Exact computation for Ising model for 1D and 2D

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This is short theoretical explanation of the test: **IsingTestExact1D.h** and **IsingTestExact2D.h**.

1 Combinatorial approach

We calculate exact solution of specific heat by finding the exact value of the partition function

$$Z(\beta) \quad = \sum_{\{\text{all configurations } \sigma_i\}} e^{-\beta E(\sigma_1, \sigma_2, \ldots, \sigma_n)}.$$

To do that we have to evaluate all possible configurations of spins. For given number n of spins on the lattice we have 2^n configurations. For example for two spins chain we have

$$\{\uparrow\uparrow, \downarrow\uparrow, \uparrow\downarrow, \downarrow\downarrow\} \quad .$$

Note that some of those configurations may have the same energy E, thus Z function can be written in a bit different way

$$Z(\beta) = \sum_{E_i} N(E_i) e^{-\beta E_i}, \tag{1}$$

where the sum runs over all possible energies E_i, and $N(E_i)$ is density of states: number of states with the same energy E_i.

To generate $N(E)$ we have to calculate E for all configurations of spins. In order to do that we use Gray code enumeration of spins (the description of the algorithm can be found e.g. in textbook: *Statistical Mechanics Algorithms and Computations*, Werner Krauth). The pseudo-code of the algorithm is following: **wyjasnienie kodu graya**

procedure `gray-flip`
input $\{\tau_0, \ldots, \tau_N\}$
$k \leftarrow \tau_0$
if $(k > N)$ **exit**
$\tau_{k-1} \leftarrow \tau_k$
$\tau_k \leftarrow k + 1$
if $(k \neq 1)$ $\tau_0 \leftarrow 1$
output $k, \{\tau_0, \ldots, \tau_N\}$
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Figure 1: Gray code for spins $\{1, ..., N\}$. The procedure returns k which is the index of next spin to flip. τ is an auxiliary vector used by the procedure. The initial value of $\tau_i = i$. Look in the code to see how to use it in practice.

Having the $N(E)$ allows us to calculate all properties of the system from (1). As an example we calculated plots of specific heat C_V in function of temperature T. The specific heat is given by expression

$$C_V = \frac{\partial \langle E \rangle}{\partial T},$$

where $\langle E \rangle = -\frac{\partial \log(Z)}{\partial \beta} = T^2 \frac{\partial \log(Z)}{\partial T}$. Thus we have

$$C_V = 2T \frac{\partial \log(Z)}{\partial T} + T^2 \frac{\partial^2 \log(Z)}{\partial T^2}.$$

For simplicity we calculate C_V using numerical differentiation using the finite difference method, which leads to following approximation

$$\begin{aligned} C_V \quad (T) \approx & \quad 2T \left(\frac{\log\left(Z(T + \Delta T)\right) - \log\left(Z(T - \Delta T)\right)}{2\Delta T} \right) \\ + & \quad T^2 \left(\frac{\log\left(Z(T + \Delta T)\right) + \log\left(Z(T - \Delta T)\right) - 2\log\left(Z(T)\right)}{\Delta T^2} \right). \end{aligned}$$

We choose small value of $\Delta T = 0.01$ (here we consider only small lattices, this guarantee that the value of ΔT is small enough to provide good approximation of derivatives even near the critical point) which should give us accurate approximation of C_V.

Note that this approach gives us exact solution to 2D Ising model, but it is limited to very small lattice sizes. The bottleneck of the algorithm is the part where we calculate $N(E)$ using Gray code. This is because we have to run over 2^n states which for lattice of size 6×6 gives $2^{36} = 68\,719\,476\,736$ number of possible configurations.

2 Results for 1D chain

The appropriate test class has name: **IsingTestExact1D**.

We calculate specific heat for three different chain lengths: N=**2, 7** and **22**. We also compared this with analytical one. For 1D the partition function is given by following equation

$$Z\left(T\right) = \left(2\cosh(\beta J)\right)^N \cdot \left(1 + \tanh(\beta J)^N\right),$$

from this we can calculate C_V per spin

$$C_V^{\text{spin}}(T) = \frac{T}{N} \frac{\partial^2 T \log\left(Z\left(T\right)\right)}{\partial T^2}. \tag{2}$$

The numerical approximation of derivative above can be found in function **exacCv()**.

The results for exact solution (Combinatorial approach) and analytical solution (2) are shown in the picture below.

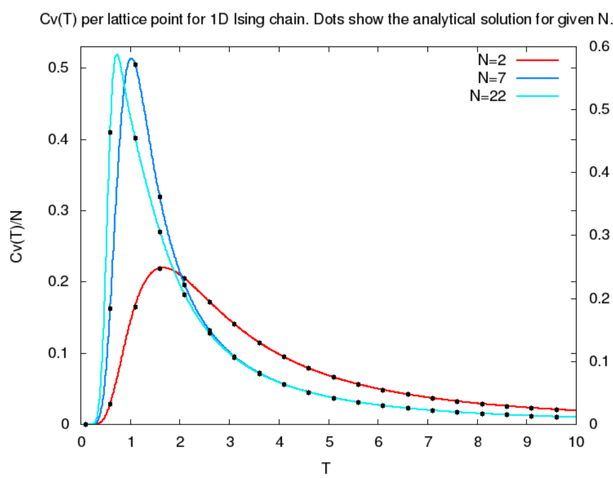

Figure 2: Specific heat for 1D Ising chain for N=2, 7 and 22. The plot is generated by IsingTestExact1D class.

From the picture above we see that for large temperatures ($T \to +\infty$) C_V tends to zero. We have the same behavior for $T \to 0$.

3 Results for 2D chain

The appropriate test class has name: **IsingTestExact2D**.

The analytical solution for 2D lattice exist but is more complicated thus we plot only the results from the combinatorial method. This method allowed us to calculate lattices up to 5x5. The results are presented below.

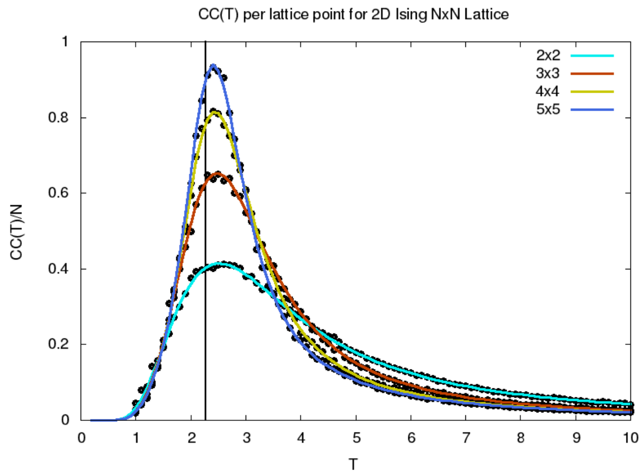

Figure 3: Specific heat for 2D Ising lattice for four different lattices size. The black dots show the results obtained from MC simulation by Wolff algorithm (for 5000 MC cycles). The plot is generated by IsingTestExact2D class. Vertical line shows the exact value of critical temperature T_C.

From figure above we see that the phase transition for small lattices occurs near the critical temperature T_C obtained from exact Onsager calculations. For 2D lattice we have the same asymptotic behavior ($T \to 0$ and $T \to +\infty$) like it was in case of 1D chain.

The numerical values of C_V from picture above can be reproduced by test: **IsingTestCC2D.h**.