

# Geometric representation of the 2D Antiferromagnetic Ising Model with topological term at $\theta = \pi$

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We study the two-dimensional Antiferromagnetic Ising Model with an imaginary magnetic field  $i\theta$  at  $\theta = \pi$ . We use a new geometric algorithm which does not present a sign problem. This allows us to perform efficient numerical simulations of this system.

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## 1. Introduction

Numerical simulations are one of the main tools that allow us to obtain quantitative results in many fields of physics, and they have played an essential part in the progress of QCD and condensed matter physics in recent years. There are, however, many interesting physical systems for which we do not have efficient numerical algorithms yet. Examples include QCD at finite density or with a non-vanishing  $\theta$  term. This situation has hindered progress in such fields for a long time, and it is thus of great interest to study novel simulation algorithms.

In the present work we develop and test a geometric algorithm which is applicable to the two-dimensional antiferromagnetic Ising model with an imaginary magnetic field  $i\theta$  (see [1] and [2]) at  $\theta = \pi$ , and which solves the sign problem that this model has when using standard algorithms.

## 2. The model and a geometric algorithm

We start with the (reduced) Hamiltonian for the Ising model in an external magnetic field,

$$H(\{s_x\}, F, h) = -F \sum_{(x,y) \in \mathcal{B}} s_x s_y - \frac{h}{2} \sum_x s_x. \quad (2.1)$$

We denote the sites of the square two-dimensional lattice by  $x = (i, j)$ , with  $i, j \in \{1, 2, \dots, N\}$ ,  $N = 2n \in \mathbb{N}$ , and the spin variables by  $s_x \in \{\pm 1\}$ . The sum  $\sum_{(x,y) \in \mathcal{B}}$  runs over the set  $\mathcal{B}$  of all nearest-neighbors  $(x, y)$ ;  $F = J/(KT)$  is the reduced coupling between spins, and  $h = 2B/(kT)$ , with  $B$  the external magnetic field. The total number of spins is  $N^2 = 4n^2$ , thus even, and therefore the quantity  $Q \equiv \frac{1}{2} \sum_x s_x$  is an integer number, taking values between  $-N^2/2$  and  $N^2/2$ , which can be thought of as playing the role of a topological charge. We are interested in studying this system for imaginary values of the reduced magnetic field  $h$ , i.e., for  $h = i\theta$ .

This model suffers from a sign problem, because the weight of a configuration is not a positive real number, and therefore we cannot apply a standard algorithm. For the special case  $\theta = \pi$  we will show how to construct an efficient geometric algorithm that circumvents this problem.

The partition function of the system at  $\theta = \pi$  is

$$\begin{aligned} Z(F, \theta = \pi) &= \sum_{\{s_x = \pm 1\}} e^{F \sum_{(x,y) \in \mathcal{B}} s_x s_y + i\frac{\pi}{2} \sum_z s_z} \\ &= i^{N^2} \sum_{\{s_x = \pm 1\}} \left\{ \prod_{(x,y) \in \mathcal{B}} [\cosh(F s_x s_y) + \sinh(F s_x s_y)] \prod_z s_z \right\} \\ &= \sum_{\{s_x = \pm 1\}} \left\{ \prod_{(x,y) \in \mathcal{B}} [\cosh(F) + \sinh(F) s_x s_y] \prod_z s_z \right\}. \end{aligned} \quad (2.2)$$

It is easy to see, by decomposing the lattice in two staggered sublattices, that  $Z(F, \pi) = Z(-F, \pi)$ ; therefore, at  $\theta = \pi$ , the ferromagnetic and antiferromagnetic models have the same partition function, and furthermore  $Z$  is in fact a function of  $|F|$ .

We can now expand the product inside the curly brackets, and assign a unique graph to each term in the expansion: to each factor  $\sinh(|F|) s_x s_y$  we assign the bond  $(x, y) \in \mathcal{B}$  in the graph, and we say that such a bond is active. Every other bond is called inactive, and corresponds to

a factor  $\cosh(|F|)$ . Each subset of active bonds describes one and only one of the terms in the expansion. After summing over spin states most of the contributions in the expansion vanish; only the graphs such that every node on the lattice has an odd number of active bonds touching it give a non-vanishing contribution. We call such graphs admissible, and we denote by  $\mathcal{G}$  the set of all admissible graphs. If we consider an admissible graph,  $g \in \mathcal{G}$ , and denote by  $\mathcal{N}_b(g)$  the number of active bonds in  $g$ , by  $\bar{\mathcal{N}}_b(g)$  the number of inactive bonds in  $g$ , and by  $\mathcal{N}$  the total number of bonds in the lattice (thus  $\mathcal{N} = \mathcal{N}_b(g) + \bar{\mathcal{N}}_b(g)$ ), the weight of such graph in the partition function is  $2^{\mathcal{N}} \sinh(|F|)^{\mathcal{N}_b(g)} \cosh(|F|)^{\bar{\mathcal{N}}_b(g)}$ . Therefore we can rewrite the partition function as:

$$\begin{aligned} Z(F, \theta = \pi) &= 2^{\mathcal{N}^2} \sum_{g \in \mathcal{G}} \cosh(|F|)^{\bar{\mathcal{N}}_b(g)} \sinh(|F|)^{\mathcal{N}_b(g)} \\ &= 2^{\mathcal{N}^2} \cosh(|F|)^{\mathcal{N}} \sum_{g \in \mathcal{G}} \tanh(|F|)^{\mathcal{N}_b(g)}. \end{aligned} \quad (2.3)$$

The important point here is that all configurations (graphs) have positive weights, and therefore this representation of the partition function does not have a sign problem. Now, generalizing the partition function (2.3) to the case where the coupling is position-dependent, we obtain:

$$Z(\{F_{xy}\}, \theta = \pi) = \sum_{\{s_x = \pm 1\}} \left\{ \prod_{(x,y) \in \mathcal{B}} [\cosh(|F_{xy}|) + \sinh(|F_{xy}|) s_x s_y] \prod_z s_z \right\}. \quad (2.4)$$

From this expression we are able to build all the correlation functions for an even number of spins (correlation functions with an odd number of spins are automatically zero). After some calculations (see [3]) we obtain the following expression for the correlation functions:

$$\begin{aligned} C(d, F) \equiv \langle s_x s_{x+d\hat{1}} \rangle &= \left[ \prod_{i=1}^d \frac{\partial}{\partial F_{x_i x_{i+1}}} \right] \log Z(\{F_{xy}\}, \theta = \pi) \Big|_{\{F_{xy}\} = \{F\}} \\ &= \langle \langle \tanh(F)^{d-2\mathcal{N}_b[g, \{x_i, y_i\}]} \rangle \rangle, \end{aligned} \quad (2.5)$$

where  $\mathcal{N}_b[g, \{x_i, y_i\}]$  is the number of active bonds along the straight path connecting  $x$  and  $x + d\hat{1}$ . However, we stress the fact that the specific choice of the path is irrelevant, as they are all equivalent, as long as the endpoints are fixed.

### 3. Simulation

In order to perform calculations by means of Monte Carlo methods, we need an efficient algorithm to explore the space of configurations, that in the geometric representation is given by the set of admissible graphs,  $\mathcal{G}$ . The essential ingredient is a local prescription<sup>1</sup> that takes the system from an admissible configuration to another admissible configuration. The simplest change that one can do to a configuration is to make an inactive bond into an active one, or viceversa. However, applying this change to an admissible configuration will not take us to another admissible configuration. Let us consider instead an arbitrary square on the lattice, and consider all possible

<sup>1</sup>Local in the sense that only a fixed number of bonds in a bounded region are changed when updating a configuration.

changes in the state of the bonds in the square. It is easy to convince oneself that if we start from an admissible configuration, the only way to arrive at another admissible configuration is either by not changing the state of any of the bonds, or by changing all of them. Using these steps and the weights of the configurations derived above, it is now easy to set up a standard Metropolis algorithm<sup>2</sup>.

Our aim is to measure how the correlation functions (2.5) depend on the distance  $d$ , choosing different antiferromagnetic couplings  $F < 0$  and varying the lattice volume  $V = L^2$ , in order to determine the staggered magnetization from their asymptotic behavior. In Figs. 1 and 2 we present some preliminary results concerning the evaluation of these correlation functions for different values of the coupling  $F$  and various lattice sizes ranging from  $L = 64$  to  $L = 1024$ . Simulations are done collecting 100k measurements for each value of  $F$ . For each run we discarded the first 10k configurations in order to ensure thermalization. The jackknife method over bins at different blocking levels was used for the data analysis.

For antiferromagnetic couplings, the behavior of the correlation functions implies that the staggered magnetization is nonzero, while the total magnetization vanishes, in the whole range of couplings that we investigated. This result is in agreement with Refs. [1, 2], and with the mean-field calculation of Ref. [4]. The apparent decrease of  $C(d, F)$ , starting from  $d \sim 10 \div 20$ , for low values of  $|F|$ , is probably due to the heavy-tailed probability distributions of the correlators, which is also the cause of their noisy behavior. In Fig. 3 we show the probability distributions of the logarithm of the correlators for lattice size  $L = 64$  and  $F = -0.4$  and  $F = -2.0$ . We can clearly notice that for a low coupling  $|F|$  the values are spread in a wider range than for  $F = -2.0$ , and also that a long tail is developed for large distances. This makes more difficult to obtain an accurate numerical evaluation of the correlators. More details will be presented in [3], where also the three-dimensional version of the model will be investigated.

## Acknowledgments

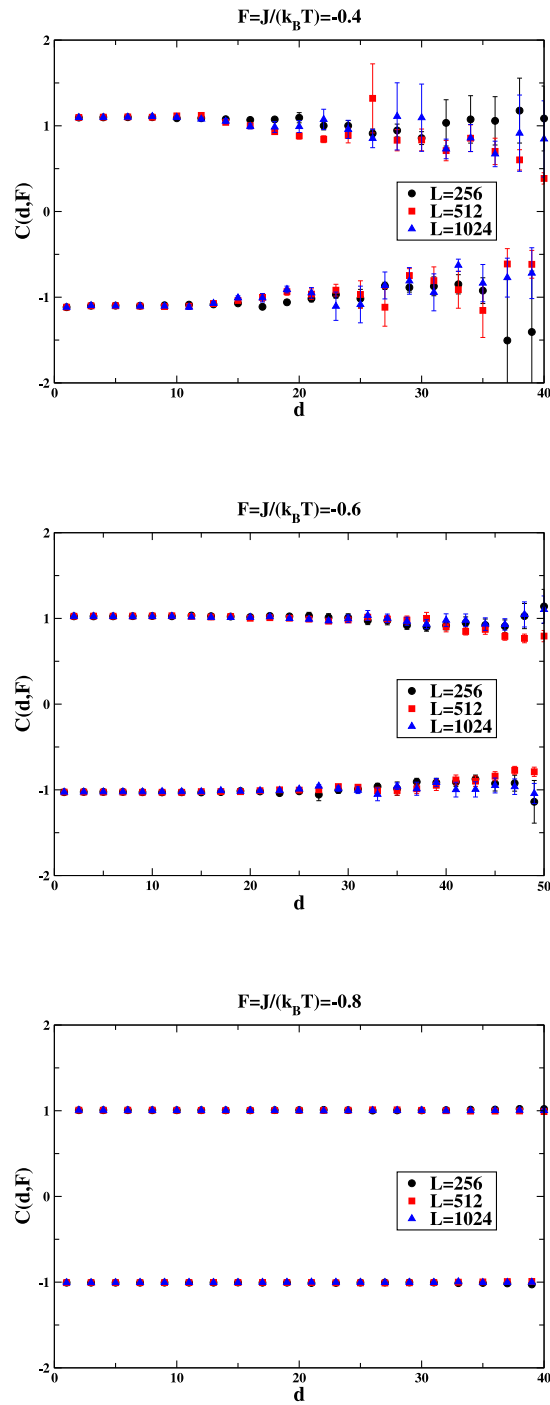
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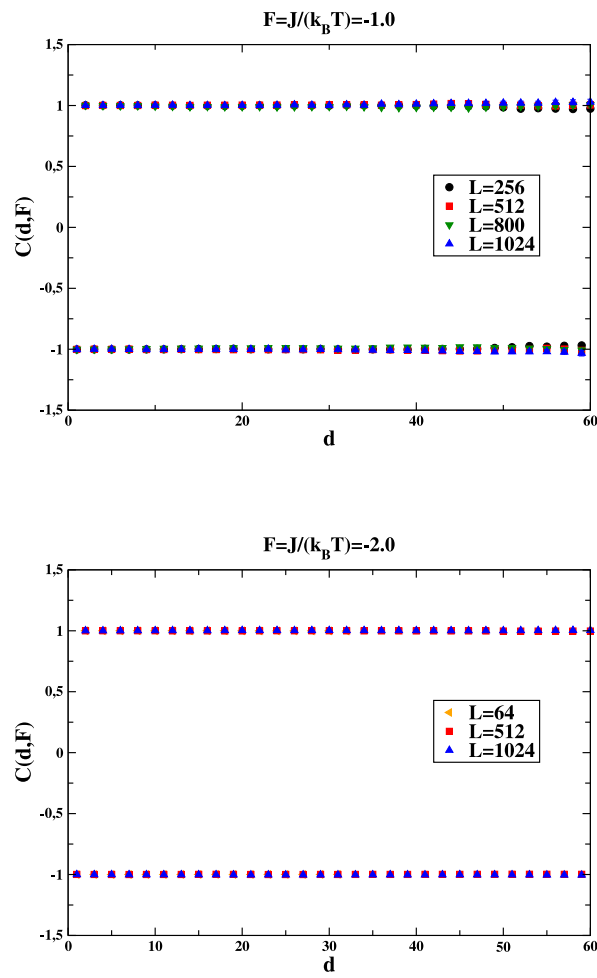
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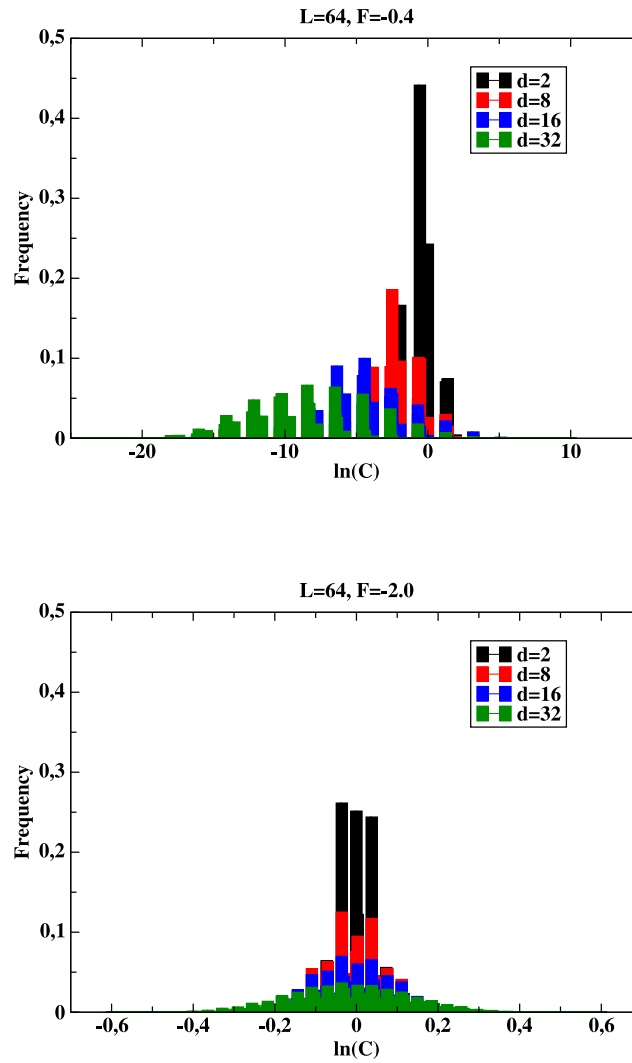
<sup>2</sup>In order to achieve ergodicity for periodic boundary conditions, we have to implement a few, global steps (more details in [3])



**Figure 1:** Dependence of the correlation functions on the distance  $d$  for different values of the coupling  $F$  and for various lattice sizes  $L$ .



**Figure 2:** Dependence of the correlation functions on the distance  $d$  for different values of the coupling  $F$  and for various lattice sizes  $L$ .



**Figure 3:** Probability distribution of the logarithm of the correlator  $C(d, F)$  for various distances  $d$ , for a lattice of size  $L = 64$ , and for coupling  $F = -0.4$  (up) and  $F = -2.0$  (down).