\setminus\{(x,y)\}}(t-1)],q^{\mathcal{T}_2}[S^{(2)}_{(x,y)}|S^{(2)}_{V'\setminus\{(x,y)\}}(t-1)]\Big)=$$

$$=\sum_{S^{(1)}_{(x,y)},S^{(2)}_{(x,y)}=1}^{8}\widetilde{\rho}(S^{(1)}_{(x,y)},S^{(2)}_{(x,y)})\cdot q^{*\ \mathcal{T}_1,\mathcal{T}_2}[S^{(1)}_{(x,y)},S^{(2)}_{(x,y)}|S^{(1)}_{V'\setminus\{(x,y)\}}(t-1)),S^{(2)}_{V'\setminus\{(x,y)\}}(t-1)]\ ; \tag{4.4}$$

the joint representation (4.3) can be exactly calculated as it is shown in Appendix A. All probability measures introduced above depend on β,V',σ' and τ'; we drop explicit dependence to simplify the notation. Notice that, of course, the $q^{\mathcal{T}_i}[\cdot|\cdot]$ are stationary. The dependence on $t-1$ in the conditioning spins is made explicit only to clarify the updating rule from the configuration at time $t-1$ to the one at time t.

5. Given $t\geq 1$ and the corresponding site $(x,y)\in V'$, the configurations $S^{(1)}(t)$ and $S^{(2)}(t)$ are obtained by choosing the pair $(S^{(1)}_{(x,y)}(t),S^{(2)}_{(x,y)}(t))$ at random according to the joint probability measure (4.3) and $S^{(i)}_{(x',y')}(t)=S^{(i)}_{(x',y')}(t-1)$ $\forall i=1,2$ and $\forall(x',y')\in V'\setminus\{(x,y)\}$.

In analogy with the terminology used in [DS1], we call this dynamics *Dynamical Surgery*; now some easy properties of this dynamics are discussed.

1. Given $t\in\mathbb{N}$, it is immediate to see that if

$$S^{(1)}_{(x',y')}(t-1)=S^{(2)}_{(x',y')}(t-1)\ \ \forall(x',y') \text{ nearest neighbors of } (x,y)$$

then

$$S^{(1)}_{(x,y)}(t) = S^{(2)}_{(x,y)}(t) \quad ; \tag{4.5}$$

in other words this means that in this case the joint representation (4.3) lies on the diagonal.

2. The evolution of the two marginal chains $S^{(1)}(t)$ and $S^{(2)}(t)$ is described by a standard Heat Bath dynamics; this is a consequence of the fact that the probability (4.3) is a joint representation of the single site probability distributions (4.2), which are the Gibbs measures of a single block–variable with boundary conditions given, respectively, by $\left(\mathcal{T}_1, S^{(1)}_{V'\setminus\{(x,y)\}}(t-1)\right)$ and $\left(\mathcal{T}_2, S^{(2)}_{V'\setminus\{(x,y)\}}(t-1)\right)$. Hence the equilibrium distributions for the two marginal chains $S^{(1)}(t)$ and $S^{(2)}(t)$ are the Gibbs measures with boundary conditions given, respectively, by $\mathcal{T}_1$ and $\mathcal{T}_2$.

3. Given $t \in \mathbb{N}$, given $Q(\cdot,\cdot) \in \mathcal{K}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,\Lambda',\sigma',\tau'}$, if the stochastic variable $X_t = (S^{(1)}(t), S^{(2)}(t))$ is such that

$$P(S^{(1)}(t) = S, S^{(2)}(t) = S') = Q(S,S') \quad \forall S, S' \in \widetilde{\Omega}_{V'} \quad ,$$

that is it is distributed according to the joint probability measure $Q(\cdot,\cdot)$, then it is easy to prove that X_{t+1} is distributed according to an element of $\mathcal{K}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,\Lambda',\sigma',\tau'}$, as well.

¿From the fact that the joint chain X_t is an ergodic, aperiodic chain with a finite state space and from properties 2 and 3, it immediately follows that there exists a unique equilibrium distribution for the Markov chain X_t; it is a joint probability measure $\bar{Q}(\cdot,\cdot) \in \mathcal{K}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,\Lambda',\sigma',\tau'}$. This means that, provided the two marginal chains have thermalized, that is they are almost described by the corresponding Gibbs measures, the joint chain, after a long enough time, is almost characterized by the distribution $\bar{Q}(\cdot,\cdot)$, which is a joint representation of the Gibbs measures $\mu^{\mathcal{T}_1}_{\beta,\Lambda',\sigma',\tau'}(S)$ and $\mu^{\mathcal{T}_2}_{\beta,\Lambda',\sigma',\tau'}(S)$. Hence, if one needs to calculate the "phase average" of an observable depending on $S^{(1)}$ and $S^{(2)}$ with the joint probability $\bar{Q}$, one can perform a sufficiently long Monte Carlo run with the dynamical surgery and calculate the "time average" of the same observable.

If it were $\bar{Q} = Q^*$ then we could perform a Monte Carlo calculation of the uniqueness parameter $\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$, but in general $\bar{Q} \neq Q^*$ and moreover we cannot say anything on how much $\bar{Q}$ is close to Q^*. Anyway we can use the joint representation $\bar{Q}$ to calculate an "upper" estimator of the uniqueness parameter ; we set:

$$\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'} := \frac{4}{l} \cdot \frac{1}{I} \sum_{s=1}^{I} \rho_{V'} \left(S^{(1)}(s \cdot |V'|), S^{(2)}(s \cdot |V'|) \right) \tag{4.6}$$

where I is the number of sweep performed during the Monte Carlo run. It is clear that $\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$ is a numerical upper bound to $\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2](\bar{x},\bar{y})}_{\beta,V',\sigma',\tau'}$.

The same Monte Carlo run can be used to estimate a “lower” bound to the uniqueness parameter like in [BMO]. Indeed, we define the quantities

$$N^{(i)}_{(x,y)}(\alpha) := \frac{1}{I}\sum_{s=1}^{I} \delta_{\alpha, S^{(i)}_{(x,y)}(s\cdot|V'|)} \quad \forall i=1,2 \ \forall (x,y)\in V' \ \forall \alpha \in \{1,...,8\} \tag{4.7}$$

and we set

$$\mathcal{L}^{[\mathcal{T}_1,\mathcal{T}_2]_{(\bar{x},\bar{y})}}_{\beta,V',\sigma',\tau'} := \frac{4}{l} \sum_{(x,y)\in V'} \frac{1}{2} \sum_{\alpha\in\{1,\ldots,8\}} |N^{(1)}_{(x,y)}(\alpha) - N^{(2)}_{(x,y)}(\alpha)| \ ; \tag{4.8}$$

see [BMO] for more details.

5. Upper and lower bound: numerical results.

In Section 4 we have developed a Monte Carlo algorithm in order to evaluate an upper and a lower bound on $\mathcal{E}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'}$ and we have denoted these two quantities respectively by $\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'}$ and $\mathcal{L}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'}$.

This algorithm cannot be used to give a direct evaluation of an upper bound to $\mathcal{E}_{\beta,V'}$; indeed, in order to calculate an upper bound to $\mathcal{E}_{\beta,V'}$ we should consider all possible constrained models and all possible pairs of boundary conditions $[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}$ (see the notation introduced in Section 2), that is we should perform $3\cdot l\cdot 2^{l^2+8l+1}$ runs of our Monte Carlo; one immediately realizes that this is an almost impossible task since it would give rise to an enormous computation even in the case of small volumes ($l=2,3$).

Indeed, two boundary conditions can differ in one site $(x,y)\in\partial V'^{+}$ in six ways: if one considers the block $B_{(x,y)}$ with $(x,y)\in\partial V'^{+}$ and gives the block–variable $S_{(x,y)}$, only two of the original spins $\sigma^i_{(x,y)}$, those adjacent from the exterior to the lattice V, influence the equilibrium properties of the system; hence the possible ways in which two boundaries may differ are the following ones

$$\begin{array}{cc} ++ & +- \\ ++ & -+ \\ ++ & -- \\ +- & -+ \\ +- & -- \\ -+ & -- \end{array} \tag{5.1}$$

where we have depicted the two couples of original spins, belonging to the block $B_{(x,y)}$ and adjacent from the exterior to V, that one can have when one considers two boundary conditions differing just in (x,y). Hence, one can easily convince himself that the total number of pairs of boundary conditions $[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}$ is given by $6\cdot 2^{2(4l-1)}$; finally, noticed that given l there exists 2^{l^2} possible constrained models and that the site (x,y) can be chosen in $4l$ different ways, it is immediate to see that considering all possible constrained models and all possible pairs of boundary conditions amounts to examine $3\cdot l\cdot 2^{l^2+8l+1}$ different situations. This number could be reduced by taking into account various symmetries; however one would still have, for interesting values of l, an excessively big computation to perform.

Hence we are forced to consider just some of the possible constrained models and some of the possible boundary conditions, that is we are forced to perform a sort of "statistics".

Let us denote by $\mathcal{U}_{\beta,V'}$ the highest value obtained for $\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'}$ and by $\mathcal{L}_{\beta,V'}$ the corresponding estimate of $\mathcal{L}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'}$.

First of all we made a preliminary evaluation of our upper and lower estimators for different values of l, by choosing completely at random a certain number of constrained models and some of all possible pairs of boundary conditions.

We describe, now, how the statistics has been performed in all cases; our numerical results are summarized in Table 1.

• $l = 1$: In this case the volume V' contains a single site, that is $V' = \{(1,1)\}$. The dynamics defined in Section 4 is based on the local updating of a single block–variable; this updating is worked out according to the probability distribution (4.3). Hence, in the case $l = 1$ the estimator (2.23) has been exactly calculated as follows:

$$\mathcal{E}_{\beta,V'} = 4\left(\sup_{\sigma' \in \Omega'_{V'}} \ \sup_{(x,y)\in\partial V'^{+}} \ \sup_{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}} \sum_{\substack{S^{(1)}_{(1,1)}, S^{(2)}_{(1,1)} \in \{1,\ldots,8\} \\ S^{(1)}_{(1,1)} \neq S^{(2)}_{(1,1)}}} q^{*\ \mathcal{T}_1,\mathcal{T}_2}[S^{(1)}_{(1,1)}, S^{(2)}_{(1,1)}] \right);$$

On the other hand since in this case the Vasserstein distance coincides with the total variation distance (see Appendix A) we could compute the same quantity by means of the expression (2.13). We got:

$$\mathcal{E}_{\beta,V'} = 2.119$$

this result means that in this case there exists at least one constrained model (we remark that there are only two constrained models, respectively corresponding to $\sigma'_{(1,1)} = +1$ and $\sigma'_{(1,1)} = -1$) and one pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(x,y)}$ such that the Dobrushin–Shlosman condition is not fulfilled. Hence, the volume V' with $l = 1$ is not "large enough" for our purposes.

In both cases $\sigma'_{(1,1)} = +1$ and $\sigma'_{(1,1)} = -1$ and for many pairs of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(x,y)}$, we have evaluated the estimator (2.21) by means of the Monte Carlo algorithm, as well; in this way we checked our computational procedure to get the best joint representation (4.3). The results that we obtained differ from the exact values by 1–2%; this shows that, at least in the case $l = 1$, our Monte Carlo procedure is very efficient.

• $l = 2$: we have considered all possible constrained models and for each model we have considered 200 different pairs of boundary conditions. By performing $1.3 \cdot 10^6$ full sweeps of our Monte Carlo, we have obtained the results in Table 1; these results show that there exists at least one constrained model σ', τ' and one pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(x,y)}$ such that $\mathcal{L}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'} > 1$. This means that there exists a constrained model, the one corresponding to σ', τ', which does not fulfill the Dobrushin–Shlosman uniqueness condition $DSU(V', \delta)$ with $\delta < 1$.

• $l = 3$: we have considered all possible constrained models and for each model we have considered 100 different pairs of boundary conditions. The results in Table 1 refer to a run of $1.3 \cdot 10^6$ sweeps. In this case there exists a particular constrained model σ', τ' and a pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(x,y)}$ such that $\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'} > 1$ and $\mathcal{L}^{[\mathcal{T}_1,\mathcal{T}_2]_{(x,y)}}_{\beta,V',\sigma',\tau'} < 1$; that is, the upper bound is "too large", while the lower bound is "too low". Hence, for this model we can neither say that the Dobrushin–Shlosman condition is fulfilled nor the opposite; we must necessarily consider larger volumes.

• $l = 4$: we have considered 50 constrained model and 60 pairs of boundary conditions; the results in Table 1 have been obtained by performing $1.3 \cdot 10^6$ full sweeps of the algorithm described in Section 4.

• $l = 8$: we have performed the same statistics as in the case $l = 4$, but in this case it is obviously less significant, because the global number of possible choices is much greater. We have performed $1.3 \cdot 10^6$ full sweeps of our Monte Carlo.

• $l = 16$: we have considered 30 constrained model and 30 pairs of boundary conditions; we had to reduce the number of runs, because of their length.

Remark.
The error $\Delta\mathcal{U}_{\beta,V'}$ in Table 1 is the usual statistical error, that is the standard deviation on the measure of the average $\mathcal{U}_{\beta,V'}$ of the Monte Carlo results. On the other hand the best estimate $\mathcal{L}_{\beta,V'}$ and the error $\Delta\mathcal{L}_{\beta,V'}$ have been obtained by fitting the Monte Carlo results with the equation

$$\mathcal{L}_{\beta,V'} + \frac{\bar{\Delta}\mathcal{L}_{\beta,V'}}{\sqrt{I}} \quad ,$$

where I is the number of full sweeps of the run (see [BMO]) and $\Delta\mathcal{L}_{\beta,V'} = \frac{\bar{\Delta}\mathcal{L}_{\beta,V'}}{\sqrt{I}}$.

The results in Table 1 suggest that in the case $l = 4$ all constrained models satisfy the Dobrushin–Shlosman condition, that is the volume V' with $l = 4$ is "large enough" for our purposes. But, strictly speaking, we cannot be sure about that, because we had to perform a statistics on the constrained models and on the boundary conditions; that is, there could exist a particular "bad" constrained model not satisfying the Dobrushin–Shlosman condition. Then we have considered values of l larger than 4 and we have shown (see Table 1) that for $l = 8, 16$ the value of $\mathcal{U}_{\beta,V'}$ is so small and the effect of the change of conditioning spin is so localized (as we will explain) to lead one to the conclusion that the existence of such a bad model can reasonably be excluded.

Our first observation refers to how the quantity $\frac{l}{4}\mathcal{U}_{\beta,V'}$, namely the average distance of the two copies of the system which evolve following the joint Monte Carlo dynamics, behaves as a function of l. Indeed, it grows from 0.530 to 0.8415 when one increases l from 1 to 3, and then it remains approximately constant when one increases the value of l; this is what one expects heuristically.

In all the above described cases the "statistics" has been performed by choosing completely at random the constrained models and the boundary conditions; in all cases we have found that the most "dangerous" models, that is the constrained models with highest values of our upper estimator, are the striped and the chessboard ones.

In order to strengthen the claim that inequality (2.23) is satisfied provided one chooses l large enough, in the case $l = 6$ we have performed a "rational" statistics, that is we have chosen the constrained models and the boundary conditions following reasonable criteria. We have chosen $l = 6$ for our final calculation, because the results listed in Table 1 suggest that in this case condition (2.23) should be fulfilled, while, on the other hand, a full sweep of the Monte Carlo algorithm takes an acceptable CPU time so that we can perform a reasonably wide statistics.

The algorithm introduced in Section 4 describes the "coupled evolution" of two copies of the same model, characterized by two different boundary conditions; we recall that at each instant of time t one and only one site $(x, y) \in V'$ is updated and we observe that the property (4.5) suggests that the differences between the two copies of the model have a unique origin: the difference of the two boundary conditions in $(\bar{x}, \bar{y}) \in \partial V'^{+}$.

Due to this fact it seems resonable to assume that during the evolution the total number $\rho_{V'}(t) := \sum_{(x,y)\in V'} \left(1 - \delta_{S^{(1)}_{(x,y)}(t), S^{(2)}_{(x,y)}(t)}\right)$ of disagreements between the two copies of the system is almost always equal to zero and sometimes these disagreements propagate in V' starting from the site $(\bar{x}, \bar{y})$ in $\partial V'^{+}$. Now, if one recalls that the average distance between the two copies is approximately equal to 0.87 for $l \geq 4$, it looks likely that the disagreements between the two copies of the system are localized in a "small" region around $(\bar{x}, \bar{y})$.

We have tested this hypothesis as indicated in the histogram in Fig. 4 which shows the spatial dependence of disagreements between the two copies. We have plotted the histogram for various constrained models, moving the site $(\bar{x}, \bar{y})$ along one of the four sides of V' and for many pairs of boundary conditions; in all cases that we have considered, we have obtained histograms similar to that depicted in Fig. 4. The results summarized in Fig. 4 strongly suggest that the disagreements between the two copies of the model are almost completely localized in a suitably chosen 3×2 rectangular block $R_{(\bar{x},\bar{y})} \subset V'$.

Now, given the constrained model corresponding to $\sigma' \in \Omega'_{V'}$ and $\tau' \in \Omega'_{\partial V'^{+}}$, the above remarks suggest that the average number of disagreements between the two copies of the system strongly depends on the values of $\sigma'_{(x,y)}$ with $(x, y) \in R_{(\bar{x},\bar{y})}$ and weakly on the values of $\sigma'_{(x,y)}$ outside $R_{(\bar{x},\bar{y})}$. Hence, we have performed the statistics on the constrained model in the case $l = 6$ by considering all possible constrained models only inside $R_{(\bar{x},\bar{y})}$. In the following we precisely describe how the statistics has been performed.

• We have considered $(\bar{x},\bar{y})=(0,3)$, $R_{(\bar{x},\bar{y})}=\{(x,y)\in V':\ x=1,2 \text{ and } 2\le y\le 4\}$, we have modified the boundary condition in $(\bar{x},\bar{y})$ in the six ways depicted in (5.1) and in each case we have considered two possible boundary conditions in $\partial V'^{+}\setminus\{(\bar{x},\bar{y})\}$.

• All possible constrained models have been considered in $R_{(\bar{x},\bar{y})}$, while in $V'\setminus R_{(\bar{x},\bar{y})}$ we have considered only the chessboard model and the model with $\sigma'_{(x,y)}=+1\ \forall (x,y)\in V'\setminus R_{(\bar{x},\bar{y})}$. Indeed, we expect that these two models are respectively the most and the less "dangerous" ones, as the results of the previous statistics suggest.

• In each run of the joint Monte Carlo algorithm we have performed 10^5 full sweeps, that is we have updated the whole lattice V' 10^5 times.

The results can be summarized by saying that the most dangerous constrained models inside $R_{(\bar{x},\bar{y})}$ appear to be the following ones

$$\begin{matrix} + & - & + \\ + & - & + \end{matrix}\qquad \begin{matrix} - & + & - \\ - & + & - \end{matrix}\qquad \begin{matrix} + & - & + \\ - & + & - \end{matrix}\qquad \begin{matrix} - & + & - \\ + & - & + \end{matrix}\ ; \tag{5.2}$$

in particular, our (indeed quite small) statistics on the boundary conditions suggests that the most dangerous model among those in (5.2) is the second one; in this case, taking the chessboard model in $V'\setminus R_{(\bar{x},\bar{y})}$ we obtain $\mathcal{U}^{[\mathcal{T}_1,\mathcal{T}_2]_{(\bar{x},\bar{y})}}_{\beta,V',\sigma',\tau'}=0.610$. The numerical results confirm the weak dependence of the estimators on the constrained model outside $R_{(\bar{x},\bar{y})}$, as well; actually the differences are of 5-10%. Finally, this set of Monte Carlo runs shows that the most dangerous ways in which one can modify the boundary conditions in $(\bar{x},\bar{y})$ are the following ones

$$++\quad --\qquad \text{and}\qquad +-\quad -+\ . \tag{5.3}$$

Once we have understood what are the worst situations inside $R_{(\bar{x},\bar{y})}$ and in $(\bar{x},\bar{y})$ we have performed the wide statistics on the possible boundary conditions described below.

• We have considered the most dangerous constrained model inside $R_{(\bar{x},\bar{y})}$.

• We have considered ten possible constrained model outside $R_{(\bar{x},\bar{y})}$; six of them are those depicted in Fig. 1, the remaining four have been chosen at random.

• In each case we have considered twenty possible pairs of boundary conditions with the original spins in $B_{(\bar{x},\bar{y})}$ and adjacent to V chosen like in (5.3).

The weak dependence of the estimator on the constrained models outside $R_{(\bar{x},\bar{y})}$ has been confirmed and we have found

$$\mathcal{U}_{\beta,V'}=0.633\quad \Delta\mathcal{U}_{\beta,V'}=0.011\ ; \tag{5.4}$$

hence we can confidently say that the condition (2.23) is satisfied if one considers the volume V' with $l=6$.

6. Conclusions.

As we explained in Section 2 the problem of proving Gibbsianness of our renormalized measure is reduced to the verification of $DSU(V, \delta)$ condition for some V and $\delta < 1$ for all possible constrained models.

It is clear that disproving the condition for a given volume V is much easier than proving it since, to disprove, it is sufficient to exhibit one constrained model and one boundary condition for which a lower bound $\mathcal{L}$ for the uniqueness parameter appearing in DSU exceeds one; moreover since this lower bound involves variation distance and then thermal averages it is naturally computable via a Monte Carlo procedure. On the other hand an upper bound has to involve the consideration of all possible constrained models as well as all possible boundary conditions. Moreover a priori it was not clear how to provide an upper bound based on a Monte Carlo computation; this motivated the idea of the dynamical surgery. The necessity of a Monte Carlo approach comes from the consideration of how fast the number of constrained models and possible boundary conditions grows as a function of l, the side of the squared volume where we try to verify DSU.

Since for $l = 2$ we find a particular constrained model and boundary condition for which $\mathcal{L}$ is greater than one, necessarily we have to go at least to $l = 3$ and already the number of independent computations is very large. Moreover since for $l = 3$ the lower bound seems always less than one whereas for at least one case the upper bound is larger than one we can neither disprove nor try to prove with our bounds the validity of DSU for a square with side 3 so that we have to go at least to $l = 4$.

It appears clear from our numerical computations that our upper estimator $\mathcal{U}$ for the uniqueness parameter has the correct behaviour with l: as a consequence of the spatial localization of the set of disagreements between our two coupled processes $\mathcal{U}$ is inversely proportional to l; thus increasing l is the correct choice to get a value of $\mathcal{U}$ so smaller than one (included the error) to be confident in the validity of DSU. Unfortunately increasing l implies an enormous increase in the number of computations; introducing some statistics becomes necessary. The right compromise between smallness of $\mathcal{U}$ and number of constrained models and boundary conditions came out to be $l = 6$. In this case we performed the "rational statistics" that we have described in Section 5 by exploiting the (numerically evident) small dependence of $\mathcal{U}$ on the constrained model and on the boundary condition far from conditioning spin that we are changing.

Our computations relative to the case $l = 6$ make us really confident on the uniform validity of DSU.

We can say that our method is successful because even the correlation length of the "worst" constrained models is very small; however it is not so small to avoid the consideration of sides l at least greater than 4.

We want to make now some general remarks on our Monte Carlo algorithm.

As it has been underlined in [DS1], the nice feature of finite size conditions like DSU, involving the behavior of Gibbs measures in finite volumes, is that they are able to imply absence of phase transitions and many nice properties of the unique *infinite volume* Gibbs state. This point of view is very helpful for example when we have to decide whether or not a given system is in the unique phase regime; especially when we do not have a natural parameter (like the inverse temperature β) whose smallness imply weak-coupling.

The "uniqueness test", based on the verification of DSU, has the advantage, w.r.t the traditional Monte Carlo test, of being based on rigorous grounds. However a real computer assisted proof seems very difficult to achieve unless the concerned volumes are really very small. If this is not the case the use of a Monte Carlo algorithm becomes essential; then the situation is somehow intermediate between a traditional Monte Carlo simulation and a computer assisted proof.

We want to remark that our algorithm to compute a numerical upper bound on the Vasserstein distance between Gibbs measures, which is based on "local readjustment" of the coupling, seems to be quite performant and probably it can be used in more general contexts. Finally it is remarkable that, due to the very nature of the coupling procedure, the statistical error on $\mathcal{U}$ is much smaller that the corresponding one on $\mathcal{L}$; indeed in this last case *all* sites of our volume and not only the disagreements, like in the computation of $\mathcal{U}$, play a role as a source of statistical errors.

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7. Appendix A.

We consider the space $S := \{1, ..., n\}$ with $n \geq 2$ and the metrics $\rho(s, s') \equiv \widetilde{\rho}(s, s') := 1 - \delta_{s,s'}$ $\forall s, s' \in S$; let us denote by λ and μ two probability measures on S and by $\mathcal{K}$ the set of the joint representations of λ and μ. Hence, given $q \in \mathcal{K}$ one has that q is a probability measure on $S \times S$ such that

$$\sum_{s \in S} q(s, s') = \mu(s') \ \forall s' \in S \ \text{ and } \sum_{s' \in S} q(s, s') = \lambda(s) \ \forall s \in S \ . \tag{A.1}$$

We recall, now, that the *total variation distance* and the *Vasserstein distance* between λ and μ are respectively given by

$$\begin{aligned} Var(\lambda, \mu) &:= \frac{1}{2} \sum_{s \in S} |\lambda(s) - \mu(s)| \\ \mathcal{D}_\rho(\lambda, \mu) &:= \inf_{q \in \mathcal{K}} \sum_{s, s' \in S} \rho(s, s') \cdot q(s, s') \end{aligned} \tag{A.2}$$

Proposition A1.

1. With the notation introduced before

$$\mathcal{D}_\rho(\lambda, \mu) = Var(\lambda, \mu) \tag{A3}$$

2. Let us consider the following partition of the set S

$$S = A \cup B \cup C \ , \tag{A.4}$$

where

$$\begin{aligned} A &:= \{s \in S : \ \lambda(s) > \mu(s)\} \\ B &:= \{s \in S : \ \lambda(s) < \mu(s)\} \\ C &:= \{s \in S : \ \lambda(s) = \mu(s)\} \end{aligned} \tag{A.5}$$

one has that

$$Var(\lambda, \mu) = \sum_{s \in A} (\lambda(s) - \mu(s)) = \sum_{s \in B} (\mu(s) - \lambda(s)) \ . \tag{A.6}$$

Proof.

1. See [D1], page 472.

2. It is an immediate consequence of the normalization of μ and λ. □

We want, now, to calculate the particular joint representation $q^* \in \mathcal{K}$ such that the following equality is satisfied

$$\mathcal{D}_\rho(\lambda, \mu) = \sum_{s,s' \in S} \rho(s,s') \cdot q^*(s,s') \quad ; \tag{A.7}$$

that is we are looking for the joint representation "optimizing" the sum in the definition of $\mathcal{D}_\rho(\lambda,\mu)$. In other words, by virtue of the above Proposition, we can say that our aim is to find an $n \times n$ square matrix

$$q^* = \begin{pmatrix} q^*_{1,n} & q^*_{2,n} & q^*_{3,n} & \cdots & q^*_{n,n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ q^*_{1,3} & q^*_{2,3} & q^*_{3,3} & \cdots & q^*_{n,3} \\ q^*_{1,2} & q^*_{2,2} & q^*_{3,2} & \cdots & q^*_{n,2} \\ q^*_{1,1} & q^*_{2,1} & q^*_{3,1} & \cdots & q^*_{n,1} \end{pmatrix} \quad , \tag{A.8}$$

such that

$$\sum_{s=1}^{n} q^*_{s,s'} = \mu_{s'} \ \forall s' = 1,...,n \quad \text{and} \quad \sum_{s'=1}^{n} q^*_{s,s'} = \lambda_s \ \forall s = 1,...,n \tag{A.9}$$

and such that the sum of the off–diagonal elements is given by

$$\sum_{s,s' :\, s \neq s'} q^*_{s,s'} = \sum_{s \in A} (\lambda_s - \mu_s) = \sum_{s \in B} (\mu_s - \lambda_s) \quad ; \tag{A.10}$$

we have introduced the notation: $\lambda_s := \lambda(s)$ and $\mu_s := \mu(s)$ $\forall s \in S$.

In order to compute all the elements of the matrix $q^*_{s,s'}$ one can follow the procedure described below; first of all we introduce the following *filling rule.* It is a construction of a matrix q^* along a sequence of steps. At each step some new set of entries of q^* will be determined whereas for the rest of the entries only some suitable sums of them will be determined. We will end up with a matrix q^* satisfying both $(A.9)$, $(A.10)$ and in this way we show that our procedure is well defined in the sense that at each step it is not empty the set of matrices satisfying our requirements.

1. If $\lambda_s = \mu_s$ $\forall s \in S$ then

$$q^*_{s,s'} = \lambda_s \delta_{s,s'} \quad \forall s, s' \in S$$

2. If $\exists s \in S$ such that $\lambda_s \neq \mu_s$ then $\forall s \in S$ one puts

$$q^*_{s,s} = \min\{\lambda_s, \mu_s\}$$

and

$$\begin{array}{l}\text{if } \mu_s = \lambda_s \text{ then } q^*_{s,s'} = 0 \; \forall s' \neq s, \; q^*_{s',s} = 0 \; \forall s' \neq s \\ \text{if } \mu_s > \lambda_s \text{ then } q^*_{s,s'} = 0 \; \forall s' \neq s \text{ and } q^*_{s',s} \text{ are subject to the condition :}\end{array}$$

$$\sum_{s' :\, s' \neq s} q^*_{s',s} = \mu_s - \lambda_s$$

$$\text{if } \lambda_s > \mu_s \text{ then } q^*_{s',s} = 0 \; \forall s' \neq s \text{ and } q^*_{s',s} \text{ are subject to the condition :}$$

$$\sum_{s' :\, s' \neq s} q^*_{s,s'} = \lambda_s - \mu_s$$

In Fig. 5 an example of application of the above filling rule is shown.

In case 1 the problem is trivially solved; indeed by means of the above filling rule one obtains a diagonal matrix fulfilling the requirements $(A.9)$ and $(A.10)$. In case 2 it is immediate to see that we construct a matrix satisfying the requirements $(A.9)$, but the problem is that in general not all off–diagonal terms are determined: many of them are set equal to zero, but for the others only some sums are specified and not the single values.

By collecting all off–diagonal non–vanishing entries one obtains an $|A| \times |B|$ rectangular matrix, whose elements are not yet determined. More correctly we should speak about a class of matrices (which at the end of our construction will be shown to be non–empty): the ones satisfying the requirements corresponding to one step of application of our filling rule.

Let us denote by $q^{(1)}_{i,j}$ with $1 \leq i \leq n_1 := |A|$ and $1 \leq j \leq n'_1 := |B|$ the elements of this new matrix. We observe that $q^{(1)}_{i,j}$ corresponds to the element $q^*_{f(i),f'(j)}$ of the original matrix, where

$$\begin{array}{l} f(1) := \min\{s \in S : \; \lambda_s > \mu_s\} \\ f(i) := \min\{s > f(i-1) : \; \lambda_s > \mu_s\} \quad \forall i > 1 \end{array} \tag{A.11}$$

and

$$\begin{array}{l} f'(1) := \min\{s \in S : \; \mu_s > \lambda_s\} \\ f'(i) := \min\{s > f'(i-1) : \; \mu_s > \lambda_s\} \quad \forall i > 1 \end{array} . \tag{A.12}$$

It is important to observe that, due to the filling rule, the elements of the new matrix must satisfy the following requirements

$$\sum_{j=1}^{n'_1} q^{(1)}_{i,j} = \lambda_{f(i)} - \mu_{f(i)} \; \forall i = 1, ..., n_1 \; \text{ and } \; \sum_{i=1}^{n_1} q^{(1)}_{i,j} = \mu_{f'(j)} - \lambda_{f'(j)} \; \forall i = 1, ..., n_1 \; . \tag{A.13}$$

¿From the fact that $q^{(1)}$ has been constructed by collecting all off–diagonal elements of q^* different from zero and from equations $(A.13)$, it follows that the $(A.10)$ is fulfilled.

In order to fill the matrix $q^{(1)}$ (by further reducing its indetermination) one applies again the filling rule stated above. Again two things may happen: all elements of $q^{(1)}$ are fixed or one obtains another $n_2 \times n_2'$ rectangular matrix $q^{(2)}$ to be filled.

One goes on applying the filling rule and in this way one obtains a sequence of rectangular matrices

$$q^*, q^{(1)}, q^{(2)}, ..., q^{(t)}, ...$$

which are smaller and smaller in the sense that

$$n \cdot n > n_1 \cdot n_1' > n_2 \cdot n_2' > ... \quad ;$$

the procedure is stopped when all elements are fixed.

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Table 1

l	$\mathcal{U}_{\beta,V'}$	$\Delta\mathcal{U}_{\beta,V'}$	$\mathcal{L}_{\beta,V'}$	$\bar{\Delta}\mathcal{L}_{\beta,V'}$
2	1.452	0.0074	1.34	-2.50
3	1.122	0.0071	0.90	+2.05
4	0.877	0.0046	0.73	+0.32
8	0.436	0.0026	0.30	+0.74
16	0.207	0.0016	0.16	+0.04

Table 1: In the table we have listed the values of $\mathcal{U}_{\beta,V'}$, $\Delta\mathcal{U}_{\beta,V'}$, $\mathcal{L}_{\beta,V'}$ and $\bar{\Delta}\mathcal{L}_{\beta,V'}$ obtained at $l = 2, 3, 4, 8, 16$. The meaning of $\Delta\mathcal{U}_{\beta,V'}$ and $\bar{\Delta}\mathcal{L}_{\beta,V'}$ is explained in the Remark in Section 5.

Fig.1: Examples of configurations of renormalized variables corresponding to constrained models which are particularly important in our calculations.

Fig.2: Specific heat for the chessboard model defined in (3.1) as a function of the inverse temperature β.

Fig.3: Specific heat for the striped model defined in (3.1) as a function of the inverse temperature β.

Fig.4: Each square of the plane **X**–**Y** represents a site (x, y) of a lattice V' with $l = 6$; the **X** axis is oriented from the left to the right, while the **Y** axis is oriented from the top of the figure to the bottom. The results contained in the histogram refer to the chessboard model: the height of each column (x, y) is given by the ratio

$$\frac{\sum_{s=1}^{I} \sum_{(x,y)\in V'} (1 - \delta_{S^{(1),s}_{(x,y)}, S^{(2),s}_{(x,y)}})}{\sum_{s=1}^{I} \sum_{(x,y)\in V'} (1 - \delta_{S^{(1),s}_{(1,3)}, S^{(2),s}_{(1,3)}})}$$

where $I = 1 \cdot 10^5$ is the number of full sweeps of the run, $S^{(1),s}_{(x,y)}$ and $S^{(2),s}_{(x,y)}$ are the block–variables of the two copies of the system on the site (x, y) and after s sweeps. The results in the histogram have been obtained considering a pair of boundary conditions $[\mathcal{T}_1, \mathcal{T}_2]_{(0,3)}$, such that the two pairs of original spins in the block $B_{(0,3)}$ are $+-$ and $-+$.

$$
\begin{array}{cccccc}
\mu_5 & 0 & 0 & 0 & 0 & \mu_5 \\
\mu_4 & \square & 0 & \square & \lambda_4 & \square \\
\mu_3 & 0 & 0 & \mu_3 & 0 & 0 \\
\mu_2 & \square & \lambda_2 & \square & 0 & \square \\
\mu_1 & \mu_1 & 0 & 0 & 0 & 0 \\
 & & & & & \\
 & \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5
\end{array}
$$

(a)

$$
\begin{array}{cccc}
q^{(1)}_{1,2} & q^{(1)}_{2,2} & q^{(1)}_{3,2} & \mu_4 - \lambda_4 \\
q^{(1)}_{1,1} & q^{(1)}_{2,1} & q^{(1)}_{3,1} & \mu_2 - \lambda_2 \\
 & & & \\
\lambda_1 - \mu_1 & \lambda_3 - \mu_3 & \lambda_5 - \mu_5 &
\end{array}
$$

(b)

Fig.5: Application of the filling rule in the case: $n = 5$, $\lambda_1 > \mu_1$, $\lambda_2 < \mu_2$, $\lambda_3 > \mu_3$, $\lambda_4 < \mu_4$ and $\lambda_5 > \mu_5$. In (a) we have depicted the matrix $q^*_{s,s'}$: the sum of the elements of one of its rows must be equal to the corresponding value depicted on the left, while the sum of the elements of one of its column must be equal to the corresponding value depicted on the bottom. The squares represent elements which are not fixed after the filling rule is applied for the first time. The collection of all squares gives rise to the matrix $q^{(1)}_{i,j}$ which is depicted in (b). The values in the right–hand column and in the bottom row are the constraints $(A.13)$ which must be satisfied by the elements, respectively, of each row and each column of the matrix.