

# Renormalization Group at Criticality and Complete Analyticity of Constrained Models: A Numerical Study

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We study the majority rule transformation applied to the Gibbs measure for the 2D 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 2D case, complete analyticity from which, as 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 the DSU condition is verified for a large enough volume  $V$  for all constrained models.

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**KEY WORDS:** Majority rule; renormalization group; non-Gibbsianness; finite-size conditions; complete analyticity; Ising model.

## 1. INTRODUCTION

In recent years much effort has 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

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

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arising from the application of a renormalization group transformation (RGT)  $T_b$ , defined “on scale  $b$ ,” to the Gibbs measure  $\mu$  is Gibbsian. In other words, we ask whether or not  $\nu$  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 the 2D Ising model at inverse temperature  $\beta$  and external magnetic field  $h \neq 0$ . Moreover, we assume that our RGT can be expressed as

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

where  $T_b(\sigma', \sigma)$  is a normalized nonnegative kernel. The system described in terms of the  $\sigma$  variables by the original measure  $\mu$  is called the “object system.” The  $\sigma'$  are the “block variables” of the “image system” described by the renormalized measure  $\nu$ .

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 ref. 12 as the basic reference for a clear and complete description of the general setup of renormalization maps from the point of view of rigorous statistical mechanics.

The above-mentioned pathological behavior (non-Gibbsianness of  $\nu$ ) can be a consequence of the violation of a necessary condition for Gibbsianness called *quasilocality*.<sup>(21, 12, 37)</sup> It is a continuity property of the finite-volume conditional probabilities of  $\nu$  which, roughly speaking, says that they are almost independent of very far away conditioning spins.

In ref. 21 it is shown that a sort of converse statement holds true, namely quasilocality + nonnullness (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  $\nu$ . The construction of the potential in Kozlov’s proof is somehow artificial: it involves reordering of a semiconvergent sum. To get a translationally invariant finite-norm potential one needs some additional, stronger assumptions on how weakly the conditional probabilities of  $\nu$  depend on far-away conditioning spins. We refer to ref. 1 for a more detailed discussion on this point.

In some situations (see, for instance, refs. 2 and 15) it is possible to use much stronger methods, based on the cluster expansion, to compute renormalized potentials, showing finiteness of their norm.

In many interesting examples<sup>(9, 11, 12)</sup> violation of quasilocality and consequently nonGibbsianness of the renormalized measure  $\nu$  are a direct

consequence of the appearance of a first-order phase transition for the original (object) system described by  $\mu$  conditioned to some particular configuration of the image system. More precisely, given a block configuration  $\sigma'$ , 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  $\sigma'$  (which here plays the role of an external parameter).

For some particular  $\sigma'$  it may happen that the corresponding measure  $\mu_{\sigma'}(\sigma)$  exhibits long-range order. See also refs. 14 and 16, where this mechanism was first pointed out.

One can ask about the “robustness” of the pathology of non-Gibbsianness. There are examples<sup>(29)</sup> in which, even though the measure  $\nu = T_b \mu_{\beta, h}$  is not Gibbsian, one has that with the same  $\beta, h$ , by choosing  $b' > b$  sufficiently large, the measure  $\nu' = T_{b'} \mu_{\beta, h}$  is Gibbsian. Alternatively, one can 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  $\beta, h$  (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  $h, \beta$ , for sufficiently large scale  $b$  any constrained model is in the one-phase region.

Another notion of robustness of the pathology<sup>(23, 30)</sup> refers to seeing whether or not it survives after application of a decimation transformation;<sup>(12)</sup> this can be relevant since a decimation transformation does not change the thermodynamic functions or the long-range correlations.

Finally, weaker notions of Gibbsianness of a renormalized measure  $\nu$  can also be considered. The usual notion of Gibbsianness requires a control of quasilocality of  $\nu$  uniform in  $\sigma'$ . It may happen that the particular  $\sigma'$  responsible for the pathology is highly nontypical with respect to  $\nu$ . It appears plausible to ask for quasilocality only for  $\nu$ -almost all configurations  $\sigma'$ .<sup>(5, 13, 24)</sup> See ref. 10 for a nice up-to-date review of all the above problematic.

Now, in many examples even though the object system is well inside the one-phase region, for some particular block configuration  $\sigma'$  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,<sup>(7,8)</sup> 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 we partition  $\mathbb{Z}^2$  into square blocks  $B_i$  of side 2. In this case the new measure  $\nu$  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, with respect to 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

$$T_b(m, \sigma) = \begin{cases} 1 & \text{if } \sum_{x \in B_i} \sigma_x = m_i \quad \forall_i \\ 0 & \text{otherwise} \end{cases}$$

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 ref. 12 that for the 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 quasilocality and then non-Gibbsianness of the renormalized measure  $\nu$ . 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 shown in ref. 12, gives an example of non-Gibbsianness of a measure  $\nu$  arising from the application of a renormalization map to a measure  $\mu$  corresponding to the very weak coupling region. We remark that, as shown in ref. 12, this non-Gibbsianness is robust with respect to the choice of the scale  $b$  (or with respect to iteration), whereas for large  $h$  it can be eliminated by applying one decimation transformation.<sup>(30)</sup>

Other interesting examples have been found.<sup>(9, 11)</sup>

We 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 ref. 3 and in ref. 1 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 van Enter showed with an example that this belief is not sufficiently justified and some extra arguments related to the specific nature of the BAT transformation are

needed to imply Gibbsianness from absence of phase transitions for the  $\{m_i=0\}$  constrained model.<sup>(9, 10)</sup>

Thus, in general, the moral is that what is relevant for Gibbsianness of  $\nu$  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 the possible very weak coupling regime of the object system) to imply non-Gibbsianness of  $\nu$ ; whereas in general, absence of phase transition in a very strong sense is needed for *all constrained models* to get a sufficient condition which implies Gibbsianness of  $\nu$  in the strong, cluster expansion, sense, as shown in ref. 15.

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 Section 2. This transformation, in the same situation of criticality, was studied by Kennedy,<sup>(19)</sup> who established 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 ref. 18. It is an “almost computer assisted proof” of absence of phase transition for these constrained models.

In the present paper we inquire after the validity, in principle for every possible constrained model, of a finite-size condition: the Dobrushin–Shlosman uniqueness condition (DSU, see Section 2), which implies (as explained in Section 2) complete analyticity, and then, using the results of ref. 15, Gibbsianness of  $\nu$ .

Strictly speaking, the proof of ref. 15 does not directly apply to our case since it requires the condition that the kernel  $T(\sigma', \sigma)$  is strictly positive for every  $\sigma', \sigma$ . Probably this is only a technical restriction that can be removed.<sup>(20)</sup> In any case in ref. 15 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 ref. 19. Our study will be numerical but, similarly to ref. 19, 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 ref. 19 some constrained models were analyzed in terms of a finite-size condition easier to satisfy than the 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 ref. 18 is not sufficient to imply complete analyticity. In the present paper, as we said

before, we try to verify the DSU condition for every constrained model, but, as will become clear in Section 5, we can, with present 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 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<sup>(1)</sup> the authors, in the context of the BAT transformation, tried, for one particularly relevant constrained model ( $\{m_i\} = 0, \forall i$ ), 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 the total variation distance can be found involving thermal averages; thus this lower bound is well adapted to study 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, a lower bound 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<sup>(6,7)</sup> that we call *dynamical surgery*. It provides an upper bound to the Vasserstein distance and so it goes in the correct direction toward *proving* the DSU condition.

Our numerical results strongly suggest that indeed the DSU condition is satisfied in our present situation for all constrained models and this, as we said before, implies Gibbsianness of the 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 the Appendix 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 neighbor interaction) 2D Ising model, with zero external field, on a finite square with

even side:  $\Lambda := \{1, \dots, 2L\}^2 \subset \mathbb{Z}^2$ , with  $L \in \mathbb{N}$ . We denote by  $\sigma \in \Omega_\Lambda := \{-1, +1\}^\Lambda$  a configuration of the system in  $\Lambda$  and by  $\tau \in \{-1, +1\}^{\partial\Lambda^+}$  a boundary condition, namely a configuration in  $\partial\Lambda^+$  defined by

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

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  $\tau$  as an extended configuration in  $\{-1, +1\}^{\mathbb{Z}^2 \setminus \Lambda}$ .

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

$$H_\Lambda^r(\sigma) := - \sum_{\substack{\langle i, j \rangle \\ i, j \in \Lambda}} \sigma_i \sigma_j - \sum_{\substack{\langle i, j \rangle \\ i \in \Lambda, j \in \partial\Lambda^+}} \sigma_i \tau_j \quad \forall \sigma \in \Omega_\Lambda \quad (2.2)$$

where the first sum runs over all pairs of nearest neighbor sites in  $\Lambda$ , while the second sum runs over all pairs  $\langle i, j \rangle$  of nearest neighbor 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  $\beta$  is denoted by  $\mu_{\beta, \Lambda}^r(\sigma)$ ,  $\forall \sigma \in \Omega_\Lambda$ , and is given by

$$\mu_{\beta, \Lambda}^r(\sigma) := \frac{\exp[-\beta H_\Lambda^r(\sigma)]}{\sum_{\eta \in \Omega_\Lambda} \exp[-\beta H_\Lambda^r(\eta)]} \quad \forall \sigma \in \Omega_\Lambda \quad (2.3)$$

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  $2 \times 2$  block whose center has coordinates  $(2x - 1/2, 2y - 1/2)$ ; 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  $(x, y) \in \{1, \dots, L\}^2$ , we get a partition of our box  $\Lambda$ . Given  $\sigma \in \Omega_\Lambda$ , we denote by  $\sigma_{(x, y)}^1, \dots, \sigma_{(x, y)}^4$  the four spins corresponding to the four sites of the block  $B_{(x, y)}$  and we define  $m_{(x, y)} := \sum_{i=1}^4 \sigma_{(x, y)}^i$ ; we suppose the four spins  $\sigma_{(x, y)}^i, \forall i=1, \dots, 4$ , ordered in the lexicographic way.

2. We define the new lattice  $\Lambda'$  by collecting the centers of all  $B_{(x, y)}$  blocks and by rescaling the lattice spacing by a factor two; the site of  $\Lambda'$ , 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  $K: (\sigma, \sigma') \in \Omega_\Lambda \times \Omega'_\Lambda \rightarrow K(\sigma, \sigma') \in \{0, 1\}$  as follows:

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

4. The *majority rule transformation* is the transformation which maps the “object” model  $(\Lambda, \Omega_{\Lambda}, \mu_{\beta, \Lambda}^{\tau}(\sigma))$  onto the “image” model  $(\Lambda', \Omega'_{\Lambda'}, \mu_{\beta, \Lambda'}^{\tau}(\sigma'))$ , where

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

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, such as BAT, the single renormalized spin variable still takes values in  $\{-1, +1\}$ .

We finally remark that in our case, where the side of the block is 2 (an even number), the majority rule transformation is not naturally defined when the magnetization inside the block happens to be zero. In order to resolve the ambiguity we choose the deterministic rule of attributing to the renormalized spin  $\sigma'$  in the  $2 \times 2$  block the value of the original spin at the left upper corner.

We could have chosen the probabilistic rule of assigning to  $\sigma'$  in the ambiguous cases the values  $\pm 1$  with equal probability  $1/2$ . We do not have *a priori* any clear criterion to prefer one of the two above options. We only observe that the probabilistic rule gives rise to a longer computation.

This transformation is well known in the physics literature and it has been widely used to investigate the properties of many spin models (see, e.g., ref. 32 and references therein).

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

$$\mu_{\beta, \Lambda, \sigma'}^{\tau}(\sigma) := \frac{K(\sigma, \sigma') \mu_{\beta, \Lambda}^{\tau}(\sigma)}{\sum_{\eta \in \Omega_{\Lambda}} K(\eta, \sigma') \mu_{\beta, \Lambda}^{\tau}(\eta)} \quad (2.6)$$

is a probability measure on  $\Omega_{\Lambda}$ . 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  $\mathcal{F}_{\beta, \sigma'}^{\tau}$  can be seen as the model

$$\left( \Lambda, \Omega_{\Lambda, \sigma'}, \mu_{\beta, \Lambda, \sigma'}^{\tau}(\sigma) = \frac{\exp[-\beta H_{\Lambda}^{\tau}(\sigma)]}{\sum_{\eta \in \Omega_{\Lambda, \sigma'}} \exp[-\beta H_{\Lambda}^{\tau}(\eta)]} \right) \quad (2.7)$$



where we have introduced the *constrained configuration space*

$$\begin{aligned} \Omega_{A, \sigma'} := \{ & \sigma \in \Omega_A : \forall (x, y) \in A' : \\ & (m_{(x, y)} \neq 0 \text{ and } m_{(x, y)} \cdot \sigma'_{(x, y)} > 0) \\ & \text{or } (m_{(x, y)} = 0 \text{ and } \sigma'_{(x, y)} \cdot \sigma'_{(x, y)} > 0) \} \end{aligned} \quad (2.8)$$

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

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  $C_+$

$$\begin{bmatrix} - & + \\ + & + \end{bmatrix} \begin{bmatrix} + & - \\ - & + \end{bmatrix} \begin{bmatrix} + & - \\ + & - \end{bmatrix} \begin{bmatrix} + & - \\ + & + \end{bmatrix} \begin{bmatrix} + & + \\ - & - \end{bmatrix} \begin{bmatrix} + & + \\ - & + \end{bmatrix} \begin{bmatrix} + & + \\ + & - \end{bmatrix} \begin{bmatrix} + & + \\ + & + \end{bmatrix} \quad (2.9)$$

- Block configurations belonging to class  $C_-$

$$\begin{bmatrix} - & - \\ - & - \end{bmatrix} \begin{bmatrix} - & - \\ - & + \end{bmatrix} \begin{bmatrix} - & - \\ + & - \end{bmatrix} \begin{bmatrix} - & - \\ + & + \end{bmatrix} \begin{bmatrix} - & + \\ - & - \end{bmatrix} \begin{bmatrix} - & + \\ - & + \end{bmatrix} \begin{bmatrix} - & + \\ + & - \end{bmatrix} \begin{bmatrix} + & - \\ - & - \end{bmatrix} \quad (2.10)$$

For any constrained model  $\mathcal{F}_{\beta, \sigma'}^\tau$  we allow, in the block  $B_{(x, y)}$ , only the configurations in the class  $C_{\text{sign } \sigma'_{(x, y)}}$ ; in order to classify these block configurations we introduce the block variable  $S_{(x, y)} \in \{1, 2, \dots, 8\}$ : to the values  $S_{(x, y)} = 1, \dots, 8$  there 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 (nonconventional) expression *block variable* referring to the variable  $S_{(x, y)}$  taking values in the set  $\{1, 2, \dots, 8\}$ ; the spin variables  $\sigma'_{(x, y)}$ , defined on the renormalized lattice  $A'$  and taking values in  $\{-1, +1\}$ , will be sometimes called *renormalized variables*.

Obviously, given any constrained model  $\mathcal{F}_{\beta, \sigma'}^\tau$ , one and only one configuration  $S \in \tilde{\mathcal{Q}}_{A'} := \{1, 2, \dots, 8\}^{A'}$  can be associated to any  $\sigma \in \Omega_{A, \sigma'}$ , and vice versa. Hence, each state of the model  $\mathcal{F}_{\beta, \sigma'}^\tau$  can be represented by a collection  $S \in \tilde{\mathcal{Q}}_{A'}$  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  $\Omega_{A, \sigma'}$ , and  $\tilde{\Omega}_{A'}$  the Hamiltonian  $H_{A'}^{\tau'}(\sigma)$  of the model  $\mathcal{F}_{\beta, \sigma'}^{\tau}$  can be thought of, for any  $\sigma \in \Omega_{A, \sigma'}$ , as a function  $H_{A', \sigma', \tau'}^{\tau}(S)$  of the block-variables configuration  $S \in \tilde{\Omega}_{A'}$ ; here by  $\tau'$  we mean a configuration of the renormalized variables in  $\partial A'^+$ , that is,  $\tau' \in \Omega'_{\partial A'^+} := \{-1, +1\}^{\partial A'^+}$ , where

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

By  $\mathcal{F} \in \tilde{\Omega}_{\partial A'^+} := \{1, \dots, 8\}^{\partial A'^+}$  we mean the boundary condition expressed in terms of the block variables in the set  $\partial A'^+$ . Notice that given the original  $\tau$  and  $\tau'$ , in general  $\mathcal{F}$  is not uniquely determined.

We remark that a block variable in  $B_{(x, y)}$ , for  $(x, y) \in A' \cup \partial A'^+$ , is completely “meaningless” if the corresponding 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  $A'$  with configuration space  $\tilde{\Omega}_{A'}$  and equilibrium measure given by

$$\mu_{\beta, A', \sigma', \tau'}^{\tau}(S) := \frac{\exp[-\beta H_{A', \sigma', \tau'}^{\tau}(S)]}{\sum_{Y \in \tilde{\Omega}_{A'}} \exp[-\beta H_{A', \sigma', \tau'}^{\tau}(Y)]} \quad \forall S \in \tilde{\Omega}_{A'} \tag{2.12}$$

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

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

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

We set

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

and, given a metric  $\rho$  on  $Y$ ,

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

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

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

For any finite set  $V \subset \mathbb{Z}^d$  we denote by  $\partial V^+$  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  $\xi \in \mathcal{S}^{\partial V^+}$ , we denote by  $\mu_V^\xi$  the Gibbs measure in  $V$  with boundary conditions  $\xi$  outside  $V$ . Given a metric  $\rho$  on  $\mathcal{S}$ , we associate to it a metric  $\rho_V$  on  $\mathcal{S}^V$  defined as follows:

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

We say that condition  $DSU_\rho(V, \delta)$  (the Dobrushin–Shlosman uniqueness condition in  $V$  with respect to the metric  $\rho$  and uniqueness parameter  $\delta$ ) 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  $\xi, \xi' \in \mathcal{S}^{\partial V^+}$  with  $\xi_i = \xi'_i, \forall i \neq j$ , one has

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

and

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

Let us consider the metric on the single site variable given by

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

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

We observe that in this case

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

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

In order to describe Dobrushin–Shlosman’s results based on the  $DSU_\rho(V, \delta)$  condition we need some more definitions. We introduce two kinds of mixing conditions, of *a priori* different strength, for Gibbs measures in a finite volume  $A$ . The first 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  $\partial A$ ; the second kind, strong mixing (SM) conditions, correspond 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 refs. 26 and 27 for a critical discussion of these different notions. It has been shown with some examples<sup>(36)</sup> 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  $A$  with uniform constants. We refer again to refs. 26 and 27 for a discussion of these points. 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<sup>(7, 8)</sup> arbitrary shapes were considered, whereas in the approach developed in refs. 33, 34, and 27 only sufficiently regular domains were involved.

We say that a Gibbs measure  $\mu_{A, \tau}^r$  on  $\Omega_A$  satisfies a *strong mixing* condition with constants  $C, \gamma$  if for every subset  $A \subset A$

$$\sup_{\tau, \tau^{(1)} \in \Omega_{A^c}} \text{Var}(\mu_{A, A}^{\tau}, \mu_{A, A}^{\tau^{(1)}}) \leq C e^{-\gamma \text{dist}(A, \tau)} \tag{2.17}$$

where  $\tau_x^{(1)} = \tau_x$  for  $x \neq y$  and  $\mu_{A, A}^{\tau}$  is the  $\mu_{A, \tau}^r$ -probability distribution of the spins in  $A$ . We denote this condition by  $SM(A, C, \gamma)$ .

We say that a Gibbs measure  $\mu_{A, \tau}^r$  satisfies a *weak mixing* condition with constants  $C, \gamma$  if for every subset  $A \subset A$

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

We denote this condition by  $WM(A, C, \gamma)$ .

**Theorem DS.**<sup>(6)</sup> Let  $DSU(V, \delta)$  be satisfied for some  $V$  and  $\delta < 1$ ; then  $\exists C > 0, \gamma > 0$  such that condition  $WM(A, C, \gamma)$  holds for every  $A$ .

**Theorem MOS.**<sup>(31)</sup> Let the dimension of the lattice be  $d = 2$ . If there exist positive constants  $C$  and  $\gamma$  such that the Gibbs measure  $\mu_{A, \tau}^r$  satisfies the weak mixing condition  $WM(A, C, \gamma)$  for any finite  $A \subset \mathbb{Z}$ , then there exist positive constants  $C'$  and  $\gamma'$  such that the Gibbs measure  $\mu_{A, \tau}^r$  satisfies the strong mixing condition  $SM(A, C', \gamma')$  for any sufficiently regular domain  $A$  and in particular for any square  $A_L$  with arbitrary side  $L$ .

Here “sufficiently regular” means “multiple of a sufficiently large square.”<sup>(26)</sup>

*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  $A_{L_0}$ , provided that  $L_0$  is large enough (depending of course on the constants  $C$  and  $\gamma$  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 all constrained models. Then if we could apply Theorem DS, we would get  $WM(A, C, \gamma)$ ,  $\forall A$ , with the same constants  $C, \gamma$  for all  $A$  and for all constrained models. Subsequently, if we could apply Theorem MOS (by exploiting the two-dimensionality), we would get  $SM(A, C', \gamma')$  for all sufficiently regular domains  $A$  with the same constants  $C', \gamma'$  for all these  $A$  and for all constrained models. This would directly imply the validity of the conclusions of Theorem 1.1 in ref. 15; indeed it immediately follows from the proof of Theorem 1.1 in ref. 15 that the authors could have obtained exactly the same result by only assuming their strong mixing hypothesis (which they express in an equivalent form, valid for Ising-like systems, as exponential decay of two-point 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  $\sigma' \in \Omega_{1,\dots}$ ) this implies, at the same time (using extended versions of Theorems DS and MOS) the validity of SM (for arbitrary sufficiently regular volumes with uniform constants) for all constrained models and then, via Theorem 1.1 in ref. 15, Gibbsianness of the renormalized measure.

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

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

and the metric on  $\tilde{\Omega}_{V'}$  given by

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

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  $\mathcal{T}_1, \mathcal{T}_2 \in \tilde{\Omega}_{\partial V'+}$  such that

$$\mathcal{T}_{1(x', y')} = \mathcal{T}_{2(x', y')} \quad \forall (x', y') \in \partial V'+ \setminus \{(x, y)\}$$

and we define

$$\begin{aligned} \mathcal{E}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{T}}_1, \bar{\mathcal{T}}_2]_{(x, y)}} &:= \mathcal{D}_{\rho_{V'}}(\mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_1}, \mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_2}) \frac{|\partial V'+|}{|V'|} \\ &= \mathcal{D}_{\rho_{V'}}(\mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_1}, \mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_2}) \frac{4}{l} \end{aligned} \quad (2.21)$$

where

$$\mathcal{D}_{\rho_{V'}}(\mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_1}, \mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{T}}_2})$$

is the Wasserstein distance between two equilibrium measures for the constrained model corresponding to  $\sigma', \tau'$  which have been obtained by modifying the boundary conditions just in one site in  $\partial V'+$ . We set

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

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

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  $\sigma', \tau'$ . 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

$$\mathcal{E}_{\beta, V'} := \sup_{\sigma' \in \Omega_{V'}} \mathcal{E}_{\beta, V', \sigma'} < 1 \quad (2.23)$$

### 3. ROUGH ESTIMATE OF CRITICAL TEMPERATURES

In the following sections we will see that two constrained models (the *chessboard* and the *striped* model, see definitions below) are particularly “dangerous,” that is, they satisfy the 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:

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

These two configurations are respectively depicted in Figs. 1b and 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  $\langle \cdot \rangle$ .

This “conventional Monte Carlo” analysis is preliminary 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 strong evidence of the fact that the critical inverse temperature of these two dangerous models is, in both cases, much greater than  $\beta_c$ .

By making use of the notation introduced in Section 2 (relative to the constrained models  $\mathcal{S}_{\beta, \sigma'}$ ), 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  $\sigma' \in \Omega'_{A'}$  and we assume periodic boundary conditions; we denote it by  $\mathcal{S}_{\beta, \sigma'}$  and its Hamiltonian by  $H_{A', \sigma'}(S)$  with  $S \in \tilde{\Omega}_{A'}$ .

2. At each step we perform a complete updating of all  $S_{(x,y)}$  block variables following the lexicographic order; in the remainder of this section this will be called a Monte Carlo *sweep*.

3. For any  $(x, y) \in A'$  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

$$S^c_{(x,y)} := S|_{(A' \cup \partial A'_+ ) \setminus B_{(x,y)}}$$

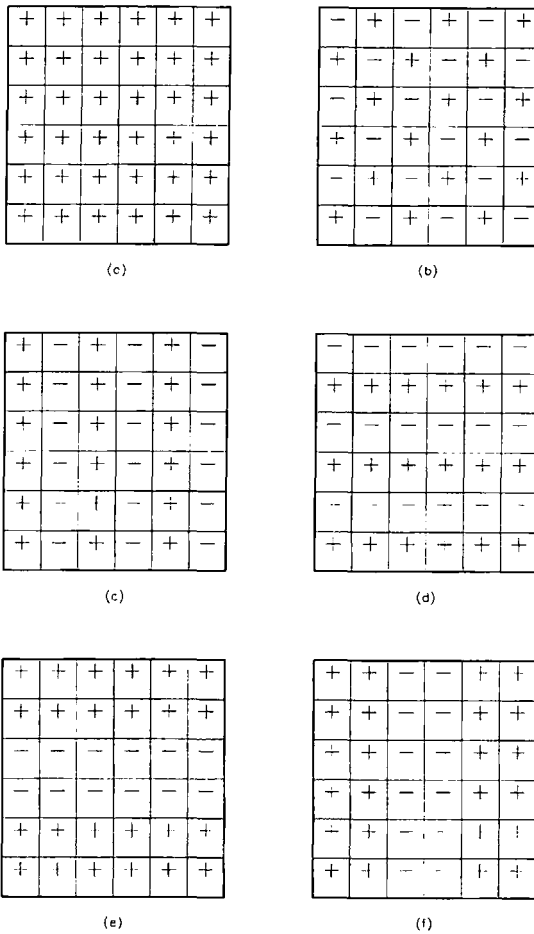


Fig. 1. Examples of configurations of renormalized variables corresponding to constrained models which are particularly important in our calculations.

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

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

We remark that in our notation there is no explicit dependence of the boundary conditions ( $\mathcal{T} - \tau'$ ), because they are supposed to be periodic.



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

$$C_{A, \sigma'} := \frac{\beta^2}{4L^2} (\langle H_{A, \sigma'}^2 \rangle - \langle H_{A, \sigma'} \rangle^2) \quad \forall \sigma' = \mathcal{C}, \mathcal{S} \quad (3.3)$$

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

Figures 2 and 3 plot the specific heat as a function of the inverse temperature  $\beta$  in the case of models  $\mathcal{J}_{\beta, \mathcal{C}}$  and  $\mathcal{J}_{\beta, \mathcal{S}}$ , 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  $\beta_c$ . Our rough estimates are

$$\beta_c^{\mathcal{C}} = 1.60 \pm 0.05 \quad \text{and} \quad \beta_c^{\mathcal{S}} \geq 2.2 \quad (3.4)$$

Notice that from the results depicted in Fig. 3 we cannot even exclude that  $\beta_c^{\mathcal{S}} = \infty$ .

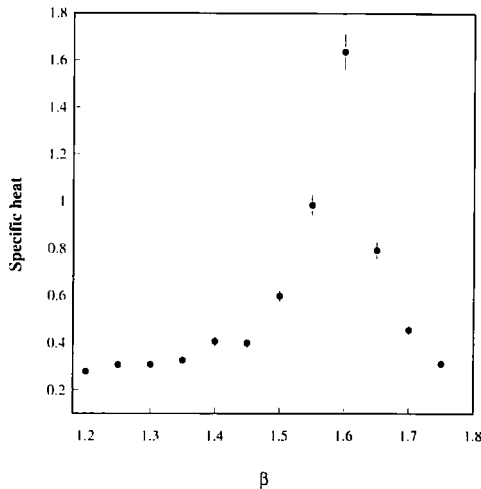


Fig. 2. Specific heat for the chessboard model defined in (3.1) as a function of the inverse temperature  $\beta$ .

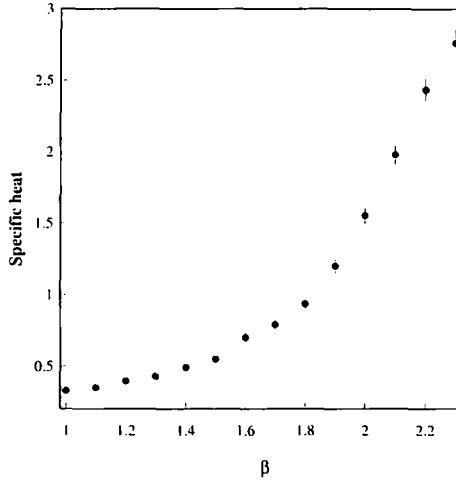


Fig. 3. Specific heat for the striped model defined in (3.1) as a function of the inverse temperature  $\beta$ .

#### 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  $[\mathcal{F}_1, \mathcal{F}_2]_{(x, \bar{y})}$ , and the two equilibrium measures  $\mu_{\beta, A', \sigma', \tau'}^{\mathcal{F}_1}$  and  $\mu_{\beta, A', \sigma', \tau'}^{\mathcal{F}_2}$ . Let us denote by

$$\mathcal{X}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, \bar{y})}}$$

the set of joint representations of  $\mu_{\beta, A', \sigma', \tau'}^{\mathcal{F}_1}$  and  $\mu_{\beta, A', \sigma', \tau'}^{\mathcal{F}_2}$ ; we want to give a numerical estimate of the quantity

$$\mathcal{E}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, \bar{y})}}$$

defined in (2.21).

A similar problem has been studied in ref. 1, where by means of a standard heat bath dynamics, a lower bound to

$$\mathcal{E}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, \bar{y})}}$$

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 we heuristically describe the idea on which the algorithm is based. In order to calculate exactly the Vasserstein distance, one should know a joint probability measure

$$Q^*(\cdot, \cdot) \in \mathcal{K}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, y)}}$$

on the space  $\tilde{\Omega}_{V'} \times \tilde{\Omega}_{V'}$  such that

$$\mathcal{D}_{V'}(\mu_{\beta, V', \sigma', \tau'}^{\mathcal{F}_1}, \mu_{\beta, V', \sigma', \tau'}^{\mathcal{F}_2}) = \sum_{S^{(1)}, S^{(2)} \in \tilde{\Omega}_{V'}} Q^*(S^{(1)}, S^{(2)}) \rho_{V'}(S^{(1)}, S^{(2)}) \quad (4.1)$$

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  $\tilde{\rho}(\alpha, \alpha') = 1 - \delta_{\alpha, \alpha'}$ ,  $\forall \alpha, \alpha' \in \{1, \dots, 8\}$  [see (2.19)] and so the Vasserstein distance coincides with the total variation distance (see ref. 4, p. 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 the two copies are updated in a single block according to the “local optimizing” joint distribution law.

The idea of a coupling of two stochastic dynamics turned out to be very useful in the theory of interacting particle systems (see ref. 22, p. 64) and also for the study of probabilistic cellular automata.<sup>(17, 25)</sup>

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  $[\mathcal{F}_1, \mathcal{F}_2]_{(x, \bar{y})}$ , 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  $\mathcal{F}_1$  and  $\mathcal{F}_2$ .

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 the *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  $\Delta t = |V'|$  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:

$$q^{\mathcal{F}_i} [S_{(x,y)}^{(i)} | S_{V' \setminus \{(x,y)\}}^{(i)}(t-1)], \quad i = 1, 2$$

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  $\mathcal{H}_{(x,y)}(t)$  the set of joint representations of

$$q^{\mathcal{F}_1} [S_{V' \setminus \{(x,y)\}}^{(1)}(t-1)] \quad \text{and} \quad q^{\mathcal{F}_2} [S_{(x,y)}^{(2)} | S_{V' \setminus \{(x,y)\}}^{(2)}(t-1)] \quad (4.2)$$

and, finally, by

$$q^{*\mathcal{F}_1, \mathcal{F}_2} [S_{(x,y)}^{(1)}, S_{(x,y)}^{(2)} | S_{V' \setminus \{(x,y)\}}^{(1)}(t-1), S_{V' \setminus \{(x,y)\}}^{(2)}(t-1)] \quad (4.3)$$

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

$$\begin{aligned} & \mathcal{D}_\beta(q^{\mathcal{F}_1} [S_{(x,y)}^{(1)} | S_{V' \setminus \{(x,y)\}}^{(1)}(t-1)], q^{\mathcal{F}_2} [S_{(x,y)}^{(2)} | S_{V' \setminus \{(x,y)\}}^{(2)}(t-1)]) \\ &= \sum_{S_{(x,y)}^{(1)}, S_{(x,y)}^{(2)} = 1}^8 \tilde{\rho}(S_{(x,y)}^{(1)}, S_{(x,y)}^{(2)}) \\ & \quad \times q^{*\mathcal{F}_1, \mathcal{F}_2} [S_{(x,y)}^{(1)}, S_{(x,y)}^{(2)} | S_{V' \setminus \{(x,y)\}}^{(1)}(t-1), S_{V' \setminus \{(x,y)\}}^{(2)}(t-1)] \end{aligned} \quad (4.4)$$

The joint representation (4.3) can be exactly calculated as shown in the Appendix. All probability measures introduced above depend on  $\beta, V', \sigma',$  and  $\tau'$ ; we drop explicit dependence to simplify the notation. Notice that, of course, the  $q^{\mathcal{F}_i}[\cdot | \cdot]$  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  $(S_{(x,y)}^{(1)}(t), S_{(x,y)}^{(2)}(t))$  at random according to the joint probability measure (4.3) and  $S_{(x',y')}^{(i)}(t) = S_{(x',y')}^{(i)}(t-1), \forall i = 1, 2$  and  $\forall (x', y') \in V' \setminus \{(x, y)\}$ .

In analogy with the terminology used in ref. 6, we call this dynamics *dynamical surgery*; our dynamics is strictly related to the *basic* (or *Vasserstein*) *coupling* used in the theory of stochastic systems of interacting particles (see ref. 22, p. 124). Now we discuss some easy properties of this dynamics.

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

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

then

$$S_{(x, y)}^{(1)}(t) = S_{(x, y)}^{(2)}(t) \tag{4.5}$$

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

$$(\mathcal{T}_1, S_{V' \setminus \{(x, y)\}}^{(1)}(t-1)) \quad \text{and} \quad (\mathcal{T}_2, S_{V' \setminus \{(x, y)\}}^{(2)}(t-1))$$

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

$$Q(\cdot, \cdot) \in \mathcal{K}_{\beta, A', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2](x, y)}$$

if the stochastic variable  $X_t = (S^{(1)}(t), S^{(2)}(t))$  is such that

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

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 also distributed according to an element of

$$\mathcal{K}_{\beta, A', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2](x, y)}$$

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

$$\bar{Q}(\cdot, \cdot) \in \mathcal{K}_{\beta, A', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2](x, y)}$$

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  $\mu_{\beta, V', \sigma', \tau'}^{\bar{\mathcal{F}}_1}(S)$  and  $\mu_{\beta, V'', \sigma', \tau'}^{\bar{\mathcal{F}}_2}(S)$ . 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 true that  $\bar{Q} = Q^*$ , then we could perform a Monte Carlo calculation of the uniqueness parameter

$$\mathcal{G}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2](x, y)}$$

but in general  $\bar{Q} \neq Q^*$  and moreover we cannot say anything on how close  $\bar{Q}$  is to  $Q^*$ . Anyway, we can use the joint representation  $\bar{Q}$  to calculate an “upper” estimator of the uniqueness parameter; we set

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2](x, y)} := \frac{4}{I} \frac{1}{I} \sum_{s=1}^I \rho_{V'}(S^{(1)}(s \cdot | V'|), S^{(2)}(s \cdot | V'')) \tag{4.6}$$

where  $I$  is the number of sweeps performed during the Monte Carlo run. It is clear that

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2](x, y)}$$

is a numerical upper bound to

$$\mathcal{G}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2](x, y)}$$

The same Monte Carlo run can be used to estimate a “lower” bound to the uniqueness parameter as in ref. 1. Indeed, we define the quantities

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

and we set

$$\mathcal{L}_{\beta, V', \sigma', \tau'}^{[\bar{\mathcal{F}}_1, \bar{\mathcal{F}}_2](x, y)} := \frac{4}{I} \sum_{(x, y) \in V'} \frac{1}{2} \sum_{\alpha \in \{1, \dots, 8\}} |N_{(x, y)}^{(1)}(\alpha) - N_{(x, y)}^{(2)}(\alpha)|_2 \tag{4.8}$$

See ref. 1 for more details.

### 5. UPPER AND LOWER BOUNDS: NUMERICAL RESULTS

In Section 4 we developed a Monte Carlo algorithm in order to evaluate an upper and a lower bound on

$$\mathcal{E}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}}$$

and we denoted these two quantities respectively by

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}} \quad \text{and} \quad \mathcal{L}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}}$$

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  $S_{(x, y)}$ , then only two of the original spins  $\sigma_{(x, y)}^i$ , 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

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

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 oneself 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, notice that given  $l$ , there exist  $2^{l^2}$  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 examining  $3 \cdot l \cdot 2^{l^2 + 8l + 1}$  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 large computation to perform.

**Table I.** Values of  $\mathcal{U}_{\beta, V'}$ ,  $\Delta\mathcal{U}_{\beta, V'}$ ,  $\mathcal{L}_{\beta, V'}$ , and  $\bar{\Delta}\mathcal{L}_{\beta, V'}$  Obtained at  $l=2, 3, 4, 8, 16^a$

$l$	$\mathcal{U}_{\beta, V'}$	$\Delta\mathcal{U}_{\beta, V'}$	$\mathcal{L}_{\beta, V'}$	$\bar{\Delta}\mathcal{L}_{\beta, V'}$
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

<sup>a</sup>The meaning of  $\Delta\mathcal{U}_{\beta, V'}$  and  $\bar{\Delta}\mathcal{L}_{\beta, V'}$  is explained in the Remark in Section 5.

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” aimed at singling out the worst possible case.

Let us denote by  $\mathcal{U}_{\beta, V'}$  the highest value obtained for

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, y)}}$$

and by  $\mathcal{L}_{\beta, V'}$  the corresponding estimate of

$$\mathcal{L}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2]_{(x, y)}}$$

First 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 was performed in all cases; our numerical results are summarized in Table I.

- $l=1$ : 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) is exactly calculated as follows:

$$\begin{aligned} \mathcal{E}_{\beta, V'} &= 4 \left( \sup_{\sigma' \in \Omega_{j'}^{(x, y)}} \sup_{(x, y) \in \partial V'^+} \sup_{[\mathcal{F}_1, \mathcal{F}_2]_{(x, y)}} \right. \\ &\quad \left. \times \sum_{\substack{S_{(1,1)}^{(1)}, S_{(1,1)}^{(2)} \in \{1, \dots, 8\} \\ S_{(1,1)}^{(1)} \neq S_{(1,1)}^{(2)}}} q^{*\mathcal{F}_1, \mathcal{F}_2} [S_{(1,1)}^{(1)}, S_{(1,1)}^{(2)}] \right) \end{aligned}$$



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

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

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 considered all possible constrained models and for each model considered 200 different pairs of boundary conditions. By performing  $1.3 \cdot 10^6$  full sweeps of our Monte Carlo, we obtained the results in Table I, these results show that there exist at least one constrained model  $\sigma', \tau'$  and one pair of boundary conditions  $[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}$  such that

$$\mathcal{L}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}} > 1$$

This means that there exists a constrained model, the one corresponding to  $\sigma', \tau'$ , which does not fulfill the Dobrushin–Shlosman uniqueness condition  $DSU(V', \delta)$  with  $\delta < 1$ .

- $l=3$ : We considered all possible constrained models and for each model we considered 100 different pairs of boundary conditions. The results in Table I refer to a run of  $1.3 \cdot 10^6$  sweeps. In this case there exists a particular constrained model  $\sigma', \tau'$  and a pair of boundary conditions  $[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}$  such that

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}} > 1 \quad \text{and} \quad \mathcal{L}_{\beta, V', \sigma', \tau'}^{[\mathcal{T}_1, \mathcal{T}_2]_{(x, y)}} < 1$$

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 consider larger volumes.

- $l=4$ : We have considered 50 constrained models and 60 pairs of boundary conditions; the results in Table I were obtained by performing  $1.3 \cdot 10^6$  full sweeps of the algorithm described in Section 4.

- $l=8$ : We 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 performed  $1.3 \cdot 10^6$  full sweeps of our Monte Carlo.

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

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

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

where  $I$  is the number of full sweeps of the run<sup>(11)</sup> and  $\Delta \mathcal{L}_{\beta, l'} = \bar{\Delta} \mathcal{L}_{\beta, l'} / \sqrt{I}$ .

The results in Table I 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 considered values of  $l$  larger than 4 and showed (see Table I) that for  $l=8, 16$  the value of  $\mathcal{U}_{\beta, l'}$  is so small and the effect of the change of conditioning spin is so localized (as we will explain) as 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  $l/4 \mathcal{U}_{\beta, l'}$ , 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 chose  $l=6$  for our final calculation, because the results listed in Table I 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

$$\rho_{1^{\cdot\cdot}}(t) := \sum_{(x, y) \in V'} (1 - \delta_{S_{(x, y)}^{(1)}(t), S_{(x, y)}^{(2)}(t)})$$

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 plot 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 considered, we 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  $3 \times 2$  rectangular block  $R_{(x, y)} \subset V'$ .

Now, given the constrained model corresponding to  $\sigma' \in \Omega'_{1^{\cdot\cdot}}$  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  $(x, y) \in R_{(x, y)}$  and weakly on the values of  $\sigma'_{(x, y)}$  outside  $R_{(x, y)}$ . Hence, we performed the statistics on the constrained model in the

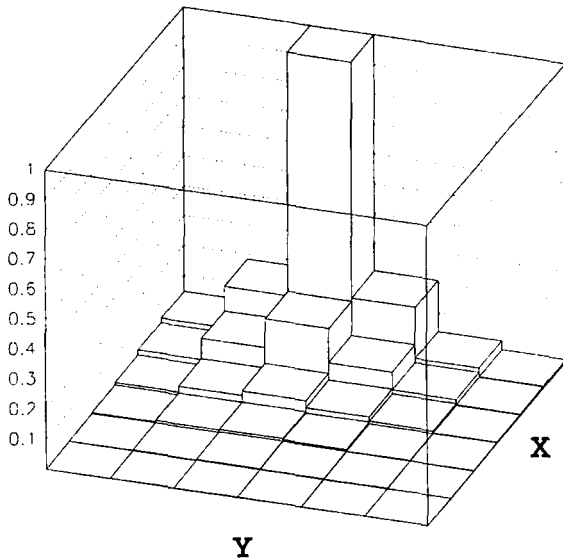


Fig. 4. Each square of the plane X-Y represents a site  $(x, y)$  of a lattice  $V'$  with  $l=6$ ; the X axis is oriented from the left to the right, while the Y axis is oriented from the top of the figure to the bottom. The results contained in the histogram refer to the chessboard model: the height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

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

where  $l=1 \cdot 10^5$  is the number of full sweeps of the run, and  $S_{(x,y)}^{(1),s}$  and  $S_{(x,y)}^{(2),s}$  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 were obtained by considering a pair of boundary conditions  $[\mathcal{F}_1, \mathcal{F}_2]_{(0,3)}$  such that the two pairs of original spins in the block  $B_{(0,3)}$  are  $+ -$  and  $- +$ .

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 was performed.

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

- All possible constrained models were considered in  $R_{(\bar{x}, \bar{y})}$ , while in  $V' \setminus R_{(\bar{x}, \bar{y})}$  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 least “dangerous” ones, as the results of the previous statistics suggest.

• In each run of the joint Monte Carlo algorithm we performed  $10^5$  full sweeps, that is, we 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

$$\begin{array}{cccc} + & - & + & - & + & - \\ + & - & + & - & - & + & - \\ + & - & + & - & - & + & - \\ + & - & + & - & + & - & + \end{array} \quad (5.2)$$

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

$$\mathcal{U}_{\beta, V', \sigma', \tau'}^{[\mathcal{F}_1, \mathcal{F}_2](\bar{x}, \bar{y})} = 0.610$$

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

$$+ + \quad - - \quad \text{and} \quad + - \quad - + \quad (5.3)$$

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

- We considered the most dangerous constrained model inside  $R_{(\bar{x}, \bar{y})}$ .
- We considered ten possible constrained models outside  $R_{(\bar{x}, \bar{y})}$ ; six of them are those depicted in Fig. 1, the remaining four were chosen at random.
- In each case we considered 20 possible pairs of boundary conditions with the original spins in  $B_{(\bar{x}, \bar{y})}$  and adjacent to  $V'$  chosen as in (5.3).

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

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

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 the  $DSU(V, \delta)$  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 the 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 the 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 the 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 behavior 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 much smaller than one (including the error) that we can be confident in the validity of the 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 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 of the uniform validity of the 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 small enough to avoid the consideration of sides  $l$  at least greater than 4.

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

As emphasized in ref. 6, the nice feature of finite-size conditions like the 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  $\beta$ ) whose smallness implies weak coupling.

The “uniqueness test” based on the verification of the DSU has the advantage, with respect to 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.

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 perform quite well 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 than the corresponding one on  $\mathcal{L}$ ; indeed, in this last case *all* sites of our volume and not only the disagreements, as in the computation of  $\mathcal{U}$ , play a role as a source of statistical errors.

## APPENDIX

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

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

We recall, now, that the *total variation distance* and the *Vasserstein distance* between  $\lambda$  and  $\mu$  are respectively given by

$$\text{Var}(\lambda, \mu) := \frac{1}{2} \sum_{s \in S} |\lambda(s) - \mu(s)| \tag{A.2}$$

$$\mathcal{D}_\rho(\lambda, \mu) := \inf_{q \in \mathcal{K}} \sum_{s, s' \in S} \rho(s, s') \cdot q(s, s')$$

**Proposition A1.**

1. With the notation introduced before

$$\mathcal{D}_\rho(\lambda, \mu) = \text{Var}(\lambda, \mu) \tag{A.3}$$

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

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

*Proof.* 1. See ref. 4, p. 472.

2. It is an immediate consequence of the normalization of  $\mu$  and  $\lambda$ . ■

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

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

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



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

such that

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

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

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

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

It is easy to see that the matrix

$$q_{s,s}^* = \min(\lambda_s, \mu_s) \tag{A.11}$$

$$q_{s,s'}^* = \frac{1}{\text{Var}(\lambda, \mu)} (\lambda_s - q_{s,s}^*)(\mu_{s'} - q_{s',s'}^*) \quad \forall s \neq s'$$

satisfies both (A.9) and (A.10).<sup>(17, 25)</sup>

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