2D and 3D Antiferromagnetic Ising Model with "topological" term at $\theta = \pi$

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Outline

- Introduction
- The Model and the algorithm
- Simulation of the system
- Results
- Conclusions

Introduction

Motivation of the work:

- Many interesting physical systems do not have an efficient numerical algorithms yet.
- An example: QCD at finite density or with a non-vanishing θ term.
- 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 and three-dimensional antiferromagnetic Ising model with an imaginary magnetic field iθ, and which solves the sign problem that this model has when using standard algorithms.

The Model and the algorithm

Reduced Hamiltonian of the system:

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

where

- $F = J/(kT) \to$ coupling
- $h = 2B/(kT) \to$ reduced magnetic field
- $Q = \frac{1}{2} \sum_x s_x$ (from $-N^2/2$ and $N^2/2$) $\to$ "topological charge"

It is then worth studying what happens for imaginary values of the reduced magnetic field h, i.e., for $h = i\theta$.

weight of a configuration not a positive real number
$\Rightarrow$ *"sign problem"*

For $\theta = \pi$ we can circumvent this problem.

$$Z(F, \theta = \pi) = \sum_{\{s_x\},\, s_x = \pm 1} e^{F \sum_{(x,y)\in\mathcal{B}} s_x s_y + i \frac{\pi}{2} \sum_z s_z}$$
$$= \sum_{\{s_x\},\, s_x = \pm 1} \prod_{(x,y)\in\mathcal{B}} [\cosh(F) + \sinh(F) s_x s_y] \prod_z s_z \,,$$

The terms that contribute to the partition function are those for which a given spin variable appears an odd number of times.

Decomposing the lattice in two staggered sublattices we can rewrite our partition function as

$$Z(F,\theta=\pi)=\sum_{\{s_x\},\, s_x=\pm 1}\prod_{(x,y)\in\mathcal{B}}\left[\cosh(F)-\sinh(F)s_xs_y\right]\prod_z s_z\,;$$

$\Rightarrow \quad Z(F,\theta=\pi)=Z(-F,\theta=\pi)$ at $\theta=\pi$;

$\Rightarrow$ the terms that survive in this expansion are those with an even number of terms s_xs_y.

Considering the contributions following these rules:

- a factor 2^N for the sum over the spins;
- a factor of $\sinh(|F|)^{\mathcal{N}[b]}$, where $\mathcal{N}[b]$ is the number of bonds for a given configuration;
- a factor $\cosh(|F|)^{\bar{\mathcal{N}}[b]}$ where $\bar{\mathcal{N}}[b] = \mathcal{N}[\mathcal{B}] - \mathcal{N}[b]$ is the number of inactive bonds;

the partition function becomes:

$$Z(F, \theta = \pi) = 2^{N^2} \cosh(|F|)^{\mathcal{N}[\mathcal{B}]} \sum_{b \in \mathcal{B}!} \tanh(|F|)^{\mathcal{N}[b]} .$$

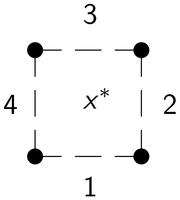
All configurations ("graphs") positive weights $\Rightarrow$ no sign problem !

Simulation of the system

Number of links at any site $\rightarrow$ odd:

- 2D $\rightarrow 1, 3$ bonds
- 3D $\rightarrow 1, 3, 5$ bonds

The dual lattice sites:



The state of bond i at the dual lattice site x^* is denoted by $A_i(x^*)$, and we set

$$A_i(x^*) \rightarrow \begin{cases} 1 & \textit{if active} \\ 0 & \textit{if inactive} \end{cases}$$

We can draw all the admissible configuration, specified by a vector $A(x^*)$.

- $S(x^*) \rightarrow$ graphs corresponding to these configurations.
- $w(x^*) = \sum_{i=1}^{4} A_i(x^*) \rightarrow$ number of active bonds at site x^* in a given configuration.

The key observation is that, as the number of external bonds touching a vertex is fixed, and the total number of bonds touching a vertex must be odd, when changing $A(x^*)$ we must be sure that the number of internal bonds that change state, touching a given vertex, is an even number, i.e., 0 or 2 (or 4 in 3D).

$S(x^*)$	$w(x^*)$	$A(x^*)$
	0	$(0, 0, 0, 0)$
	1	$(1, 0, 0, 0)$
	1	$(0, 1, 0, 0)$
	1	$(0, 0, 1, 0)$
	1	$(0, 0, 0, 1)$
	2	$(1, 1, 0, 0)$
	2	$(1, 0, 1, 0)$
	2	$(1, 0, 0, 1)$

Active bonds $\rightarrow$ solid line, inactive bonds $\rightarrow$ no line.

$w(x^*) = \sum_{i=1}^{4} A_i(x^*) \rightarrow$ number of active bonds.

Updating the configurations:

$$A(x^*) \to \begin{cases} \mathcal{I}A(x^*) = A(x^*)\,, \\ \mathcal{C}A(x^*) = I - A(x^*) \end{cases}$$

where

- $\mathcal{I} \to$ *identity*
- $\mathcal{C} \to$ *conjugation*

The variation $\Delta w(x^*)$ of the number of active bonds is given by

$$\Delta w(x^*) = \sum_{i=1}^{4} \mathcal{C}A_i(x^*) - A_i(x^*) = \sum_{i=1}^{4} I_i - 2A_i(x^*) = 2[2 - w(x^*)]\,.$$

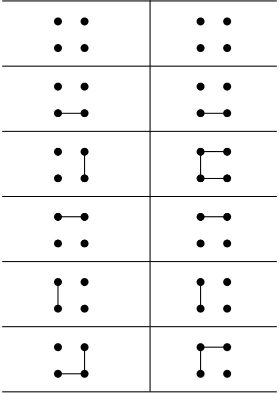
To pass to another admissible configuration, we have only two possibilities: either leave everything unchanged, or change the state of all the bonds at the given square/dual lattice site (next table).

$S(x^*)$	$\hat{\mathcal{C}}S(x^*)$	$\Delta w(x^*)$
		4
		2
		2
		2
		2
		0
		0
		0

Transformation under $\mathcal{C}$

Ergodicity

$S(x^*)$	$\hat{\mathcal{R}}S(x^*)$



Reduction: it coincides with the identity if $A_2 = 0$, and with conjugation if $A_2 = 1$

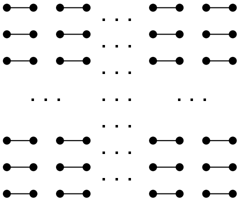
Open boundary conditions: Ergodicity

Figure: (Left) Right-most colum after the first step of reduction. (Right) Two right-most columns after the second step of reduction.

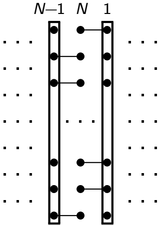
Open boundary conditions: Ergodicity

Figure: (Left) Right-most colum after the first step of reduction. (Right) Two right-most columns after the second step of reduction.

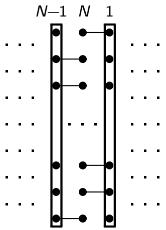
Reduced configuration →

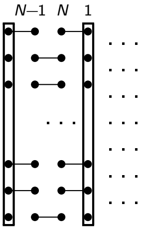


Periodic boundary conditions: Ergodicity



Periodic boundary conditions: Ergodicity





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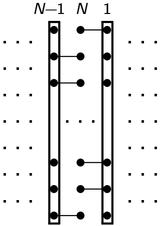

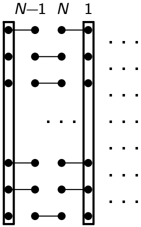

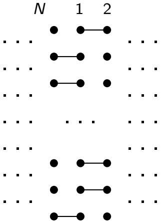

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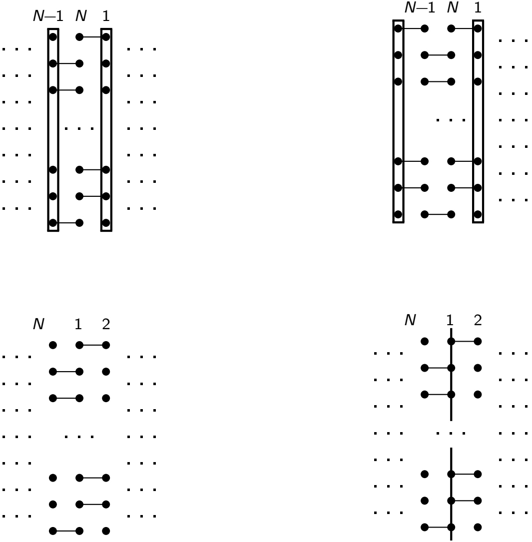
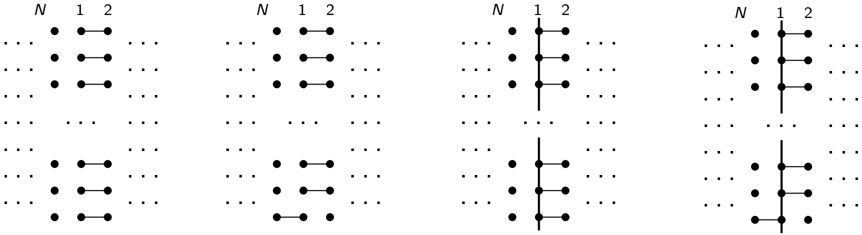


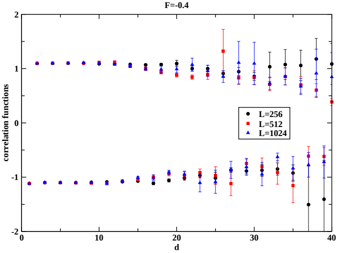
Periodic boundary conditions: Ergodicity

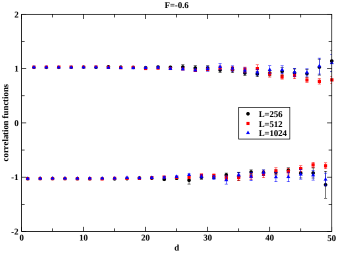


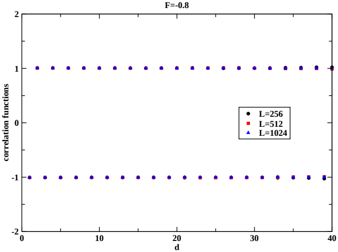
4 inequivalent reduced configurations in 2D

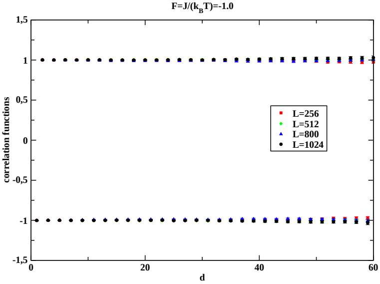
Results: Correlation function in the 2D model

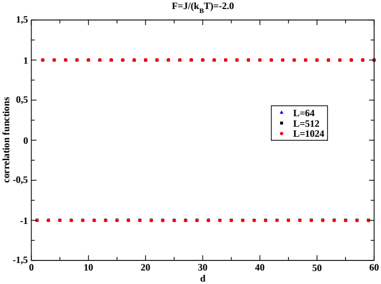
$$C(d, F) \equiv \langle s_x s_{x+d\hat{1}} \rangle$$

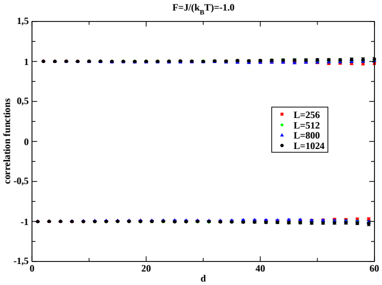


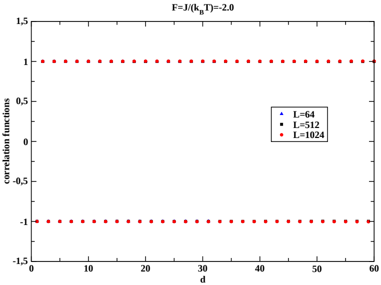




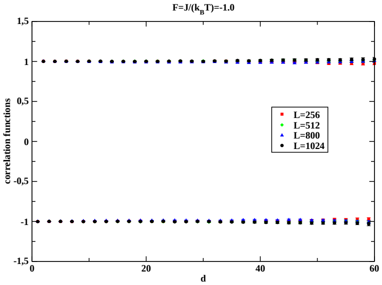

F=J/(k_B T)=-1.0
correlation functions
d
L=256
L=512
L=800
L=1024
1,5
1
0,5
0
-0,5
-1
-1,5
0
20
40
60

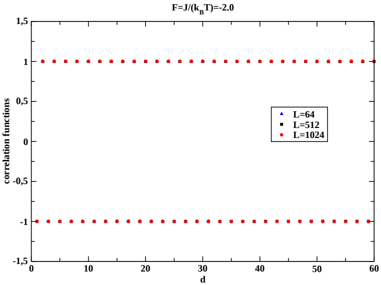

F=J/(k_B T)=-2.0
correlation functions
d
L=64
L=512
L=1024
1,5
1
0,5
0
-0,5
-1
-1,5
0
10
20
30
40
50
60





Results is in agreement with B. M. McCoy and T. T. Wu, *Phys. Rev.* **155** (1967) 438 T. D. Lee and C. N. Yang, *Phys. Rev.* **87** (1952) 410, V. Matveev and R. Shrock, *J. Phys. A* **28** (1995) 4859 and with the mean-field calculation done by V. Azcoiti, E. Follana, and A. Vaquero, *Nucl. Phys. B* **851** (2011) 420.





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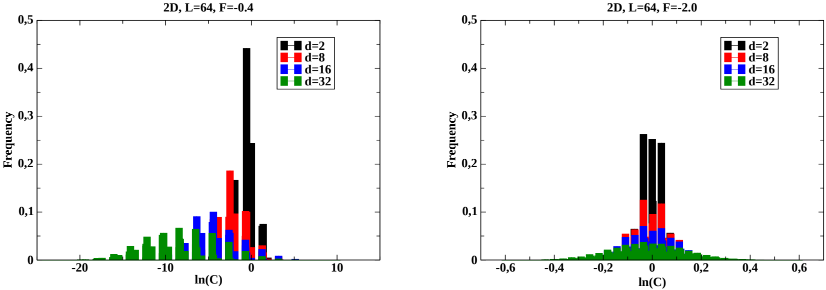
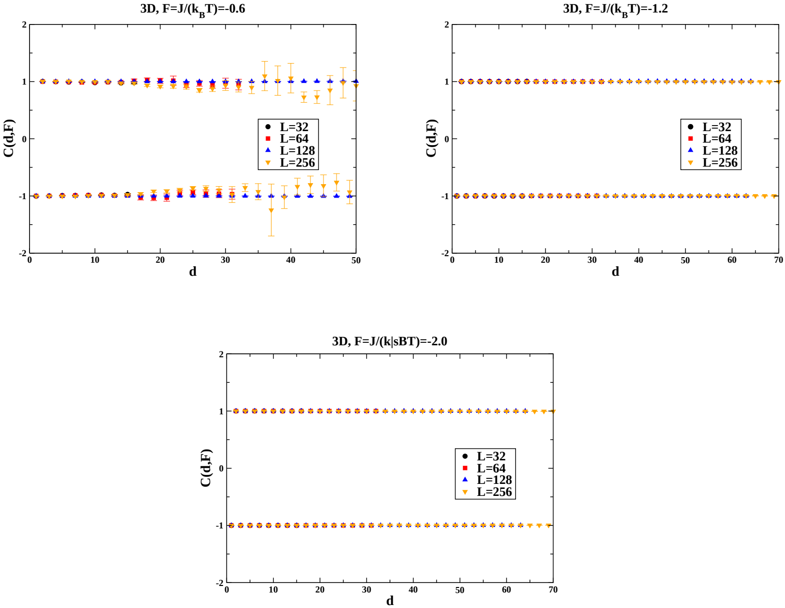
- the apparent decrease of $C(d, F)$ is probably due to the heavy-tailed probability distributions of the correlators

Probability distributions of the logarithm of the correlators

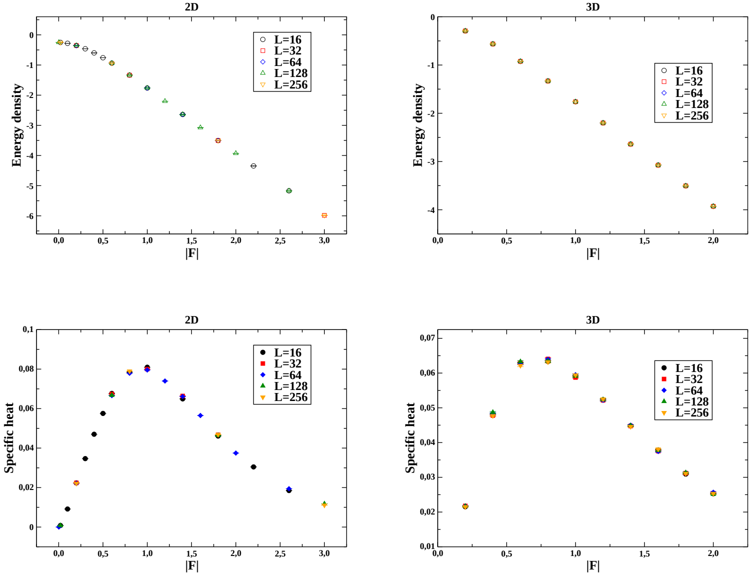


For a low coupling $|F|$ the values are spread in a wider range than for $F = -2.0$, and also that a long tail is developed for large distances.

Results: Correlation function in the 3D model



Energy density and Specific Heat



Conclusions

- We developed, for a model not free from the sign problem, a new algorithm able to circumvent this obstacle
- We tested successfully for the $2D$ antiferromagnetic Ising model and we studied also the $3D$ version
- The behavior of the correlation function as well the specific heat are in agreement with the predictions
- No phase transitions for these models at $\theta = \pi$
- This technique maybe can be applied to study other interesting models