Two-dimensional antiferromagnetic Ising model as a toy model for usual θ physics

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Work in collaboration with [1]

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[1] arXiv:1612.08598

Outline

A brief introduction

- The Sign Problem: a major difficulty
  - θ-QCD
  - $\mu > 0$ QCD
  - Chains of quantum spins with AF interactions $\leftrightarrow O(3)_\theta NL\sigma M$
  - Hubbard model
- Usual importance sampling techniques fail, other methods needed
- It is convenient to have a set of benchmark calculations

Motivation

- Analytical solution in few systems
  - 1d Ising model within an imaginary magnetic field
  - 2d compact $U(1)$-model with a topological term
  - 2d Ising model with $H/KT = i\pi/2$
- Reformulation of variables, overcoming the sign problem
  - $U(1)$ / Z_3 gauge-Higgs model, $\mu > 0$[2]

Our motivation: to provide a benchmark calculation for a system both without an analytical solution or a known reformulation, the 2d AF Ising model within a pure imaginary field.

[2] [Mercado, Gattringer and Schmidt, 2013]

What we have done

A study of the 2d AF Ising model within a pure imaginary field, which partition function is

$$\mathcal{Z} = \sum_{\{s_i\}} \exp\left(i\theta \frac{1}{2} \sum_i s_i + F \sum_{<ij>} s_i s_j \right). \tag{1}$$

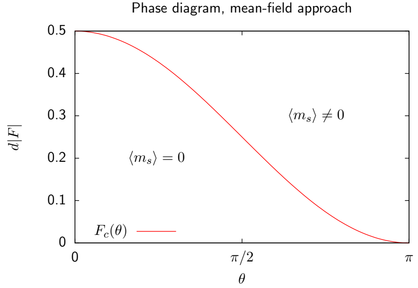
- Exact cumulant expansion to 8th order
- Analytic computation of $\mathcal{Z}$ and other observables for a large number of DOFs
- Analyze the phase structure of the model

What we expect

A mean-field study[3] of the 2d AF Ising model within a pure imaginary field was performed. The resulting partition function was

$$\mathcal{Z}_{MF}(F,\theta) = \sum_{\{s_i\}} \exp\left(i\theta \frac{M_1 + M_2}{2} - \frac{Fd}{N}(M_1 - M_2)^2 \right), \qquad (2)$$

Applying saddle-point techniques, the critical line is $dF_c = \cos^2(\theta_c/2)/2$.



[3] [Azcoiti et al, NPB 851, 2011]

Reformulating $\mathcal{Z}$

- First, we divide the lattice into two sublattices Ω_1, Ω_2, and define the magnetization densities m_1 and m_2 as

$$m_j \equiv \frac{M_j}{N/2} \equiv \frac{\sum_{i\in\Omega_j} s_i}{N/2} \qquad j = 1, 2, \tag{3}$$

and the density of states $g(m_1, m_2)$ as the number of microstates with magnetization densities m_1, m_2.

- Then, we reformulate $\mathcal{Z}$ as

$$\mathcal{Z} = \sum_{m_1,m_2} g(m_1, m_2) \left\langle \exp\left(i\frac{\theta}{2} \sum_i s_i + F \sum_{<ij>} s_i s_j \right) \right\rangle_{m_1,m_2} . \tag{4}$$

Cumulant expansion

$$\mathcal{Z} = \sum_{m_1,m_2} g(m_1,m_2) e^{\frac{1}{4} N i\theta(m_1+m_2)} \left\langle \exp\left(F \sum_{<ij>} s_i s_j \right) \right\rangle_{m_1,m_2} . \quad (5)$$

- We recall the definition of the cumulants κ_n,

$$\left\langle e^{tX} \right\rangle \equiv \exp\left(\sum_{n=1}^{\infty} \kappa_n \frac{t^n}{n!} \right), \quad (6)$$

- The n-th cumulant is an n-th degree polynomial in the first n non-central moments of X,

$$\kappa_n = \mu'_n - \sum_{m=1}^{n-1} \binom{n-1}{m-1} \kappa_m \mu'_{n-m}, \qquad \mu'_n \equiv \langle X^n \rangle . \quad (7)$$

Final $\mathcal{Z}$ and cumulant expressions

$$\mathcal{Z} = \sum_{m_1,m_2} g(m_1,m_2) \exp\left(\frac{1}{4}Ni\theta(m_1+m_2) + \sum_{n=1}^{\infty} \kappa_n(m_1,m_2)\frac{F^n}{n!}\right) \quad (8)$$

$$\begin{aligned}
\kappa_1 &= 2Nm_1m_2, \\
\kappa_2 &= 2N({m_1}^2-1)({m_2}^2-1), \\
\kappa_3 &= 8Nm_1m_2({m_1}^2-1)({m_2}^2-1), \\
\kappa_4 &= 4N(21{m_1}^2{m_2}^2 - 9({m_1}^2+{m_2}^2)+5) \\
&\quad \times({m_1}^2-1)({m_2}^2-1), \\
&\quad (\cdots)
\end{aligned} \quad (9)$$

Computing the observables

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \sum_{m_1, m_2} \mathcal{O}(m_1, m_2) g(m_1, m_2) \times \exp\left\{ i\theta \frac{M_1 + M_2}{2} + \sum_{n=1}^{n_{max}} \frac{F^n}{n!} \kappa_n(m_1, m_2) \right\} \quad (10)$$

- The complex valued exponentials in (8) and (10) give rise to a SSP.
- Multiprecision libraries (GMP, GNU MPFR, GNU MPC, gmpy2) are used to sum over m_1, m_2.
- $\mathcal{Z} > 0?$[4]

[4] [Seung-Yeon Kim, 2004]

Observables of interest

- We have computed several observables, including the density of free energy ϕ, the density of internal energy e, the specific heat c_v and both usual and staggered magnetizations $\langle m \rangle, \langle m_s \rangle$.

$$\phi \equiv -\frac{1}{NF} \log \mathcal{Z}, \tag{11}$$

$$e \equiv -\frac{1}{2N} \frac{d \log \mathcal{Z}}{dF}, \qquad c_v \equiv -F^2 \frac{d}{dF} e, \tag{12}$$

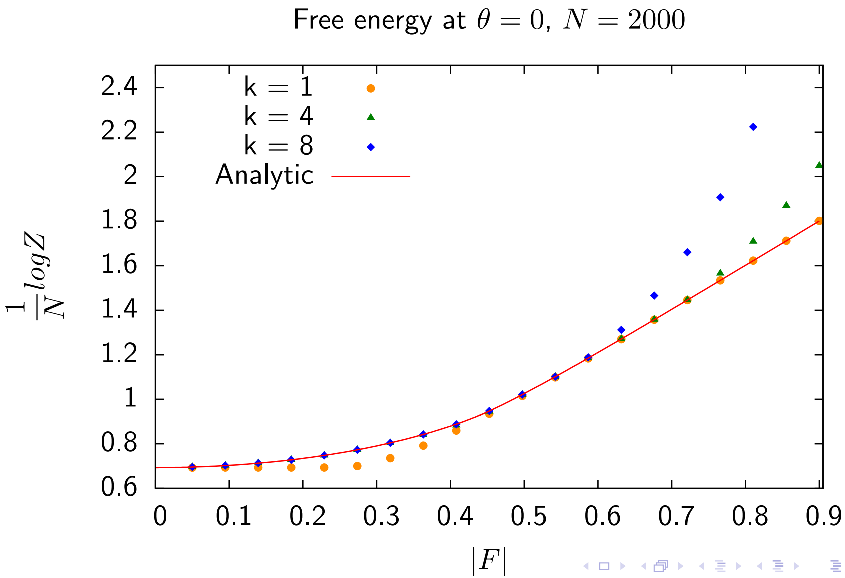
$$\langle m \rangle \equiv \left\langle \frac{m_1 + m_2}{2} \right\rangle, \qquad \langle m_s \rangle \equiv \left\langle \frac{m_1 - m_2}{2} \right\rangle. \tag{13}$$

- For symmetry reasons, the *natural* order parameter $\langle m_s \rangle$ is always zero, and we compute instead the expected value of its square, $\langle m_s^2 \rangle$.

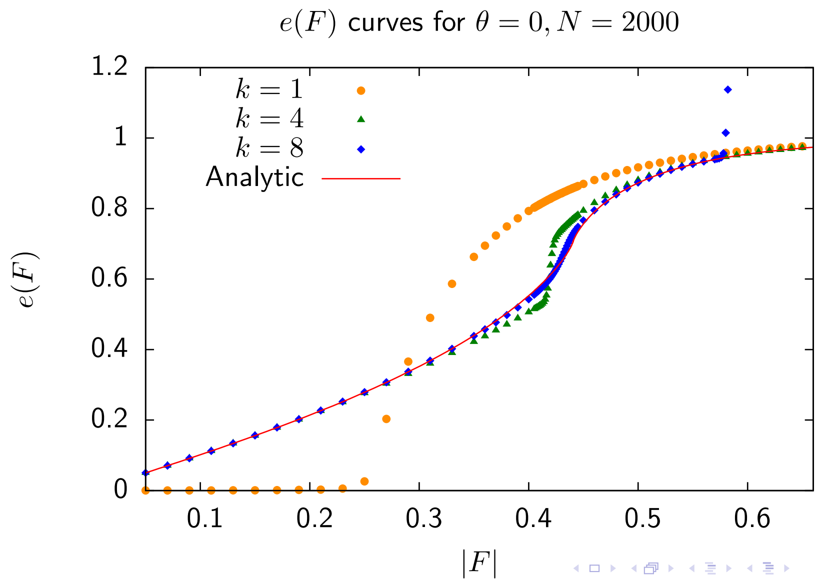
Results

- We show results keeping one, four and eight cumulants
- For clarity we plot just the largest N calculated
- At $\theta = 0$ and $\theta = \pi$ we have analytical solutions

Results

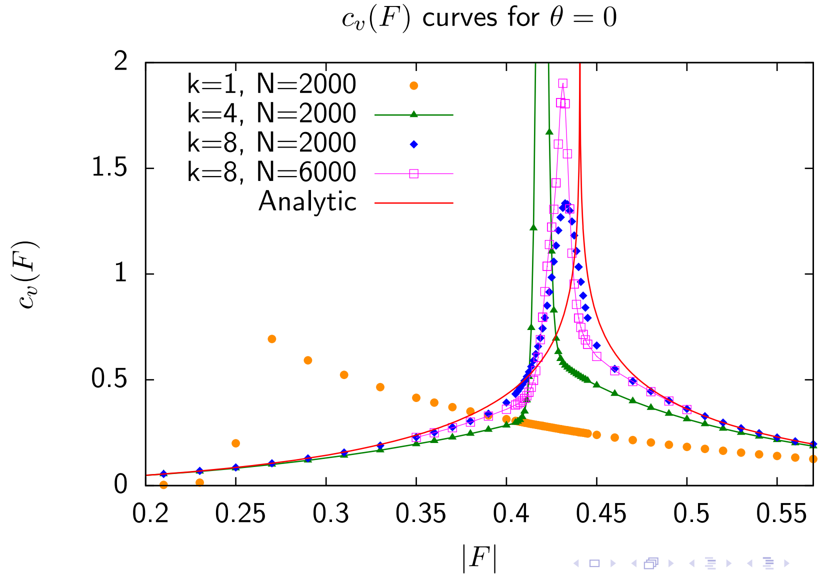

Free energy at $\theta = 0,\ N = 2000$
k = 1
k = 4
k = 8
Analytic
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
$\frac{1}{N} log Z$
$|F|$

Results

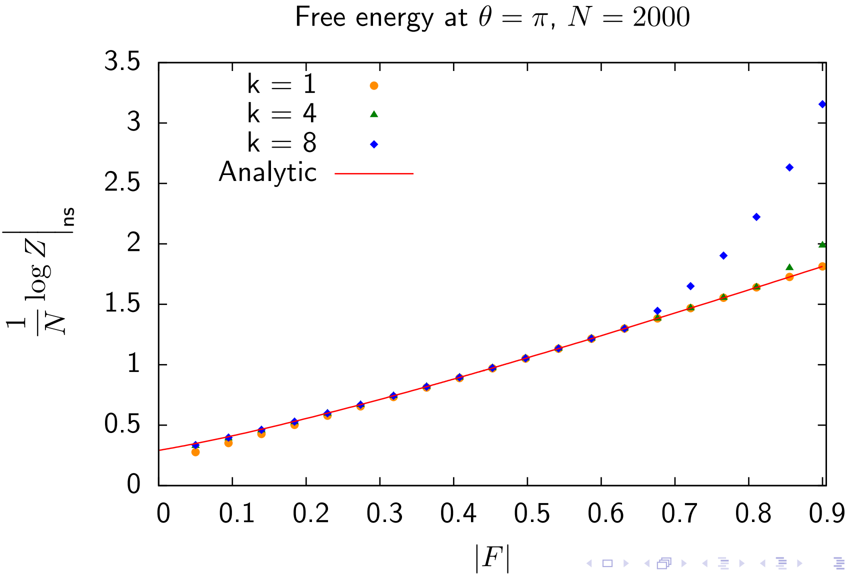


$e(F)$ curves for $\theta = 0, N = 2000$
$k = 1$
$k = 4$
$k = 8$
Analytic
$e(F)$
$|F|$
1.2
1
0.8
0.6
0.4
0.2
0
0.1
0.2
0.3
0.4
0.5
0.6

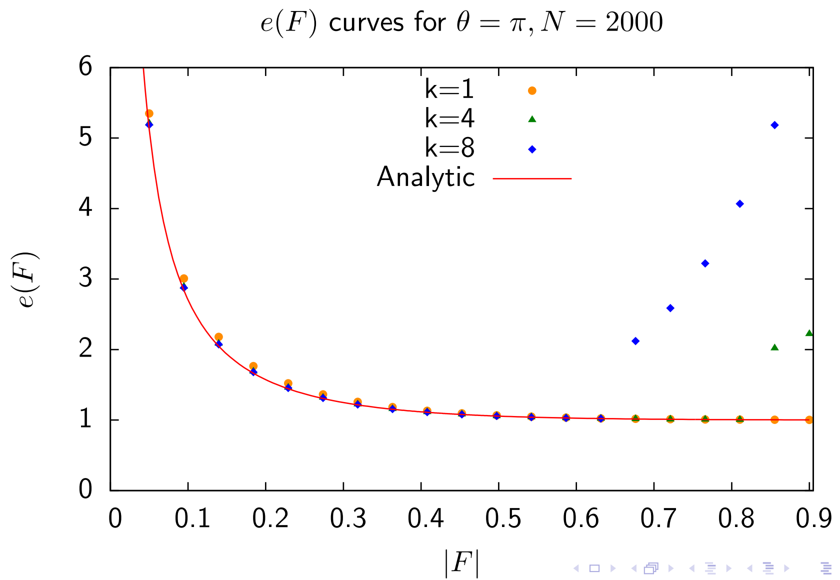
Results


$c_v(F)$ curves for $\theta = 0$
2
1.5
1
0.5
0
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55
k=1, N=2000
k=4, N=2000
k=8, N=2000
k=8, N=6000
Analytic
$c_v(F)$
$|F|$

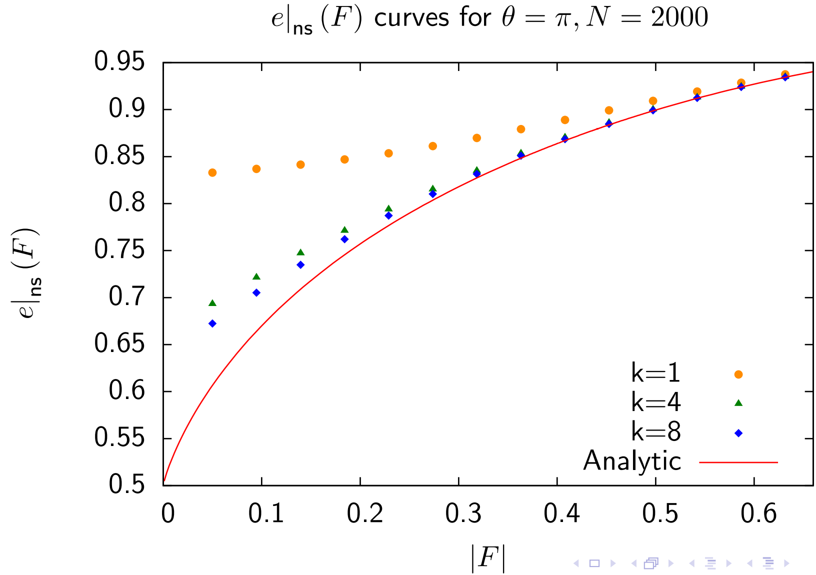
Results



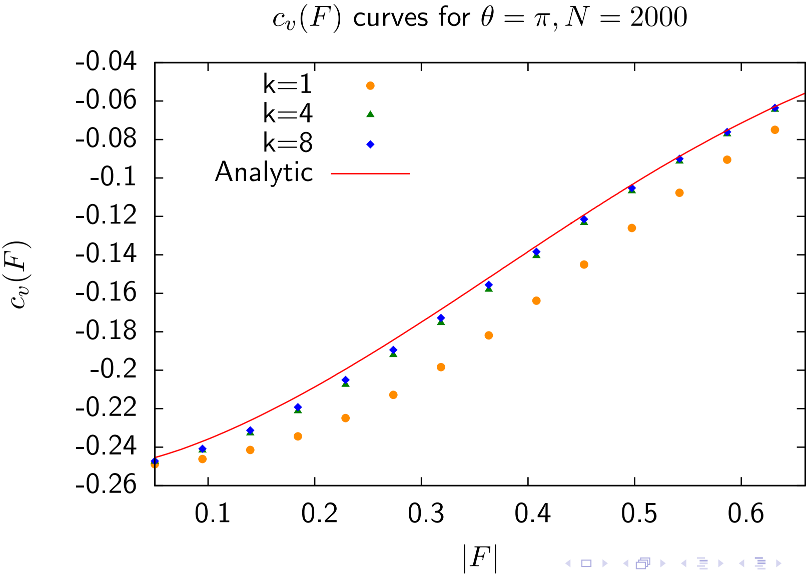
Free energy at $\theta = \pi$, $N = 2000$
3.5
3
2.5
2
1.5
1
0.5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
k = 1
k = 4
k = 8
Analytic
$\frac{1}{N} \log Z \big|_{\text{ns}}$
$|F|$


$e(F)$ curves for $\theta = \pi, N = 2000$
k=1
k=4
k=8
Analytic
$e(F)$
$|F|$
0
1
2
3
4
5
6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

Results


$e|_{\text{ns}}(F)$ curves for $\theta = \pi, N = 2000$
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
$e|_{\text{ns}}(F)$
$|F|$
k=1
k=4
k=8
Analytic

Results

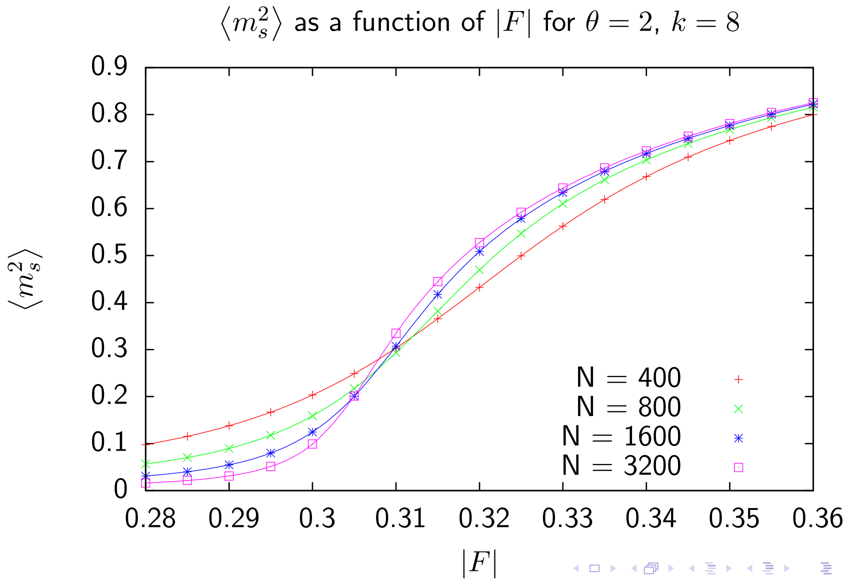


$c_v(F)$ curves for $\theta = \pi, N = 2000$
-0.04
-0.06
-0.08
-0.1
-0.12
-0.14
-0.16
-0.18
-0.2
-0.22
-0.24
-0.26
0.1
0.2
0.3
0.4
0.5
0.6
$c_v(F)$
$|F|$
k=1
k=4
k=8
Analytic

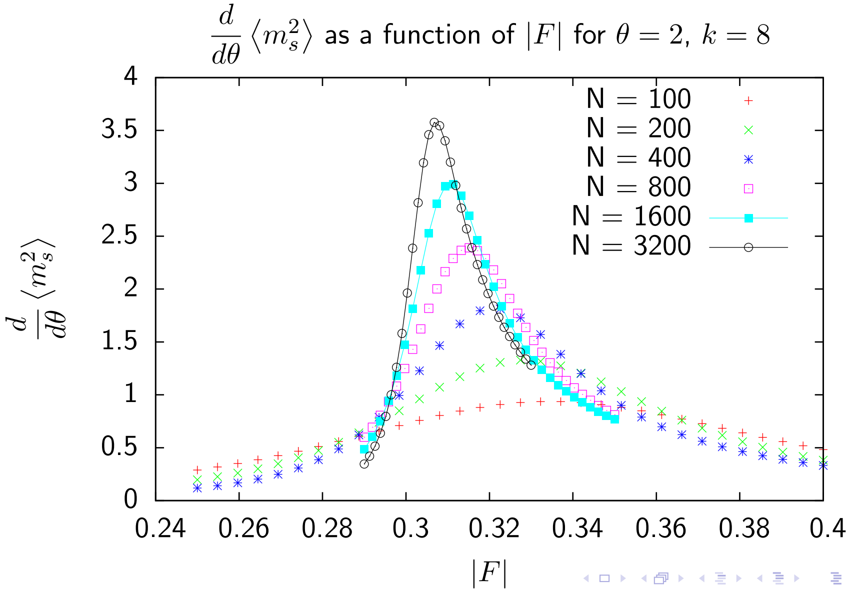
Results

- The agreement with the exact results both at $\theta = 0$ and $\theta = \pi$ suggests that the cumulant expansion can be trusted at all values of θ, as long as $|F| \lesssim 0.57$
- Now with the results for $\theta = 2$...

Results

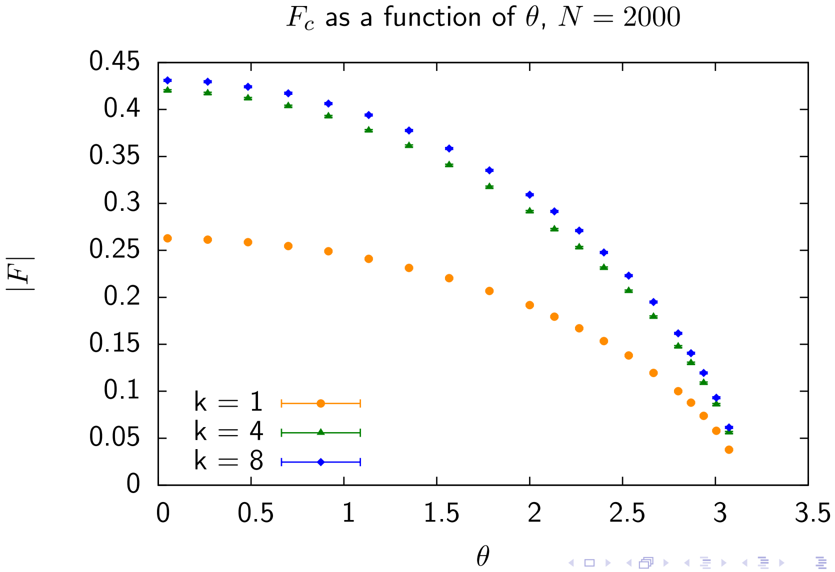


$\langle m_s^2 \rangle$ as a function of $|F|$ for $\theta = 2$, $k = 8$
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
$\langle m_s^2 \rangle$
0.28
0.29
0.3
0.31
0.32
0.33
0.34
0.35
0.36
$|F|$
N = 400
N = 800
N = 1600
N = 3200



$\frac{d}{d\theta}\langle m_s^2\rangle$ as a function of $|F|$ for $\theta = 2$, $k = 8$
N = 100
N = 200
N = 400
N = 800
N = 1600
N = 3200
$\frac{d}{d\theta}\langle m_s^2\rangle$
$|F|$
0
0.5
1
1.5
2
2.5
3
3.5
4
0.24
0.26
0.28
0.3
0.32
0.34
0.36
0.38
0.4

Results


F_c as a function of θ, $N = 2000$
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
0.5
1
1.5
2
2.5
3
3.5
$|F|$
θ
k = 1
k = 4
k = 8

Summary and conclusions

- We have analyzed the two-dimensional antiferromagnetic Ising model within an imaginary magnetic field by analytical techniques.
- By means of a reformulation of $\mathcal{Z}$ and a cumulant expansion to 8-th order in F, we have computed physical quantities for a large number of DOFs with the help of multiprecision algorithms.

- Comparisons with the analytical results at $\theta = 0, \pi$, give reliability to our results.
- The qualitative picture described in previous works, predicting the existence of two phases whith the staggered magnetization as an order parameter.
- This model could be a good laboratory to check proposals to simulate physical systems afflicted by a SSP.