Susceptibility computation for Ising model for 1D and 2D

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This is short theoretical explanation of the test: **IsingTestChi1D.h** and **IsingTestChi2D.h**.

1 Theory

Magnetic susceptibility (χ) is defined by the relationship:

$$\chi = \frac{\partial M}{\partial h},$$

where M is magnetization of the system

$$M = \sum_i s_i$$

and h is magnetic field strength. We focus on calculating the magnetic susceptibility at zero magnetic field:

$$\chi_0 = \frac{\partial M}{\partial h}|_{h=0},$$

calculated per one site.

For the system of spins s_i in external magnetic field h, the Hamiltonian is:

$$\hat{H} = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i,$$

where $\beta = 1/(k_B T)$, J is interaction energy between the adjacent spins and the first sum runs over pairs of neighboring sites s_i.

We can calculate χ_0 as:

$$\chi_0 = \frac{\partial \langle M \rangle}{\partial h}.$$

Here the value of magnetization is averaged over the configurations $\{s\}$ of spins:

$$\langle M\rangle = \frac{1}{Z}\sum_{\{s\}} M \exp(\beta J \sum_{\langle i,j\rangle} s_i s_j + \beta h \sum_i s_i), \tag{1}$$

where

$$Z = \sum_{\{s\}} \exp(\beta J \sum_{\langle i,j\rangle} s_i s_j + \beta h \sum_i s_i).$$

To obtain a formula useful for the numerical calculation of χ_0, let us take the derivative of the (1) with respect to h.

$$\frac{\partial \langle M\rangle}{\partial h} = \frac{\beta}{Z}\sum_{\{s\}} M^2 \exp(-\beta \hat{H}) + \frac{\beta}{Z^2}\left[\sum_{\{s\}} M \exp(-\beta \hat{H})\right]^2 = \beta\left(\left\langle M^2\right\rangle - \langle M\rangle^2\right).$$

In zero field:

$$\chi_0 = \beta\left(\left\langle M^2\right\rangle|_{h=0} - \langle M\rangle^2|_{h=0}\right).$$

This formula allows for calculation of the χ_0 in the Monte Carlo simulation of Ising model.

For comparison of the numerical results with the theoretical values of the magnetization, let us consider the behavior of χ_0 in function of the temperature. In one dimension, for a chain of Nspins the analytical formula is:

$$\chi_0 = \frac{\beta}{N}\exp\left(2\beta J\right). \tag{2}$$

For 2D square lattice of N spins we don't have the exact formula for the susceptibility, but we know the behavior in the critical temperature:

$$\chi \sim |t|^{-\gamma},$$

where $t = \frac{T-T_c}{T_c}$, T_c being the critical temperature, and γ is the critical exponent. For an infinite 2D lattice their values are:

$$T_c = 2.269,\ \gamma = 7/4.$$

It means that for the critical temperature the magnetic susceptibility diverges at $T = T_c$. For finite lattice the critical temperature is slightly different and the susceptibility is finite.

2 Results for 1D chain

The appropriate test class has name: IsingTestChi1D.

We performed the calculations of $\chi_0$versus the temperature for a chain of $N = 500$ spins with 10000 Monte Carlo cycles for each T. We compared the results with the analytical solution. The dependence is shown in the figure (2).

For high temperatures we find a good agreement with the analytical solution. However, for low temperatures there is a significant difference between the numerical and analytical results. We attribute this behavior to the low acceptance ratio of Metropolis algorithm, which lowers the number of configurations used in the averaging.

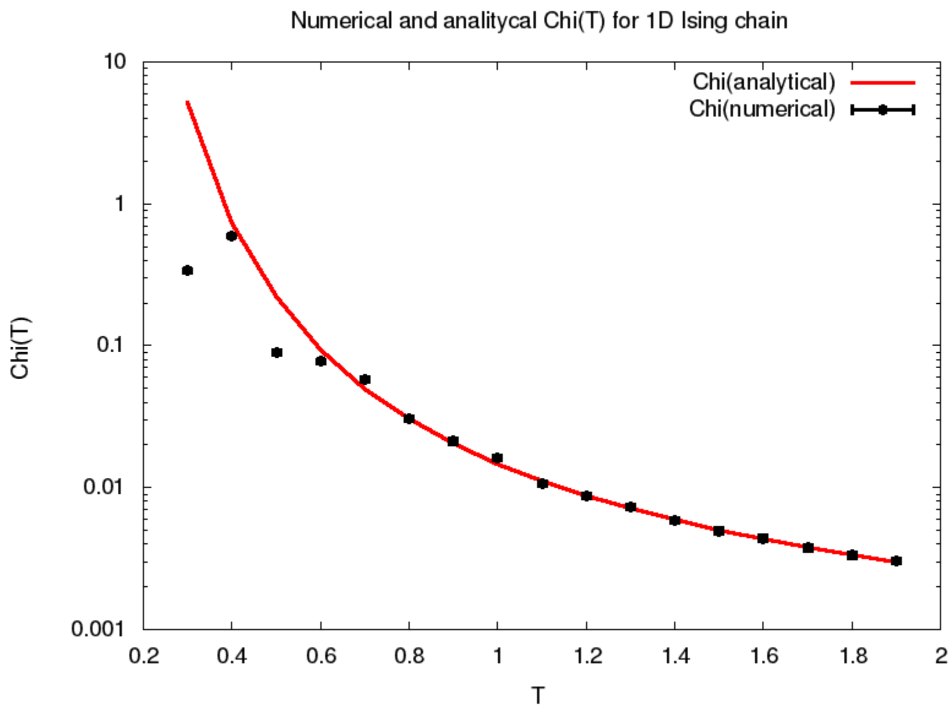

Figure 1: The numerical and analytical results for susceptibility versus the temperature. The plot is generated by the IsingTestChi1D class.

Also, we performed the calculations of the magnetic susceptibility versus the number of spins at $T = 1$ K. According to (2), χ_0 is proportional to inverse N. Results are shown on Fig. 2. We find a good agreement with the analytical solution.

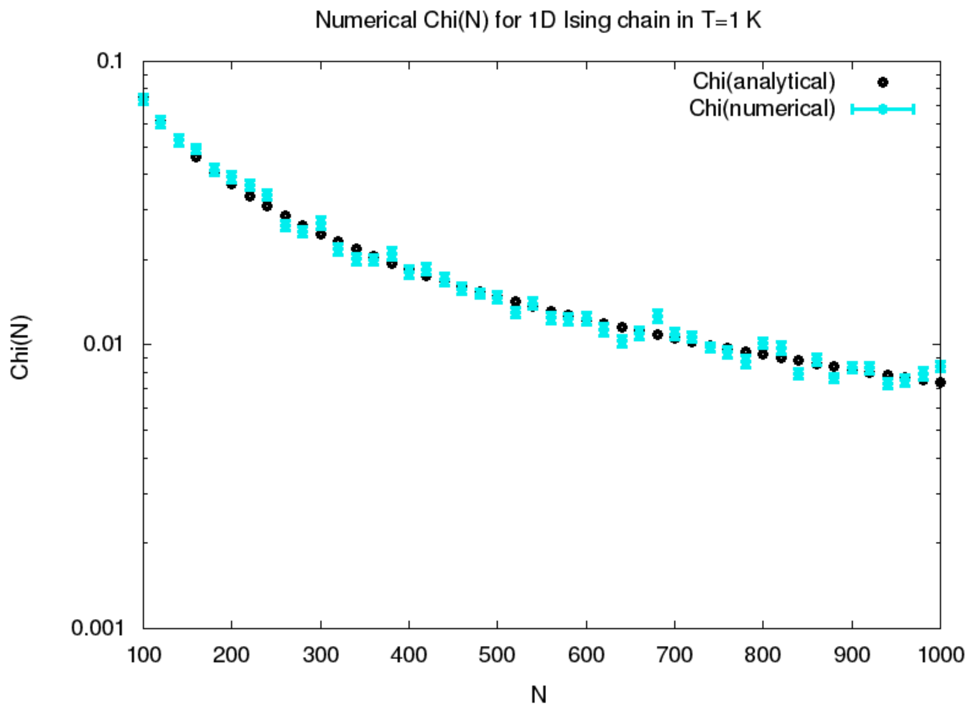

Figure 2: The numerical and analytical results for susceptibility versus the size of chain.

3 Results for 2D lattice

The appropriate test class has name: IsingTestChi2D.

We computed the susceptibility versus temperature for a square lattice consisting of 100 spins. The results are shown in figure 3. For each T we did 100000 cycles for Metropolis and 1000 Wolff cycles.

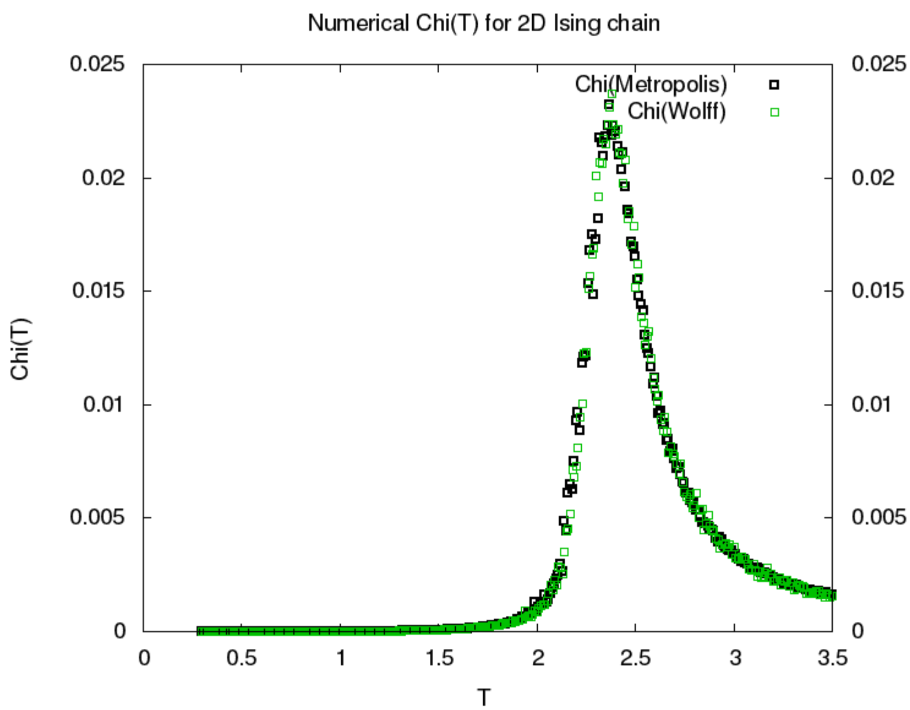

Figure 3: Results for susceptibility versus the temperature. Green points show the result for Wolff algorithm.