# New algorithm for the computation of the partition function for the Ising model on a square lattice

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# 1 Introduction

- A calculation of the partition function $Z$ exactly in the thermodynamic limit $N \longrightarrow \infty$ is equivalent to knowledge of all equilibrium properties of a given system.

- Even for a finite system of $N$ spins our computational ability is limited by the number of the system configurations, which is $2^N$.

# 1.1 The Ising Model

- only two spin states are possible, say “up” and “down” ($S_i = \pm 1$)

$$E = -J \sum_{<ij>} S_i S_j - H \sum_i S_i$$

$$J_{ij} = \begin{cases} J_{ji} = J & \text{for NN} \\ 0 & \text{otherwise} \end{cases}$$

1D: $H = 0$ — $T_C^{1D} = 0$

2D: $H = 0$

$$T_C^{2D} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.2691 \; [J/k_B]$$

$$m(T) = \sqrt[8]{1 - \sinh^{-4}(2J/k_B T)}$$

3D: $H = 0$ — $T_C^{3D} \approx 4.5115 \; [J/k_B]$

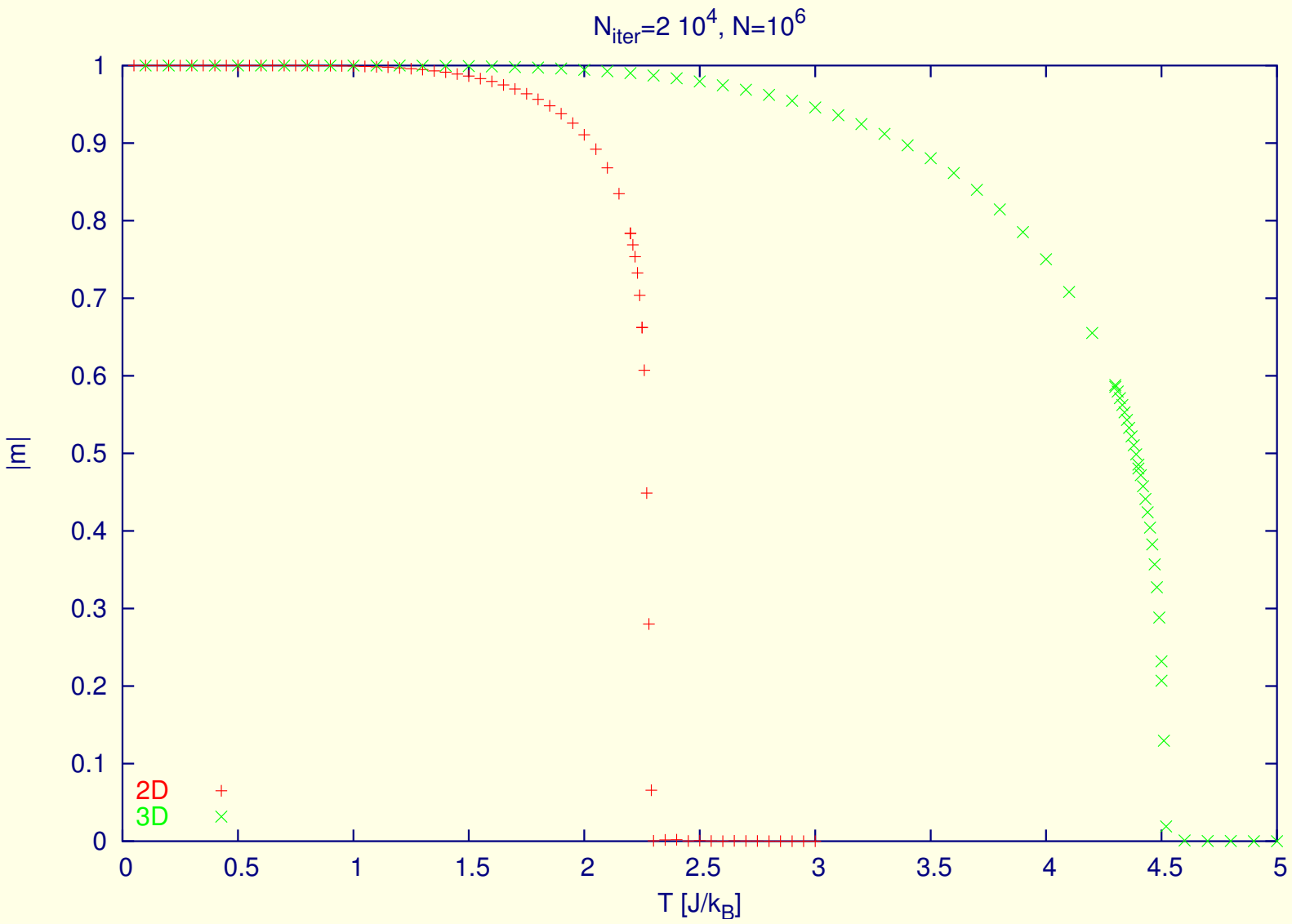
N_iter=2 10^4, N=10^6
|m|
T [J/k_B]
2D
3D
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

Figure 1: $m(T)$

## 1.2 The Energy $E$ of a Given Spin Configuration

$$E(n,k) = 2J(k - L^2 + L) - H(L^2 - 2n), \qquad (1)$$

- $n$ — # of spins pointing "up" (say $S_i = +1$)
- $k$ — # of anti-parallel bonds between the NN $(S_i S_j = -1)$
- $L$ — the linear size of the lattice.

## 1.3 The Partition Function

$$Z = \sum_{n,k} \Omega(n,k) \cdot \exp[-\beta E(n,k)] \qquad (2)$$

- $\Omega(n,k)$ — # of lattice configurations with given numbers $n$ and $k$
- $1/\beta = k_B T$
- $k_B$ is a Boltzmann constant
- and $T$ is temperature

Then, the average value of any quantity $A$ may be calculated as

$$\langle A \rangle = \frac{1}{Z} \sum_{n,k} A(n,k) \cdot \Omega(n,k) \cdot \exp[-\beta E(n,k)]. \quad (3)$$

The magnetic susceptibility per spin $\chi$ may be also expressed in the terms of $n$, $k$ and $L$:

$$\begin{aligned} \chi/N &= \beta\left(\langle S_i^2\rangle - \langle S_i\rangle^2\right) = \\ &= \beta\left(\langle (2n - L^2)^2\rangle - \langle 2n - L^2\rangle^2\right), \end{aligned} \tag{4}$$

where the index $k$ enters through the averaging procedure.

A computation of the partition function (2) requires an evaluation of the histogram $\Omega(n,k)$.

The CPU time $t$ [sec] necessary for investigation of $M$ different configurations of $8\times 8$ large 2D Ising lattice on SGI 2800 machine.

| $10^5$ | $10^6$ | $10^7$ | $10^8$ | $10^9$ | $10^{10}$ |
|---|---|---|---|---|---|
| 0.86 | 6.90 | 66.4 | 660 | 6648 | 65752 |

$$2^{64}\approx 10^{19}\rightarrow t=4.5\times 10^6 \text{ [years]!}$$

# 2 Calculations

## 2.1 The algorithm

$$\Omega_{4\times4}(n,k) + \Omega_{4\times4}(n,k) \longrightarrow \Omega_{8\times4}(n,k)$$

$$\Omega_{8\times4}(n,k) + \Omega_{8\times4}(n,k) \longrightarrow \Omega_{8\times8}(n,k)$$

or

$$4 \times \Omega_{4\times4}(n,k) \longrightarrow \Omega_{8\times8}(n,k)$$

$$\begin{array}{cccc} 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{array}$$

$$0011\ 0101\ 1001\ 0110_{\mathsf{bin}} = 13718_{\mathsf{dec}}$$

$$L = 4 \rightarrow \texttt{net} \in [-2^{15}, 2^{15})$$

$$
\begin{array}{cccc|cccc}
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\
\multicolumn{4}{c}{+} & & & & \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
\hline
0 & 1 & 1 & 0 & 1 & 1 & 1 & 0
\end{array}
$$

However, the procedure requires storing information on the $\Omega$ dependence not only on $n$ and $k$, but also on $b^r$ — the state of the $r$-sites-long lattice border.

$$\begin{array}{cccccccc} 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \end{array}$$

$$0 \leq b^8 \leq 255$$

$$\begin{array}{cccc} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{array}$$

$$0110\ 0011\ 0101\ 1001$$

$$0 \leq b^7 \leq 127$$

$$\Omega_{8\times 4}(b^8, n_1+n_2, k_1+k_2+k') =$$

$$= \sum_{\substack{b_1^7, n_1, k_1 \\ b_2^7, n_2, k_2}} \Omega_{4\times 4}(b_1^7, n_1, k_1)\cdot \Omega_{4\times 4}(b_2^7, n_2, k_2), \quad (5)$$

where $0 \le k' \le 4$ is the additional number of anti-parallel bonds and $b^8$ is combined from $b_1^7$ and $b_2^7$.

$$\Omega_{8\times 8}(n_1+n_2, k_1+k_2+k'') =$$

$$= \sum_{\substack{b_1^8, n_1, k_1 \\ b_2^8, n_2, k_2}} \Omega_{8\times 4}(b_1^8, n_1, k_1) \cdot \Omega_{8\times 4}(b_2^8, n_2, k_2), \quad (6)$$

and again $0 \leq k'' \leq 8$ is the number of additional anti-parallel bonds.

## 2.2 The implementation

```
  n=n+IAND(ISHFT(net,-i),1)
  k=k+IEOR(IAND(ISHFT(net,-i+1),1),
&          IAND(ISHFT(net,-i),1))
  k=k+IEOR(IAND(ISHFT(net,-i+L),1),
&          IAND(ISHFT(net,-i),1))
```

1001 1010 1100 0110

```
  iborder_7=IAND(net,15)
& +16*IAND(ISHFT(net,-7),1)
& +32*IAND(ISHFT(net,-11),1)
& +64*IAND(ISHFT(net,-15),1)
```

$$15_{\text{dec}} = 1111_{\text{bin}}$$

```
iborder_4_1=IAND(iborder_7_1,15)
iborder_4_2=IAND(iborder_7_2,15)
link=IEOR(iborder_4_1,iborder_4_2)
kk=0
DO i=0,3
  kk=kk+IAND(ISHFT(link,-i),1)
ENDDO
```

```
   iborder_8
& =ISHFT(IAND(iborder_7_1,120),-3)
& +ISHFT(IAND(iborder_7_2,120),+1)
```

$$120_{\text{dec}} = 1111000_{\text{bin}}$$

$$15_{\text{dec}} = 0001111_{\text{bin}}$$

```
DO iborder_8_1=0,255
DO n_1=0,2*L*L
DO k_1=0,4*L*L+4
DO iborder_8_2=0,255
link=IEOR(iborder_8_1,iborder_8_2)
kk=0
  DO i=0,7
  kk=kk+IAND(ISHFT(link,-i),1)
  ENDDO
```

```
  DO n_2=0,2*L*L
  DO k_2=0,4*L*L+4
  omega_8x8(n_1+n_2,k_1+k_2+kk)=
& omega_8x8(n_1+n_2,k_1+k_2+kk)+
& 1.0q0*omega_8x4(iborder_8_1,n_1,k_1)
&       *omega_8x4(iborder_8_2,n_2,k_2)
  ENDDO
  ...
  ENDDO
```

- This procedure on SGI 2800 machine takes only 22 hours of the machine time instead of a few million years in case of the usage of the traditional/direct method.
- Successive merging may be repeated recursively to obtain the partition function for larger lattices.

## 2.3 Monte Carlo simulation

- Standard Monte Carlo Metropolis algorithm is applied to determine the magnetic spin susceptibility of a $1000 \times 1000$ Ising lattice.
- After getting equilibrium, each point of the plot is obtained as the time average over a thousand of time steps.

## 2.4 Mean field approach

For two sublattices $\alpha$ and $\gamma$:

$$\begin{cases} m_\alpha = & \tanh\left(\beta(Jm_\gamma + H)\right) \\ m_\gamma = & \tanh\left(\beta(Jm_\alpha + H)\right) \end{cases} \tag{7}$$

where $J < 0$

$T_C = -J/k_B$

$\chi = (m_\alpha + m_\gamma)/H$ for $H \to 0$.

## 2.5 Experimental data

- The experimental data are collected from Ref. [2]. They concern two-dimensional Ising antiferromagnets $Rb_2CoF_4$ and $K_2CoF_4$ where $S = \pm 1$.

- The Van Vleck susceptibility is subtracted to obtain a pure spin contribution.

# 3 Results

- $\Omega_{8\times 8}(n,k)$
- $\chi(T)$ for $J < 0$

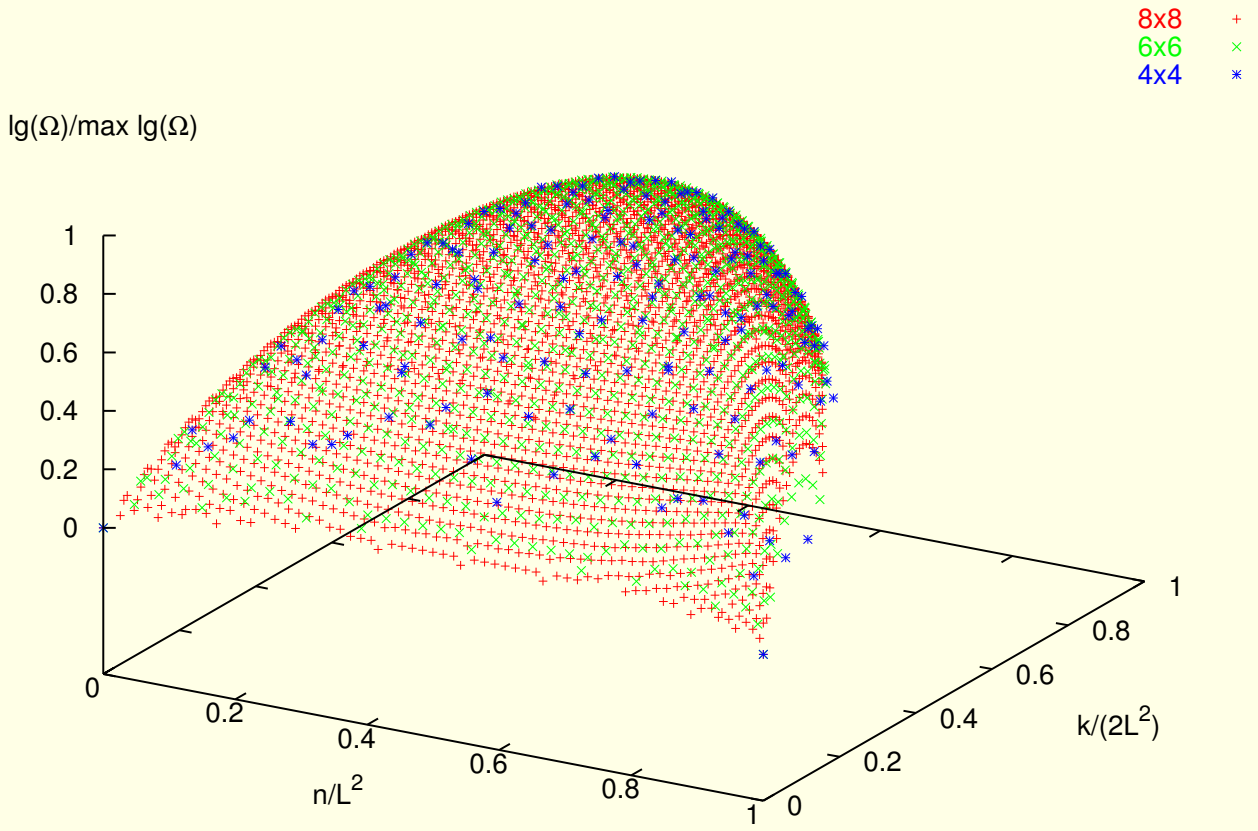


Figure 2: $\Omega_{4\times4}(n,k)$, $\Omega_{6\times6}(n,k)$, $\Omega_{8\times8}(n,k)$

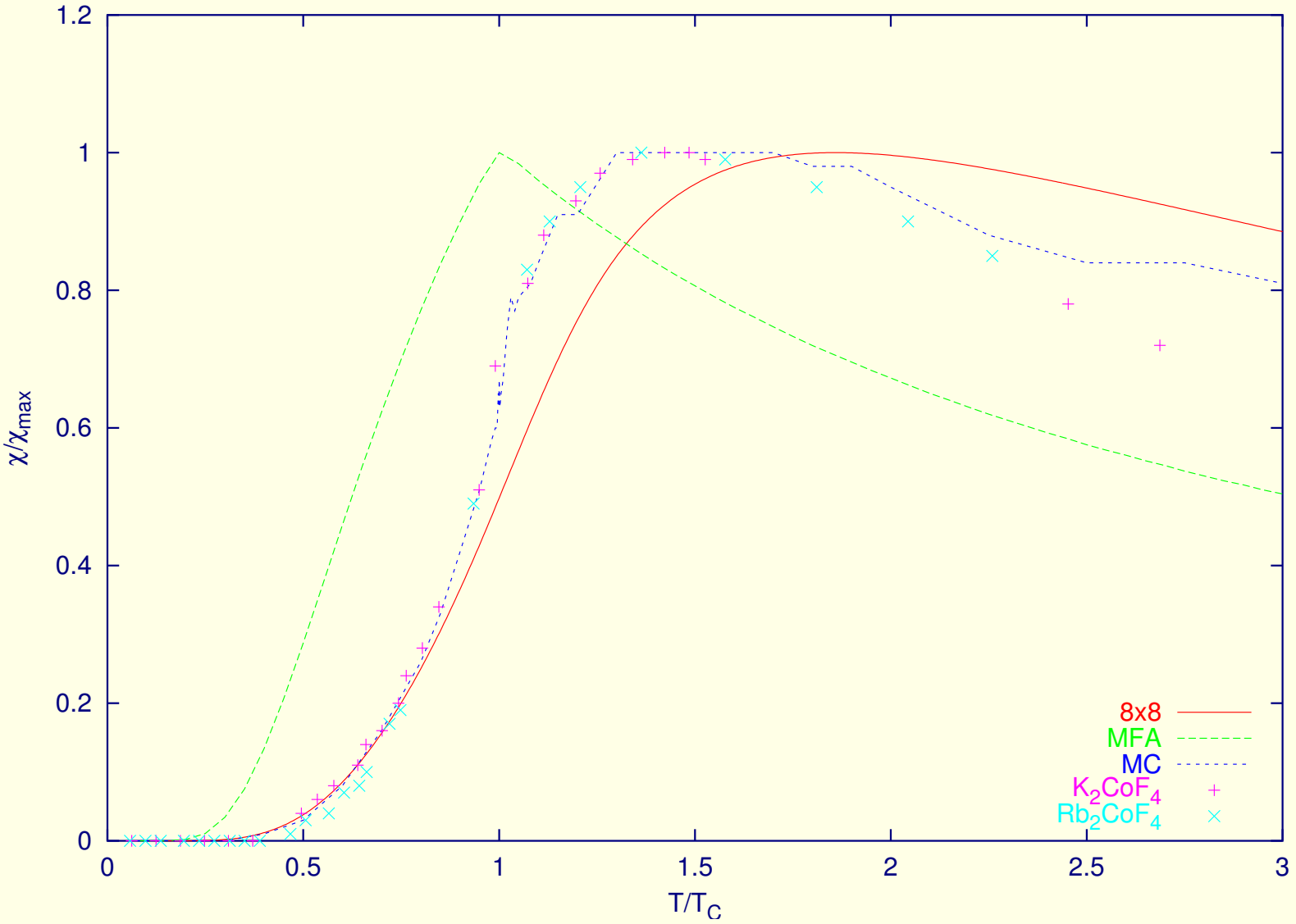


Figure 3: $\chi(T)$

# 4 Conclusions

- The function $\Omega(n,k)$, once known, can be easily used for the calculation of all equilibrium thermodynamic properties, for ferro- and antiferromagnets, various values of temperature and magnetic field.
- The summation over $n$ and $k$ is much faster, than the summation over $2^{64}$ spin configurations.

- As for our knowledge, the partition function has never been calculated exactly for the lattice as large as $8 \times 8$.
- In principle, the algorithm can be applied to larger lattices, with a cost of more time and memory.
- The computational mountain remains infinite, but its slope is a little bit reduced.

# References


[1] K.Malarz et al, Int. J. Mod. Phys. **C13** (2003) 689.

[2] D.J.Breed, K.Gilijamse and A.R.Miedema, Physica **45** (1969) 205.

[3] `http://www.zis.agh.edu.pl/omega/`

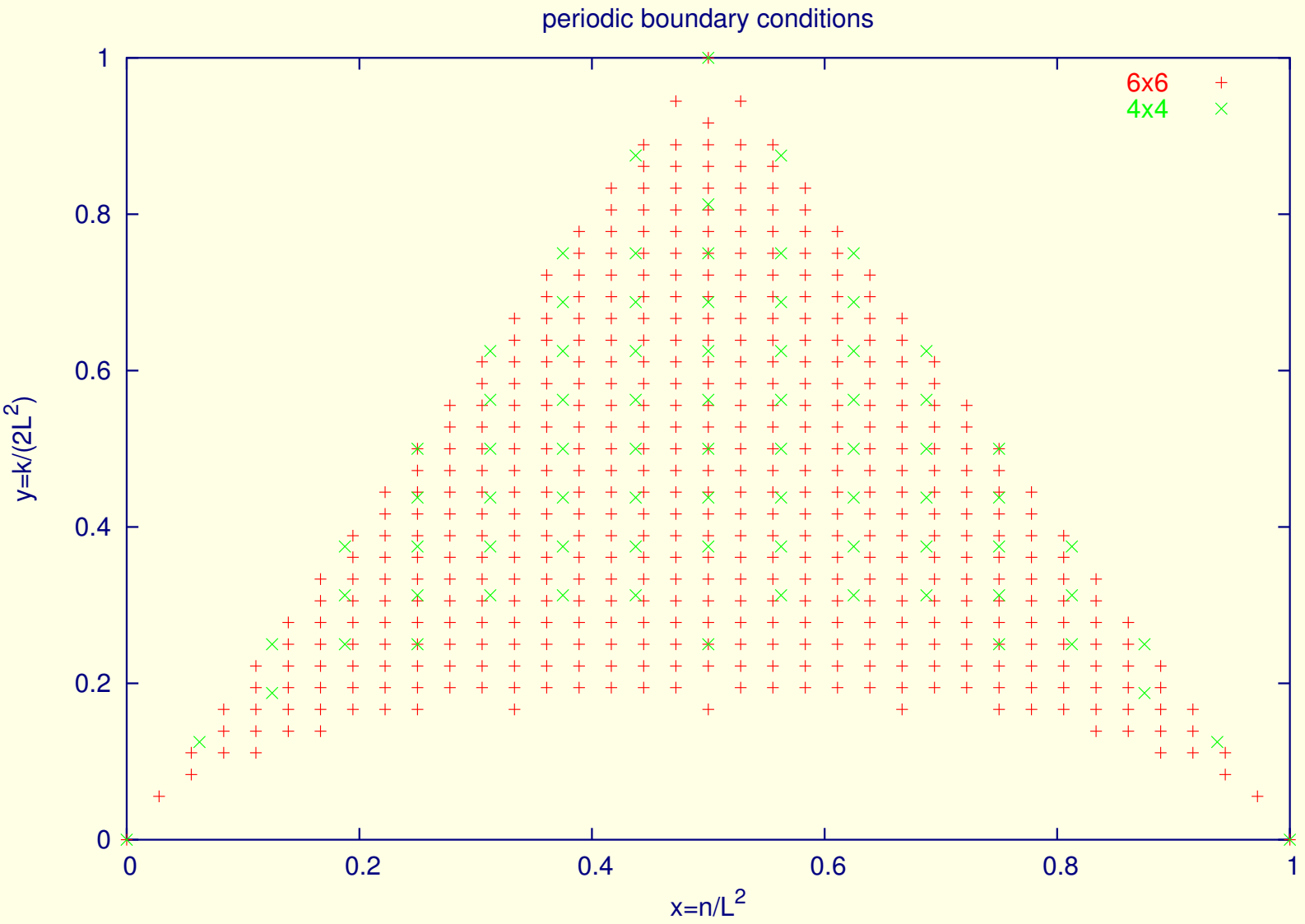


Figure 4: $\Omega_{4\times4}(n,k)$, $\Omega_{6\times6}(n,k)$

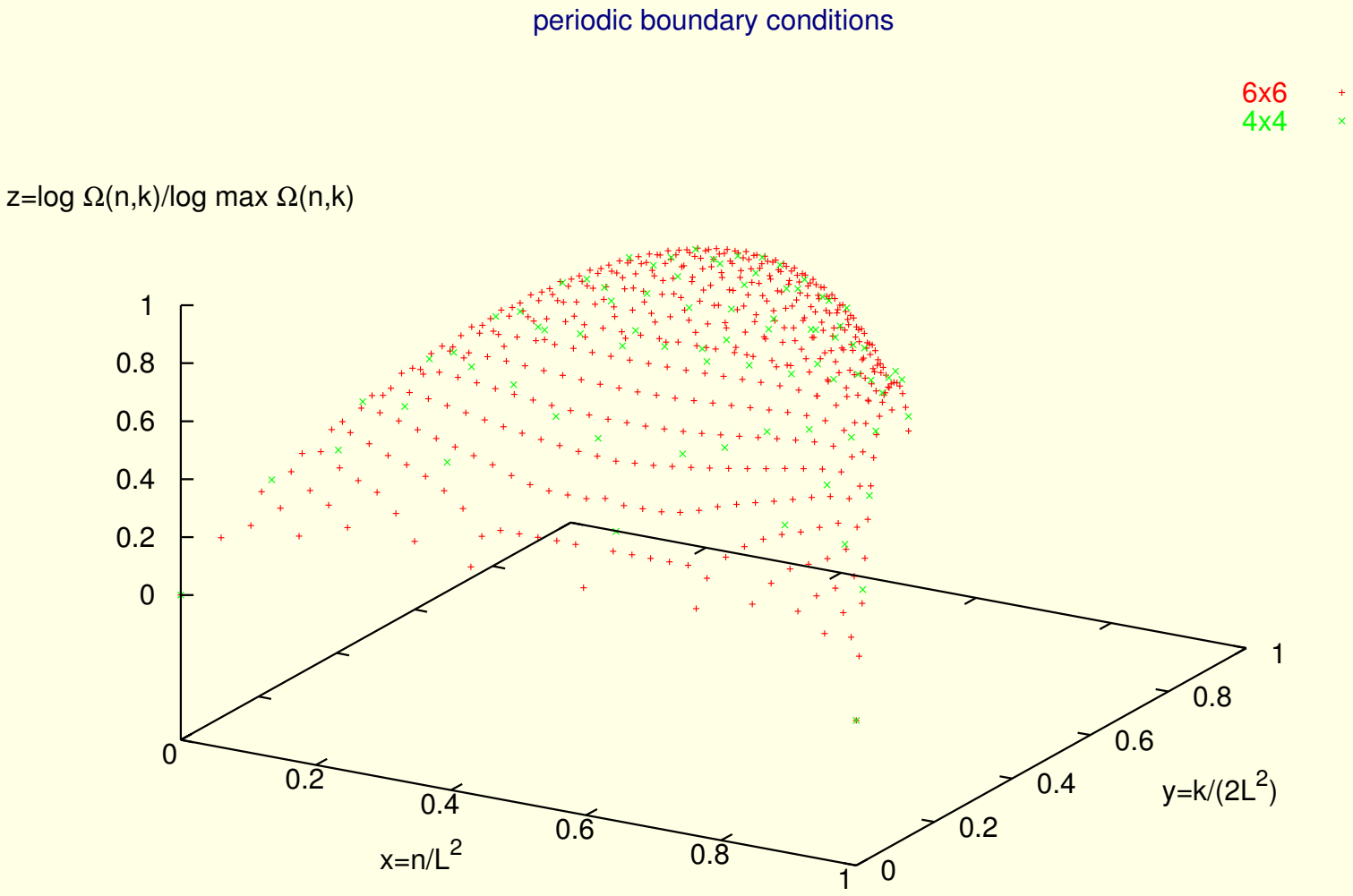


Figure 5: $\Omega_{4\times4}(n,k)$, $\Omega_{6\times6}(n,k)$