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Probabilistic Cellular Automata for Low-Temperature 2-d Ising Model

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Abstract We construct a parallel stochastic dynamics with invariant measure converging to the Gibbs measure of the 2-d low-temperature Ising model. The proof of such convergence requires a polymer expansion based on suitably defined Peierls-type contours.

Keywords Ising model · Probabilistic celluar automata · MCMC

1 Introduction

The goal of this paper is to construct parallel stochastic dynamics to sample the Gibbs measure of the nearest neighbors Ising model at low-temperature on a finite volume. More precisely we explicitly control the total variation distance between the Gibbs measure of the low-temperature Ising model and the invariant measure of suitable parallel stochastic dynamics defined on the same finite volume. In particular we show that such total variation distance tends to zero when the size of the volume tends to infinity.

The parallel dynamics described in this paper are homogeneous discrete time Markov chains on a product space $S^\Lambda =: \mathcal{X}$, where $S = \{-1, 1\}$ and Λ is a finite square of $\mathbb{Z}^2$, with transition probabilities:

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$$P(\sigma, \tau) = \prod_{i\in\Lambda} p_i(\tau_i|\sigma). \tag{1}$$

This kind of dynamics are known in the literature as Probabilistic Cellular Automata (PCA).

Parallel dynamics on finite volume is a challenging topic in Markov Chain Monte Carlo (MCMC) methods and statistical mechanics because they are very promising algorithms and the efficiency of parallel computing can be exploited in their simulation. From a theoretical point of view there are few results in the literature on the convergence to equilibrium of parallel dynamics. This is in general a difficult task, since the high mobility related to parallelization, implies that it is much more complicated to identify possible bottlenecks or saddle configurations in the tunneling between different configurations on which the invariant measure can be concentrated than in the single-spin-flip dynamics. We mention here two examples where the efficiency of parallel dynamics has been proved to be clearly higher than the efficiency of single-spin-flip dynamics. The first example is given in [5] where a control of the mixing time of an irreversible PCA related to the 2d Ising model is given in a particular regime of low-temperature in a finite box of side L with periodic boundary conditions. In this case the mixing time turns out to be polynomial in L. A second example is the Swendsen–Wang dynamics on the Ising model [21] (see also the review [17]). In this case the updating rule is not given in the form (1) of a PCA, but there is fast mixing because it is possible to update in a single step of the Markov chain a large amount of spins.

However there is a preliminary more difficult problem in the use of parallel dynamics in MCMC or in statistical mechanics: the control of their invariant measures. This is the reason why their use is not widespread, even if PCA have been introduced in Equilibrium Statistical Mechanics a long time ago, see for instance [2,3,11,12,16]. Invariant measures for infinite-volume PCA's may be non-Gibbsian [8] and even in the finite-volume case they are usually completely different compared to the invariant measures of Markov chains obtained by the random updating of a single site i, with the same probability $p_i(\tau_i|\sigma)$ used in (1).

In a previous paper [4], given a quite general spin system, a PCA was introduced with an invariant measure converging, in the thermodynamic limit, to the Gibbs measure of the Ising model at high temperature. The main tool used in the proof was the Dobrushin uniqueness Theorem.

In the present paper we use completely different tools to prove a similar result in the low-temperature regime. Indeed we will use a polymer expansion based on suitably defined Peierls-type contours. We present the results in the simple case of two dimensions:

- with plus boundary conditions in the reversible case;
- with periodic boundary conditions in the reversible case;
- with periodic boundary conditions in the irreversible case.

In the irreversible case a similar result was obtained in [5] in a very particular regime of low-temperature, where the inverse temperature suitably increases with the volume. In this paper we are in a standard low-temperature regime, with a temperature small enough, independently of the volume.

In our discussion the temperature will be associated to the interaction parameter J, and therefore obviously the low-temperature regime will correspond to large J.

We finally remark that in this paper estimates are not optimized and that a generalization to higher dimensions using the same technics should be possible. The study of interactions beyond the nearest neighbor could be also possible but it would imply a generalization of the concept of contours much more involved.

1.1 Definitions

1.1.1 Ising Model and Gibbs Measure

Henceforth Λ denotes a two-dimensional $L \times L$ square lattice in $\mathbb{Z}^2$ and B_Λ denotes the set of all nearest neighbor pairs in Λ, i.e., $B_\Lambda = \{\langle i, j\rangle : \ i, j \in \Lambda, \ |i - j| = 1\}$ with $|i - j|$ being the usual lattice distance in $\mathbb{Z}^2$. We denote by $\partial^{ext}\Lambda$ ($\partial^{int}\Lambda$) the external (internal) boundary of Λ, i.e., $\partial^{ext}\Lambda = \{i \in \mathbb{Z}^2 \setminus \Lambda : \ \exists j \in \Lambda \text{ s.t. } |i - j| = 1\}$ ($\partial^{int}\Lambda = \{i \in \Lambda : \exists j \in \mathbb{Z}^2 \setminus \Lambda \text{ s.t. } |i - j| = 1\}$) and we set $\bar{\Lambda} = \Lambda \cup \partial^{ext}\Lambda$.

Let B_Λ^{per} be the set of all nearest neighbors in Λ plus the pairs of sites at opposite faces of the square Λ, so that the pair $(\Lambda, B_\Lambda^{per})$ is homeomorphic to the two-dimensional discrete torus $(\mathbb{Z}/(L\mathbb{Z}))^2$.

We set $B_{\bar{\Lambda}}^{+} = \{ < i, j\rangle : \ i, j \in \bar{\Lambda} : \ |i - j| = 1\}$, i.e., $B_{\bar{\Lambda}}^{+}$ is the set of all nearest neighbors in $\bar{\Lambda}$. We finally recall that $\mathcal{X}$ denotes the set of spin configurations in Λ., i.e., $\mathcal{X}$ is the set of all functions $\sigma : \Lambda \to \{-1, 1\}$.

In the two cases of periodic and $+$ boundary conditions (b.c.) define the Ising Hamiltonian with interaction $J > 0$ as follows. Given $\sigma \in \mathcal{X}$,

$$H^{per}(\sigma) = -J \sum_{\langle i,j\rangle \in B_\Lambda^{per}} \sigma_i \sigma_j, \qquad H^{+}(\sigma) = -J \sum_{\langle i,j\rangle \in B_{\bar{\Lambda}}^{+}} \sigma_i \sigma_j \tag{2}$$

where in $H^+(\sigma)$ we fix $\sigma_i = +1$ when $i \in \partial^{ext}\Lambda$.
Using the notation $H^*(\sigma)$ with either $* = per$ or $* = +$, we denote

$$w_G^*(\sigma) = e^{-H^*(\sigma)}, \quad Z_G^* = \sum_{\sigma \in \mathcal{X}} e^{-H^*(\sigma)} \tag{3}$$

so that the standard Gibbs measure with $* = per, +$ is

$$\pi_G^*(\sigma) = \frac{w_G^*(\sigma)}{Z_G^*} \tag{4}$$

Note that since Λ is a finite volume the Gibbs measure is uniquely defined.

The case of minus boundary conditions could be treated in the same way.

1.1.2 Pair Hamiltonian

We use here the same construction of the parallel dynamics introduced in [4] (see also [9,13,15]).

The previous Hamiltonians can be *lifted* to Hamiltonians on $\mathcal{X} \times \mathcal{X}$ as follows:

$$H^{per}(\sigma, \tau) = -\frac{J}{2} \sum_{i \in \Lambda} \sum_{\substack{j \in \Lambda \\ \langle i,j\rangle \in B_\Lambda^{per}}} \sigma_i \tau_j + q \sum_{i \in \Lambda} (1 - \sigma_i \tau_i) \tag{5}$$

$$H^{+}(\sigma, \tau) = -\frac{J}{2} \sum_{i \in \Lambda} \sum_{\substack{j \in \Lambda: \\ \langle i,j\rangle \in B_\Lambda}} \sigma_i \tau_j - \frac{J}{2} \sum_{i \in \partial^{int}\Lambda} \sum_{\substack{j \in \partial^{ext}\Lambda: \\ |i-j|=1}} (\sigma_i + \tau_i) + q \sum_{i \in \Lambda} (1 - \sigma_i \tau_i) \tag{6}$$

where $q > 0$ is a volume-dependent parameter controlling the average number of spin-flips in a single step of the dynamics that we will choose later (see Theorem 1.1 ahead). Note that

$\sum_{\substack{j\in\partial^{ext}\Lambda:\\|i-j|=1}}$ has a single term in each site $i \in \partial^{int}\Lambda$ which is not a corner and has two terms in the four corners of $\partial^{int}\Lambda$.

Clearly, for $* = +, per$, $H^*(\sigma,\tau)$ is symmetric, i.e., $H^*(\sigma,\tau) = H^*(\tau,\sigma)$. Moreover observing that $H^{per}(\sigma)$ and $H^+(\sigma)$ can be rewritten respectively as

$$H^{per}(\sigma) = -\frac{J}{2}\sum_{i\in\Lambda}\sum_{\substack{j\in\Lambda\\ \langle i,j\rangle\in B_\Lambda^{per}}}\sigma_i\sigma_j \tag{7}$$

$$H^+(\sigma) = -\frac{J}{2}\sum_{i\in\Lambda}\sum_{\substack{j\in\Lambda\\ \langle i,j\rangle\in B_\Lambda}}\sigma_i\sigma_j - J\sum_{i\in\partial^{int}\Lambda}\sum_{\substack{j\in\partial^{ext}\Lambda\\ |i-j|=1}}\sigma_i \tag{8}$$

we also get immediately that $H^*(\sigma,\sigma) = H^*(\sigma)$.

Let us write

$$\partial_i = \frac{J}{2}\mathbf{1}_{\{i\in\partial^{int}\Lambda\}}\sum_{\substack{j\in\partial^{ext}\Lambda:\\ |i-j|=1}} 1, \qquad G(\sigma) = \sum_{i\in\Lambda}\partial_i\sigma_i \tag{9}$$

and define

$$h_i^+(\sigma) = \frac{J}{2}\sum_{\substack{j\in\Lambda:\\ \langle i,j\rangle\in B_\Lambda}}\sigma_j + \partial_i, \qquad h_i^{per}(\sigma) = \frac{J}{2}\sum_{\substack{j\in\Lambda:\\ \langle i,j\rangle\in B_\Lambda^{per}}}\sigma_j. \tag{10}$$

Then we can rewrite

$$H^*(\sigma,\tau) = -\sum_{i\in\Lambda}(h_i^*(\sigma)+\sigma_i q)\tau_i - G^*(\sigma) + q|\Lambda| \tag{11}$$

with $G^+(\sigma) = G(\sigma)$ and $G^{per}(\sigma) = 0$.

1.1.3 Parallel Dynamics

We can now define parallel dynamics, that are called *PCA dynamics*, with the following transition probabilities, for $* = per, +$

$$P^*_{PCA}(\sigma,\tau) = \frac{e^{-H^*(\sigma,\tau)}}{\sum_{\tau\in\mathcal{X}} e^{-H^*(\sigma,\tau)}} \tag{12}$$

It is a standard task to show that this PCA dynamics is reversible with respect to the measure

$$\pi^*_{PCA}(\sigma) = \frac{\sum_{\tau\in\mathcal{X}} e^{-H^*(\sigma,\tau)}}{\sum_{\tau,\tau'\in\mathcal{X}} e^{-H^*(\tau,\tau')}} \tag{13}$$

Due to (11), the transition probabilities of this Markov chain can be written as products of the transition probabilities of each component τ_i of the new configuration τ, as usual for PCAs:

$$P^*_{PCA}(\sigma,\tau) = \prod_{i\in\Lambda} p_i^*(\tau_i|\sigma)$$

with

$$p_i^*(\tau_i|\sigma) = \frac{e^{(h_i^*(\sigma)+\sigma_i q)\tau_i}}{2\cosh(h_i^*(\sigma)+\sigma_i q)}.$$

1.1.4 Irreversible Parallel Dynamics

In the case of periodic boundary conditions we will also consider an *irreversible* parallel dynamics, denoted with I for irreversible, by considering the following pair Hamiltonian

$$H^I(\sigma,\tau) = -\sum_{i\in\Lambda}\left[J\sigma_i(\tau_{i^\uparrow}+\tau_{i^\rightarrow})+q\sigma_i\tau_i\right] = -\sum_{i\in\Lambda}\left[J\tau_i(\sigma_{i^\downarrow}+\sigma_{i^\leftarrow})+q\sigma_i\tau_i\right] \quad (14)$$

where $i^\uparrow, i^\rightarrow, i^\downarrow, i^\leftarrow$ are respectively the up, right, down, left nearest neighbors of the site i on the torus $(\Lambda, B_\Lambda^{per})$. We have $H^I(\sigma,\sigma) = H^{per}(\sigma) - q|\Lambda|$ but note that now $H^I(\sigma,\tau) \neq H^I(\tau,\sigma)$. However, as shown in [5,15], the following *weak symmetry condition (dynamical balance)* holds

$$\sum_{\tau\in\mathcal{X}} e^{-H^I(\sigma,\tau)} = \sum_{\tau\in\mathcal{X}} e^{-H^I(\tau,\sigma)}. \quad (15)$$

so that the parallel dynamics defined by

$$P^I_{PCA}(\sigma,\tau) = \prod_{i\in\Lambda}\frac{\exp\left\{\tau_i\left[J(\sigma_{i^\downarrow}+\sigma_{i^\leftarrow})+q\sigma_i\right]\right\}}{2\cosh(J(\sigma_{i^\downarrow}+\sigma_{i^\leftarrow})+q\sigma_i)}$$

is irreversible with a unique stationary distribution π^I_{PCA} given by

$$\pi^I_{PCA}(\sigma) := \frac{Z^I_\sigma}{Z^I_{PCA}}, \qquad Z^I_\sigma = \sum_{\tau\in\mathcal{X}} e^{-H^I(\sigma,\tau)} \quad (16)$$

with $Z^I_{PCA} := \sum_\sigma Z^I_\sigma$.

1.2 Remarks

It is possible to find in literature a lot of results about PCA defined directly on the whole lattice (infinite volume), see e.g. [11,20]. This problem is not directly faced in this paper.

The idea to extend the state space by considering products of the configuration space $\mathcal{X}$ is not new in PCA literature related to interacting particle systems. An important idea has been to increase the dimension of the state space, considering a copy of $\mathcal{X}$ for each discrete time (see for instance the widely cited paper [16] and [22]).

Pair Hamiltonians were also already present in the literature (see [6,20]), and sometimes their use was related to generalizations of the detailed balance condition, see for instance [18, p. 336], where the notion of "approximately reversible non degenerate" Markov chain has been introduced. In the latter case a pair Hamiltonian was introduced in order to write

$$P(\sigma,\tau) \propto e^{-[H(\sigma,\tau)-H(\sigma)]}$$

where as usual the symbol $\propto$ stands for proportionality, so that reversibility w.r.t. the Gibbs measure was immediately related to the symmetry condition $H(\sigma,\tau) = H(\tau,\sigma)$.

Here (as in [4,9,13,15]) the pair Hamiltonian $H(\sigma,\tau)$ has a completely different role since it is a necessary ingredient to define the dynamics. More precisely, to define the dynamics we want to consider a Gibbs measure $\mu(\sigma,\tau) \propto e^{-H(\sigma,\tau)}$ on the space of pairs of configurations $(\sigma,\tau) \in \mathcal{X}^2$ instead of the Gibbs measure for single configurations, looking at pairs of configurations as possible moves of the dynamics.

The "lifting" given by the definition of pair Hamiltonian is due to the quadratic form of $H(\sigma)$ so that it is possible to consider $H(\sigma) = H(\sigma,\sigma)$.

Once the pair Hamiltonian is given, it is natural to define the probability measure on $\mathcal{X} \times \mathcal{X}$:

$$\mu(\sigma, \tau) = \frac{e^{-H(\sigma,\tau)}}{Z} \qquad \text{with} \quad Z = \sum_{\sigma,\tau} e^{-H(\sigma,\tau)}.$$

The marginal of $\mu(\sigma, \tau)$ is the measure on $\mathcal{X}$:

$$\sum_{\tau} \frac{e^{-H(\sigma,\tau)}}{Z} =: \nu(\sigma) \equiv \frac{Z_\sigma}{Z}$$

and if $H(\sigma, \tau) = H(\tau, \sigma)$, i.e., in the *reversible case*, we have $\mu(\sigma, \tau) = \mu(\tau, \sigma) = \mu(\{\sigma, \tau\})$ and $\nu(\sigma)$ can be also written as $\nu(\sigma) = \sum_\tau \frac{e^{-H(\tau,\sigma)}}{Z}$.

Hence, for a given $\sigma \in \mathcal{X}$ the transition probabilities of the PCA can be interpreted as a conditioned probability of the pair Gibbs measure $\mu(\sigma, \tau)$, namely

$$P(\sigma, \tau) = \mathbb{P}((\sigma, \tau)|\sigma) := \frac{\mu(\sigma, \tau)}{\nu(\sigma)} = \frac{e^{-H(\sigma,\tau)}}{Z_\sigma} \equiv P_{PCA}(\sigma, \tau) \tag{17}$$

and $\nu(\sigma) = \frac{Z_\sigma}{Z} = \pi_{PCA}(\sigma)$ is clearly its invariant measure.

In the *irreversible case*, when $H(\sigma, \tau) \neq H(\tau, \sigma)$, we need to consider periodic boundary conditions. Then, imposing for instance completely asymmetric interactions, see (14), it is possible to prove that (see [5,15])

$$\nu(\sigma) := \sum_{\tau} \frac{e^{-H(\sigma,\tau)}}{Z} = \sum_{\tau} \frac{e^{-H(\tau,\sigma)}}{Z}$$

and this implies again that the marginal measure ν is the stationary measure of the dynamics defined in equation (17). Unfortunately, this identity strongly depends on the translational invariance of the system (i.e., periodic boundary conditions) and therefore we are not able to identify the stationary measure for $+$ boundary conditions.

Note however that in this periodic case the same construction holds in the reversible and non-reversible case. This is an interesting feature of our approach, introducing a unique promising language to treat equilibrium and non-equilibrium statistical mechanics.

1.3 Results

We can now give our general results. Define the total variation distance, or L_1 distance, between the Gibbs measure π_G and the stationary measure π_{PCA} of the parallel dynamics as

$$\|\pi_{PCA} - \pi_G\|_{TV} = \frac{1}{2} \sum_{\sigma \in \mathcal{X}} |\pi_{PCA}(\sigma) - \pi_G(\sigma)|. \tag{18}$$

The first theorem states that this distance tends to zero as the square Λ tends to infininity.

Theorem 1.1 *Set $\delta = e^{-2q}$, and let δ be such that*

$$\lim_{|\Lambda|\to\infty} \delta^2 |\Lambda| = 0, \tag{19}$$

then, there exist J_c such that for any $J > J_c$

$$\lim_{|\Lambda|\to\infty} \|\pi^*_{PCA} - \pi^*_G\|_{TV} = 0 \qquad * = +, per \tag{20}$$

The second theorem deals with the irreversible case, with periodic boundary conditions

Theorem 1.2 *Under the assumption* (19), *there exist* J_c *such that for any* $J > J_c$

$$\lim_{|\Lambda|\to\infty} \|\pi^{I}_{PCA} - \pi^{per}_{G}\|_{TV} = 0 \tag{21}$$

Remark We make some comments and comparisons with similar results obtained in [4,5].

(i) First note that (19) means that the parameter q goes to infinity faster than $\frac{1}{4}\ln|\Lambda|$. Note that this condition implies that typically at each step of the dynamics the number of updated spin is of the order of $\delta|\Lambda| = |\Lambda|^{1/2-\varepsilon}$. This is not a fraction of the volume, but nevertheless it can be a large quantity, and then it is possible to tune the parameter q in order to update a large number of spins at each step, exploiting optimally the computing resources. As far as Theorem 1.1 is concerned, as mentioned in the introduction, a similar result was obtained in [4] but in the opposite regime of high-temperature (uniqueness of phase for the infinite volume Gibbs measure).

(ii) As far as Theorem 1.2 is concerned a similar result was obtained in [5] but with a very particular choice of the parameters. In that paper indeed a low-temperature regime was defined by fixing $J(L)$ and $q(L)$ as functions of the side length L of the square Λ. In the present paper we want to stress that we are in a true low-temperature regime, i.e., we prove the convergence of the invariant measures of the PCA to the Gibbs measure in the thermodynamical limit for any J large enough provided that the hypothesis (19) on the parameter q is satisfied.

(iii) The strategy of the proofs of Theorems 1.1 and 1.2, as in [4,5], is to show that the following inequality holds

$$\|\pi^{*}_{PCA} - \pi^{*}_{G}\|_{TV} = \mathcal{O}(\delta|\Lambda|^{1/2}) \tag{22}$$

and then the proof immediately follows by using the hypothesis (19). However the proof of (22), is based on Lemmas 2.2 and 2.3 below which are completely different from the tools used in the previous papers [4,5].

2 Proof of Theorems 1.1 and 1.2

Let us start with Theorem 1.1. We first prove that there exists J_c such that for any fixed $J > J_c$ there exist δ_J such that for any $\delta < \delta_J$ (22) holds.

Let, for $* = per, +$

$$w^{*}_{PCA}(\sigma) = \sum_{\tau\in\mathcal{X}} e^{-H^{*}(\sigma,\tau)} \tag{23}$$

Then, recalling (11), we have (up to a constant $e^{-q|\Lambda|}$ which cancels out in the ratio $w^{*}_{PCA}(\sigma)/\sum_{\sigma} w^{*}_{PCA}(\sigma)$)

$$w^{*}_{PCA}(\sigma) = e^{G^{*}(\sigma)} \sum_{\tau\in\mathcal{X}} e^{\sum_{i\in\Lambda}[(h^{*}_{i}(\sigma)+q\sigma_i)\tau_i)]}.$$

We now rewrite the sum on $\tau \in \mathcal{X}$ in the following way. Given $\sigma \in \mathcal{X}$, to sum over all $\tau \in \mathcal{X}$ is the same as to sum over all subsets $I \subset \Lambda$ such that $\tau_i = -\sigma_i$ if $i \in I$ while $\tau_i = \sigma_i$ otherwise. Hence we can write

$$\begin{aligned} w^*_{PCA}(\sigma) &= e^{G^*(\sigma)} \sum_{I\subset\Lambda} e^{\sum_{i\in\Lambda} h^*_i(\sigma)\sigma_i - 2\sum_{i\in I} h^*_i(\sigma)\sigma_i - 2q|I|} \\ &= e^{\sum_{i\in\Lambda} h^*_i(\sigma)\sigma_i + G^*(\sigma)} \sum_{I\subset\Lambda}\prod_{i\in I} e^{-2h^*_i(\sigma)\sigma_i - 2q} = e^{\sum_{i\in\Lambda} h^*_i(\sigma)\sigma_i + G^*(\sigma)} \prod_{i\in\Lambda}(1+\delta\phi^*_i) \end{aligned} \tag{24}$$

where, recalling that $\delta = e^{-2q}$, we have defined

$$\phi^*_i = e^{-2(h^*_i(\sigma))\sigma_i} \tag{25}$$

By definitions (7), (8), (9) and (10) it is easy to check that

$$\sum_{i\in\Lambda} h^*_i(\sigma)\sigma_i + G^*(\sigma) = -H^*(\sigma)$$

The following lemma shows that the invariant measure $\pi^*_{PCA}(\sigma)$ of the PCA dynamics can be expressed in terms of the Ising Gibbs measure $\pi^*_G(\sigma)$.

Lemma 2.1 *Let*

$$f^*(\sigma) = \prod_{i\in\Lambda}(1+\delta\phi^*_i), \tag{26}$$

then

$$\pi^*_{PCA}(\sigma) = \frac{\pi^*_G(\sigma) f^*(\sigma)}{\pi^*_G(f^*)}$$

where $\pi^*_G(f^*) = \sum_{\sigma\in\mathcal{X}} w^*_G(\sigma) f^*(\sigma)$.

Proof We have, by (24)

$$w^*_{PCA}(\sigma) = w^*_G(\sigma) f^*(\sigma) \tag{27}$$

and therefore, by definitions (23), (4) and (13) we get

$$\begin{aligned} \pi^*_{PCA}(\sigma) &= \frac{w^*_{PCA}(\sigma)}{\sum_{\sigma'\in\mathcal{X}} w^*_{PCA}(\sigma')} = \frac{w^*_G(\sigma) f^*(\sigma)}{\sum_{\sigma'\in\mathcal{X}} w^*_G(\sigma') f^*(\sigma')} \\ &= \frac{\frac{w^*_G(\sigma)}{Z^*_G} f^*(\sigma)}{\sum_{\sigma'\in\mathcal{X}} \frac{w^*_G(\sigma')}{Z^*_G} f^*(\sigma')} = \frac{\pi^*_G(\sigma) f^*(\sigma)}{\pi^*_G(f^*)} \end{aligned}$$

□

By Lemma 2.1 we have

$$\begin{aligned} \|\pi^*_{PCA} - \pi^*_G\|_{TV} &= \sum_\sigma \pi^*_G(\sigma)\left|\frac{f^*(\sigma)}{\pi^*_G(f^*)} - 1\right| = \pi^*_G\left(\left|\frac{f^*(\sigma)}{\pi^*_G(f^*)} - 1\right|\right) \\ &\le \frac{(\mathrm{var}_{\pi^*_G}(f^*))^{1/2}}{\pi^*_G(f^*)} = \left(\Delta^*(\delta)\right)^{1/2} \end{aligned} \tag{28}$$

with

$$\Delta^*(\delta) = \frac{\pi_G((f^*)^2)}{(\pi_G(f^*))^2} - 1 \tag{29}$$

so that we need to prove that $\Delta^*(\delta) = O(\delta^2|\Lambda|)$. By writing

$$\Delta^*(\delta) = \exp\Big[\ln \pi^*_G((f^*)^2) - 2\ln \pi^*_G(f^*)\Big] - 1$$

this follows if we show that the argument of the exponential divided by $|\Lambda|$ is analytic in δ, and that the first order in δ of its expansion cancels out.

Therefore Theorem 1.1 is proved by the following:

Lemma 2.2 *There exists J_c such that for any $J > J_c$*

(i) $\dfrac{\ln \pi_G^*((f^*)^2)}{|\Lambda|}$ *and* $\dfrac{\ln \pi_G^*(f^*)}{|\Lambda|}$ *are analytical functions of δ for $|\delta| < \delta_J$.*

(ii) $\dfrac{\ln \pi_G^*((f^*)^2)}{|\Lambda|} - 2\dfrac{\ln \pi_G^*(f^*)}{|\Lambda|} = O(\delta^2)$

Proof

Part (i)

We will show the analyticity of $\frac{\ln \pi_G^*((f^*)^2)}{|\Lambda|}$ and $\frac{\ln \pi_G^*(f^*)}{|\Lambda|}$ by showing that both these quantities may be written as partition functions of an abstract polymer gas. Then the analyticity will follow by standard cluster expansion, see [7], Theorem 1, p. 128.

We have

$$\pi_G^*((f^*)^k) = \frac{1}{Z_G^*}\sum_{\sigma\in\mathcal{X}} e^{-H^*(\sigma)}\prod_{i\in\Lambda}(1+\delta\phi_i^*)^k, \quad k=1,2 \tag{30}$$

and, recalling (10), (25), note that

$$\phi_i^* = \exp\{-2h_i^*(\sigma)\sigma_i\} = \exp\left\{-J\sum_{\substack{j\in\Lambda^*\\ \langle i,j\rangle\in B_\Lambda^*}}\sigma_i\sigma_j\right\} \tag{31}$$

with $\Lambda^{per} = \Lambda$, $\Lambda^+ = \bar{\Lambda}$ and we agree that $\sigma_j = +1$ when $j \in \partial^{ext}\Lambda$.

+ boundary conditions

We first consider $\pi_G^+((f^+)^k)$, $k = 1, 2$. Then, by (31), we can write

$$\pi_G^+((f^+)^k) = \frac{1}{Z_G^+}\sum_{\sigma\in\mathcal{X}}\exp\left\{J\sum_{\langle i,j\rangle\in B_\Lambda^+}\sigma_i\sigma_j\right\}\prod_{i\in\Lambda}\left(1+\delta\exp\left\{-J\sum_{j\in\bar{\Lambda},|j-i|=1}\sigma_i\sigma_j\right\}\right)^k \tag{32}$$

We rewrite the l.h.s. of (32) via a standard Peierls contour gas (for the definition of standard Peierls contours see e.g. [19] or [10]). This is possible because we are considering nearest neighbor interactions. Following the usual construction, for a fixed configuration σ, let Γ be the set of unit segments perpendicular to the center of each bond of nearest neighbors in $\bar{\Lambda}$ having opposite spins at their extremities (again with the convention that $\sigma_i = 1$ if $i \in \partial^{ext}\Lambda$). Any unit segment $e \in \Gamma$ is a nearest neighbor bond of a $(L+1)\times(L+1)$ square with vertices in the dual unit square lattice $\mathbb{Z}^{*2}$ (translated by the vector $(\frac{1}{2}, \frac{1}{2})$ respect to the original lattice $\mathbb{Z}^2$). As far as + b.c are concerned, the correspondence $\sigma \mapsto \Gamma$ is one-to-one and the unit segments of Γ form a collection of closed polygons which separate regions where the spins are positive from regions where they are negative. These polygons possibly intercept themselves in such a way that the degree of each vertex is even. Let us denote by $\mathcal{G}_\Lambda$ the set of all possible Γ. Then we can write

$$J\sum_{\langle i,j\rangle\in B_{\bar{\Lambda}}}\sigma_i\sigma_j = |B_{\bar{\Lambda}}| - 2J|\Gamma|$$

Moreover, calling $l_s(\Gamma)$, for $s = 1, ..., 4$, the set of vertices $i \in \Lambda$ having exactly s edges $\langle i, j\rangle$ with dual in Γ, we have

$$\prod_{i\in\Lambda}\left(1+\delta\exp\left\{-J\sum_{j\in\bar\Lambda,|j-i|=1}\sigma_i\sigma_j\right\}\right)^k = \prod_{i\in\Lambda\setminus\cup_{s=1}^4 l_s(\Gamma)}\left(1+\delta e^{-4J}\right)^k\times\prod_{i\in l_1(\Gamma)}\left(1+\delta e^{-2J}\right)^k \times\prod_{i\in l_2(\Gamma)}(1+\delta)^k\times\prod_{i\in l_3(\Gamma)}\left(1+\delta e^{+2J}\right)^k \times\prod_{i\in l_4(\Gamma)}\left(1+\delta e^{+4J}\right)^k$$

Therefore (32) can be rewritten as follows

$$\pi_G^+((f^+)^k) = \frac{1}{Z_G^+}e^{J|B_{\bar\Lambda}|}(1+\delta e^{-4J})^{k|\Lambda|}\,\Xi_\Lambda^{+(k)}(J,\delta) \tag{33}$$

where

$$\Xi_\Lambda^{+(k)}(J,\delta) = \sum_{\Gamma\in\mathcal{G}_\Lambda}\left[e^{-2J|\Gamma|}\xi_k(\Gamma)\right] \tag{34}$$

with

$$\xi_k(\Gamma) = \left[\frac{1+\delta e^{-2J}}{1+\delta e^{-4J}}\right]^{k|l_1(\Gamma)|}\left[\frac{1+\delta}{1+\delta e^{-4J}}\right]^{k|l_2(\Gamma)|}\left[\frac{1+\delta e^{+2J}}{1+\delta e^{-4J}}\right]^{k|l_3(\Gamma)|}\left[\frac{1+\delta e^{+4J}}{1+\delta e^{-4J}}\right]^{k|l_4(\Gamma)|} \tag{35}$$

From (33) we obtain that

$$\frac{1}{|\Lambda|}\ln\pi_G^+((f^+)^k) = -\frac{\ln Z_G^+}{|\Lambda|} + J\frac{|B_{\bar\Lambda}|}{|\Lambda|} + k\ln(1+\delta e^{-4J}) + \frac{1}{|\Lambda|}\ln\Xi_\Lambda^{+(k)}(J,\delta)$$

The first two terms of the r.h.s. of the identity above do not depend on δ and are uniformly bounded as $|\Lambda| \to \infty$ and the third term is analytic in δ and independent of $|\Lambda|$. It thus remains to analyze the term $\frac{1}{|\Lambda|}\ln\Xi_\Lambda^{+(k)}(J,\delta)$. In order to do that, we regard each $\Gamma \in \mathcal{G}_\Lambda$ as the disjoint union of its suitably defined *p-connected components* $\gamma_1, ..., \gamma_n$ in such a way that any vertex of $l_s(\Gamma)$, $s = 1, ..., 4$, is associated to at most one p-connected component γ_i. We introduce the notion of p-connection as an extension of the usual notion of connection. Namely we define two unit segments of Γ as *p-connected* if they share a common vertex *or if they are parallel and at distance 1*. We denote by $\mathcal{P}_\Lambda$ the set of all such p-connected components, i.e., $\gamma_i \in \mathcal{P}_\Lambda$. For $\gamma, \gamma' \in \mathcal{P}_\Lambda$ we write $\gamma \sim \gamma'$ if $\gamma\cup\gamma' \notin \mathcal{P}_\Lambda$. With these notations (34) can be written as follows

$$\Xi_\Lambda^{+(k)}(J,\delta) = \sum_{n\geq 0}\frac{1}{n!}\sum_{\substack{(\gamma_1,...,\gamma_n)\in\mathcal{P}_\Lambda^n\\ \gamma_i\sim\gamma_j}}\prod_{i=1}^n\left[e^{-2J|\gamma_i|}\xi_k(\gamma_i)\right] \tag{36}$$

where the $n = 0$ contribution is 1, and it corresponds of course to the configuration $\sigma \equiv 1$.

The r.h.s. of (36) is the grand canonical partition function of a hard-core polymer gas, where the polymers are the elements of $\mathcal{P}_\Lambda$ defined above and their activity $\rho_k(\gamma)$ is

$$\rho_k(\gamma) = \xi_k(\gamma)e^{-2J|\gamma|} \tag{37}$$

It is well known that the logarithm of $\Xi_\Lambda^{+(k)}(J,\delta)$ divided by $|\Lambda|$ can be written as an absolutely convergent series uniformly in Λ for $\rho_k(\gamma)$ sufficiently small. For the sake of simplicity, and since we are not seeking optimal bounds, we will use the Kotecky-Preiss (KP) condition [14] (see also [1,7] for better conditions). In its general form, the KP condition reads

$$\sum_{\gamma \not\sim \gamma'} \rho(\gamma) e^{a(\gamma)} \le a(\gamma') \tag{38}$$

where $a(\gamma)$ is any positive function of γ. Choosing $a(\gamma) = a|\gamma|$, $a > 0$, and noting that

$$\sum_{\gamma \not\sim \gamma'} \rho(\gamma) e^{a|\gamma|} \le 3|\gamma'| \sup_{x \in \mathbb{Z}^2} \sum_{\gamma \ni x} \rho(\gamma) e^{a|\gamma|} \tag{39}$$

we have that equation (38) is satisfied if

$$\sup_{x \in \mathbb{Z}^2} \sum_{\substack{\gamma \in \mathcal{P} \\ x \in \gamma}} \rho_k(\gamma) e^{a|\gamma|} \le \frac{a}{3} \tag{40}$$

where $\mathcal{P}$ is the set of all p-connected contours in $\mathbb{Z}^2$. The factor 3 in the r.h.s. of (39) comes from the fact that the contour γ is anchored to γ' if there exists a vertex x of γ' of degree 2 in γ' such that either x is also a vertex of γ or the edge exiting from x in γ', when γ' is traveled in a given direction, is parallel and at distance 1 to an edge of γ. In the latter case there are two possible choices, hence the factor 3.

As we said in the introduction it is not our intention to look for optimal estimates. We thus choose $a = 1$ (which is not optimal) and hence condition (40) becomes

$$\sup_{x \in \mathbb{Z}^2} \sum_{\substack{\gamma \in \mathcal{P} \\ x \in \gamma}} \rho_k(\gamma) e^{|\gamma|} \le \frac{1}{3} \tag{41}$$

To check (41), let first obtain an upper bound for $\rho_k(\gamma)$. Recalling the definition (35), we get, for $|\delta| < e^{4J}$

$$\rho_k(\gamma) \le e^{-2J|\gamma|} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^{k \sum_{s=1}^{4} |l_s(\gamma)|} \tag{42}$$

Observing that

$$\sum_{s=1}^{4} |l_s(\gamma)| \le 2|\gamma|$$

we get, for any $k = 1, 2$

$$\rho_k(\gamma) \le e^{-2J|\gamma|} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^{2k|\gamma|} \le \left(e^{-2J} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^4 \right)^{|\gamma|} \tag{43}$$

Let us call

$$A(J, \delta) = e^{-2J} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^4$$

When the p-connected contour $\gamma \in \mathcal{P}_\Lambda$ is composed by several different connected components we define a new connected contour by adding edges between adjacent contours. We define a rule. For instance we order the vertices of Λ and we consider the consequent order of edges with lexicographic ordering. Given a contour γ, we add to the contour pairs of edges corresponding to the set of smallest edges in order to obtain a connected graph. The resulting graph $\bar{\gamma}$ is then a connected graph with possible multiple edges (the added pairs), with even degree at each vertex, with maximal degree 4. Since each connected component of γ has at least 4 edges, the number of added pairs of edges is at most $\frac{|\gamma|}{4}$.

Then

$$\sup_{x\in\mathbb{Z}^2}\sum_{\gamma\ni x}\rho_k(\gamma)e^{|\gamma|}\leq\sum_{n\geq 4}A(J,\delta)^n e^n\sum_{\substack{\bar{\gamma}\ni 0\\|\gamma|=n}}1\leq\sum_{n\geq 4}[e\cdot 3^{3/2}A(J,\delta)]^n$$

Here the factor $3^{3n/2}$ comes from the estimate of the number of graphs $\bar{\gamma}$ of $3n/2$ edges passing through a fixed vertex. Indeed the graph $\bar{\gamma}$ has a Eulerian circuit and, as usual, each new step has three possible choices. Therefore (41) is surely fulfilled for $k=1,2$ if

$$\frac{[e\cdot 3^{3/2}A(J,\delta)]^4}{1-e\cdot 3^{3/2}A(J,\delta)}\leq\frac{1}{3}\qquad\Longrightarrow\qquad A(J,\delta)<\frac{1}{2e3^{3/2}}\tag{44}$$

Rough estimates give that (44) is satisfied when

$$e^{2J}>4e3^{3/2},\quad|\delta|<\frac{1}{12e^{4J}}\tag{45}$$

this proves Part (i) of Lemma 2.2 in the + b.c. case.

Periodic Boundary Conditions

The only difference is that now the map $\sigma\mapsto\Gamma$ is two-to-one (i.e., σ and $-\sigma$ yield the same Γ). Each Γ is, as before, the union of p-connected contours γ where the connection is the same as in the + b.c. case, and denote by $\mathcal{P}_\Lambda^{per}$ the set of all contours, which now also includes contours winding around the torus Λ^{per}. Therefore, we can write

$$\pi_G^{per}((f^{per})^k)=\frac{2}{Z_G^{per}}e^{J|B_\Lambda|}(1+\delta e^{-4J})^{k|\Lambda|}\Xi_\Lambda^{per(k)}(J,\delta)\tag{46}$$

where the factor 2 is due to the fact that a contour can be filled in two ways and

$$\Xi_\Lambda^{per(k)}(J,\delta)=\sum_{n\geq 0}\frac{1}{n!}\sum_{\substack{(\gamma_1,\ldots,\gamma_n)\in(\mathcal{P}_\Lambda^{per})^n\\\gamma_i\nsim\gamma_j}}\prod_{i=1}^n\left[e^{-2J|\gamma_i|}\xi_k(\gamma_i)\right]$$

This implies that

$$\frac{1}{|\Lambda|}\ln\pi_G^{per}((f^{per})^k)=-\frac{\ln(Z_G^{per}/2)}{|\Lambda|}+J\frac{|B_\Lambda|}{|\Lambda|}+k\ln(1+\delta e^{-4J})+\frac{1}{|\Lambda|}\ln\Xi_\Lambda^{per(k)}(J,\delta)$$

with $\frac{1}{|\Lambda|}\ln\Xi_\Lambda^{per(k)}(J,\delta)$ being absolutely convergent if the same condition (41) is satisfied. Therefore $\frac{1}{|\Lambda|}\ln\pi_G^{per}((f^{per})^k)$ is analytic in δ uniformly in Λ whenever J and δ satisfy, as before, the condition given in (45).

Part (ii)

The first order in δ of $\pi_G^*((f^*)^k),\ k=1,2$, can be directly computed. Recalling (30), we have

$$\pi_G^*((f^*)^k)=\frac{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)(\prod_{i\in\Lambda}(1+\delta\phi_i^*))^k}{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)}=\frac{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)(1+k\sum_{i\in\Lambda}\delta\phi_i^*+O(\delta^2))}{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)}$$
$$=1+k\delta\frac{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)\sum_{i\in\Lambda}\phi_i^*}{\sum_{\sigma\in\mathcal{X}}w_G^*(\sigma)}+O(\delta^2)=1+k\delta\sum_{i\in\Lambda}\pi_G^*(\phi_i^*)+O(\delta^2)$$

Therefore, for $k = 1, 2$, we get that the first order in δ of $\frac{1}{|\Lambda|} \ln \pi^*_G((f^*)^k)$ is given by

$$k\delta \frac{\sum_{i\in\Lambda} \pi^*_G(\phi^*_i)}{|\Lambda|}$$

from which Part (ii) easily follows. □

The proof of theorem 1.2 is similar, and even easier, because the number of possible configurations to analyze is smaller, and in particular the Peierls contours are in this case the standard ones, i.e., we don't need to introduce the notion of p-connectedness (see below). Here we list the few changes needed in this case. We define

$$h^I_i(\sigma) = J(\sigma_{i\downarrow} + \sigma_{i\leftarrow}), \tag{47}$$

$$\phi^I_i = e^{-2(h^I_i(\sigma)\sigma_i} \tag{48}$$

and

$$f^I(\sigma) = \prod_{i\in\Lambda}(1 + \delta\phi^I_i) \tag{49}$$

The theorem follows exactly in the same way if we prove

Lemma 2.3 *There exists J_c such that for any $J > J_c$*

(i) $\dfrac{\ln \pi^{per}_G((f^I)^2)}{|\Lambda|}$ *and* $\dfrac{\ln \pi^{per}_G(f^I)}{|\Lambda|}$ *are analytical functions of δ for $|\delta| < \delta_J$.*

(ii) $\dfrac{\ln \pi^{per}_G((f^I)^2)}{|\Lambda|} - 2\dfrac{\ln \pi^{per}_G(f^I)}{|\Lambda|} = O(\delta^2)$

Proof The proof of the lemma uses the same ideas. We have

$$\pi^{per}_G((f^I)^k) = \frac{1}{Z^{per}_G} e^{J|B_\Lambda|}(1 + \delta e^{-4J})^{k|\Lambda|} \sum_{\Gamma\in\mathcal{G}_\Lambda} \left[e^{-2J|\Gamma|}\xi^I_k(\Gamma)\right] \tag{50}$$

where now, due to (47), (48)

$$\xi^I_k(\Gamma) = \left[\frac{1+\delta}{1+\delta e^{-4J}}\right]^{k|l_1(\Gamma)|} \left[\frac{1+\delta e^{+4J}}{1+\delta e^{-4J}}\right]^{k|l_2(\Gamma)|} \tag{51}$$

Then we split Γ in its connected components $\gamma_1, \ldots, \gamma_n$, where the notion of connection is in this case the usual one (since if $i \in l_2(\Gamma)$ then, due to (47), the two segments of Γ at distance $1/2$ from i must form an elbow.). Denoting by $\mathcal{P}^I_\Lambda$ the set of standard contours in Λ, we can therefore write

$$\sum_{\Gamma\in\mathcal{G}_\Lambda} e^{-2J|\Gamma|}\xi^I_k(\Gamma) = \Xi^{I(k)}_\Lambda(J,\delta) = \sum_{n\geq 0}\frac{1}{n!} \sum_{\substack{(\gamma_1,\ldots,\gamma_n)\in(\mathcal{P}^I_\Lambda)^n \\ \gamma_i\not\sim\gamma_j}} \prod_{i=1}^{n}\left[e^{-2J|\gamma_i|}\xi^I_k(\gamma_i)\right]$$

So, as before, we have to analyze the absolute convergence of the logarithm of the quantity $\Xi^{I(k)}_\Lambda(J,\delta)$, the grand-canonical partition function of a hard core polymer gas in which polymers are now standard contours in the set $\mathcal{P}_\Lambda$ with activity

$$\rho^I_k(\gamma) = \xi^I_k(\gamma)e^{-2J|\gamma|}$$

and we have to prove that

$$\sum_{\substack{\gamma \in \mathcal{P} \\ x \in \gamma}} |\rho_k^I(\gamma)| e^{|\gamma|} \le 1 \tag{52}$$

where $\mathcal{P}$ is now the set of usual contours in $\mathbb{Z}^2$ and x is any fixed vertex of $\mathbb{Z}^2$, due to the translation invariance of the model. We can easily find a bound for $|\rho_k^I(\gamma)|$: we get, for $|\delta| < e^{4J}$

$$\rho_k^I(\gamma) \le e^{-2J|\gamma|} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^{k \sum_{s=1}^2 |l_s(\gamma)|} \tag{53}$$

Observing that in this case

$$\sum_{s=1}^{2} |l_s(\gamma)| \le |\gamma|$$

we get, for any $k = 1, 2$

$$\rho_k^I(\gamma) \le e^{-2J|\gamma|} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^{k|\gamma|} \le e^{-2J|\gamma|} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^{2|\gamma|} \tag{54}$$

We call then

$$A(J, \delta) = e^{-2J} \left[\frac{1 + |\delta| e^{+4J}}{1 - |\delta| e^{-4J}} \right]^2$$

and we obtain

$$\sum_{\substack{\gamma \in \mathcal{P} \\ x \in \gamma}} \rho_k^I(\gamma) e^{|\gamma|} \le \sum_{n \ge 4} A^I(J, \delta)^n e^n \sum_{\substack{\gamma \ni x \\ |\gamma| = n}} 1 \le \sum_{n \ge 4} [3eA^I(J, \delta)]^n$$

Here the factor 3^n comes from the usual estimate on Peierls contours. The rest of the proof is identical. □

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