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Homework 2

1 Exact enumeration of Partition Functions

1.1 Derivation

For two spins our partition function will have in total four states, two spins up, two spins down and two states with one spin up and one down. The partition function Z_2 is given then by

$$Z_2 = 2e^{\beta J} + 2e^{-\beta J} = 4cosh(\beta J)$$

For N spins we can write the following relation for a chain of spins with free boundary conditions

$$Z_N = \sum_{s_1=\pm1} \cdots \sum_{s_N=\pm1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}}$$

showing that we have 2^N microstates for N spins.
To show how our ennumeration will work though, we should have a look at a simple chain, for example of three spins

$$Z_3 = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} e^{\beta J s_1 s_2 + \beta J s_2 s_3}$$

We can take the sum over s_3 independently of s_1 and s_2 and get

$$Z_3 = \sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2} \left[e^{\beta J s_2} + e^{-\beta J s_2} \right] = \sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2} 2cosh(\beta J s_2)$$

We can see that since $cosh$ is an even function, we can ignore the dependence of s_2's sign in $cosh(\beta J s_2)$, thus giving us

$$Z_3 = 2 \sum_{s_1=\pm1} \sum_{s_2=\pm1} e^{\beta J s_1 s_2} cosh(\beta J)$$

In the case of the s_1 and s_2 summation though, we will not ignore the dependence of s_1, since it's the only time we use it in the boundary conditions, thus the end result being

$$Z_3 = 2 \sum_{s_1=\pm1} \left(e^{\beta J s_1} + e^{-\beta J s_1} \right) cosh(\beta J) = 2(2e^{\beta J} + 2e^{-\beta J}) cosh(\beta J) = 2(2cosh(\beta J))^2$$

Thus our enumeration technique will involve taking a sum of $e^1 + e^{-1}$ for all spins and multiplying it by two, so our algorithm will be

$$2(e^{\beta J} + e^{-\beta J})^{N-1}$$

1.2 The Code and Results

I decided to go with a *for* loop instead of nested *do* loops just to save some writing, but the idea is identical. Since all loops would be the same, even after the proposed changes in the problem (for the temperature and magnetic field), it's not really worth it to write them down separately.
As a slight optimisation, the exponents could be calculated outside of the loop, instead of every time it runs, but this won't really affect anything in our case.

```
using System.Collections;
using System;
using System.Linq;

public class ExactIsingModel {

        // NOTE: The strength of interaction J and beta =
          ↪ 1/(kT) are defaulted to 1
        double[] partitionFunctionElements;

        public double partitionFunctionEnumeration(int n)
        {
                partitionFunctionElements = new double[n
                  ↪ - 1];

                for (int i = 0; i < n - 1; i++)
                {
                        partitionFunctionElements [i] =
                          ↪ Math.Exp (1) + Math.Exp
                          ↪ (-1);
                }

                return 2 * partitionFunctionElements.
                  ↪ Aggregate (1d, (a, b) => a * b);

        }

        public double partitionFunctionAnalytic(int n)
        {
                return 2 * Math.Pow (2 * Math.Cosh (1), n
                  ↪ - 1);
        }
```

The results for different N, as would be expected, agree with each other, no matter the method used:

N	Enumeration	Analytical	By Hand
5	181.428	181.428	181.428
10	50792.261	50792.261	-
15	14219706.400	14219706.400	-
20	3980922408.725	3980922408.725	-

As for the proposed changes, to include the temperature all we have to do is include a variable in the exponents, so that they include βJ, and then we can run it for different temperatures.
To include different magnetic fields, we need to refactor our partition function into periodic boundary conditions, and build a matrix of the type

$$P = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}$$

and bring it to a power N by using our loops to multiply it to itself N times. Then we take the trace of it, and that would give us the partition function for the Ising Model in 1D with magnetic field under periodic boundary conditions.

2 Finite-size corrections for the 1D Ising Model

As was discussed in Homework 1, the free boundary conditions introduce sizable finite-size effects, which only completely disappear at the thermodynamic limit $N \to \infty$. Here we endeavour to put some perspective on the effects, using the free energy per spin as our guide.

2.1 Derivation of finite-size corrections

The free energy per spin for the 1D Ising Model without a magnetic field at the thermodynamic limit $N \longrightarrow \infty$ is given by

$$\beta f_\infty = \lim_{N\to\infty} \frac{1}{N} \ln Z = \ln 2 + \ln\cosh(\beta J)$$

The partition functions under for the same model under free and periodic boundary conditions are respectively

$$Z_{free} = 2(2\cosh(\beta J))^{N-1}$$
$$Z_{per} = (2\cosh(\beta J))^N + (2\sinh(\beta J))^N = \left(2\cosh(\beta J)^N\right)\left[1 + (\tanh(\beta J))^N\right]$$

giving us the following expressions for the free energy per spin

$$\beta f_{free} = \frac{1}{N}\ln Z_{free} = \ln 2 + \frac{1}{N}\left[(N-1)\ln\cosh(\beta J)\right]$$

$$\beta f_{per} = \frac{1}{N}\ln Z_{per} = \ln 2 + \ln\cosh(\beta J) + \frac{1}{N}\ln\left[1 + (\tanh(\beta J))^N\right]$$

The finite-size correction $\beta f_N - \beta f_\infty$ then reads

$$\beta f_{free} - \beta f_\infty = -\frac{1}{N}\ln\cosh(\beta J)$$
$$\beta f_{per} - \beta f_\infty = \frac{1}{N}\ln\left[1 + (\tanh(\beta J))^N\right]$$

2.2 Linear plots of the finite-size corrections

As a disclaimer the values of the free boundary condition corrections are forced to their absolute values, to make the visual comparison between the free and periodic boundary conditions easier.

First is the comparison between the free and periodic boundary conditions with $\beta = 1$. In this case the difference is visible, but hardly critical, and the periodic boundary conditions take a slight edge over the free ones at $N > 2$.

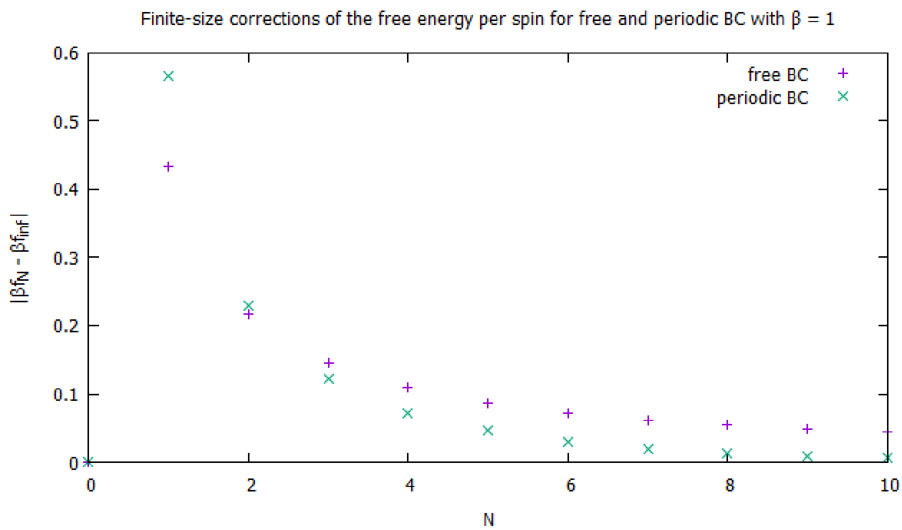

Figure 1: Free boundary conditions vs periodic boundary conditions for $\beta = 1$

Next we compare the same boundary conditions with $\beta = 10$. Here the superiority of the periodic boundary conditions is clearly visible over all Ns.

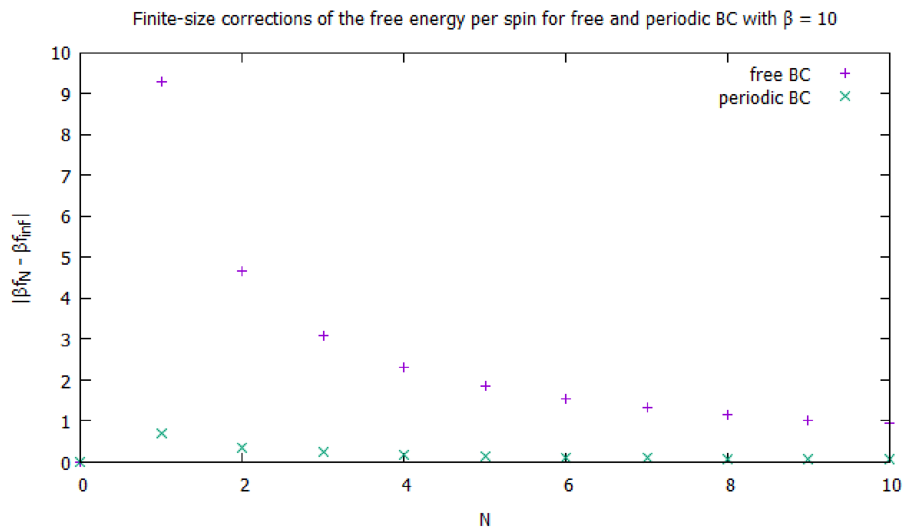

Figure 2: Free boundary conditions vs periodic boundary conditions for $\beta = 10$

In fact the periodic boundary conditions for $\beta = 10$ deserve a plot of their own, so we can see the values of the correction more clearly:

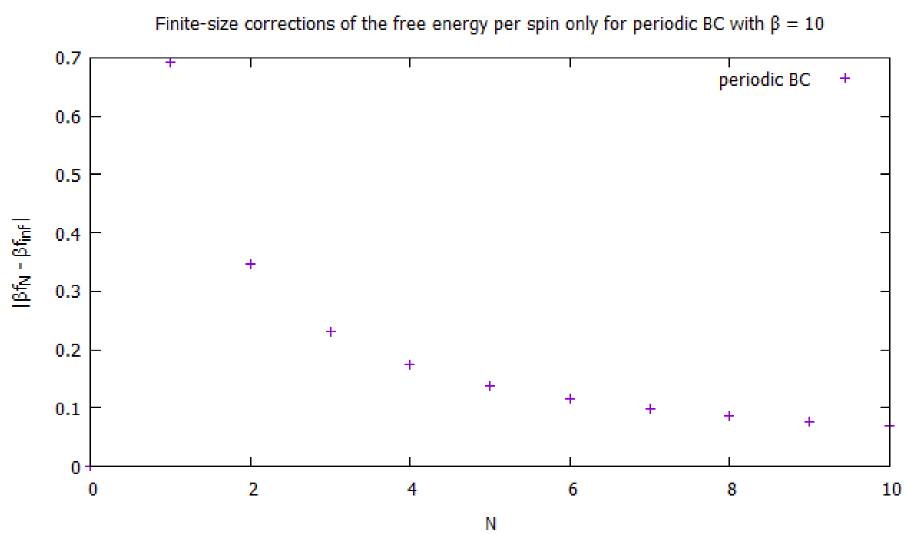

Figure 3: Periodic boundary conditions for $\beta = 10$

2.3 Logarithmic plots of the finite-size corrections

To see more clearly the rate of change of the correction as N increases, we will use logarithmic scale for $\delta\beta f$ and check again for $\beta = 1$ and $\beta = 10$

First we compare the results for $\beta = 1$. We see that the correction in the case of the periodic boundary conditions continues to decrease at a steady exponential rate as N increases. Meanwhile the correction for free boundary conditions slows down considerably.

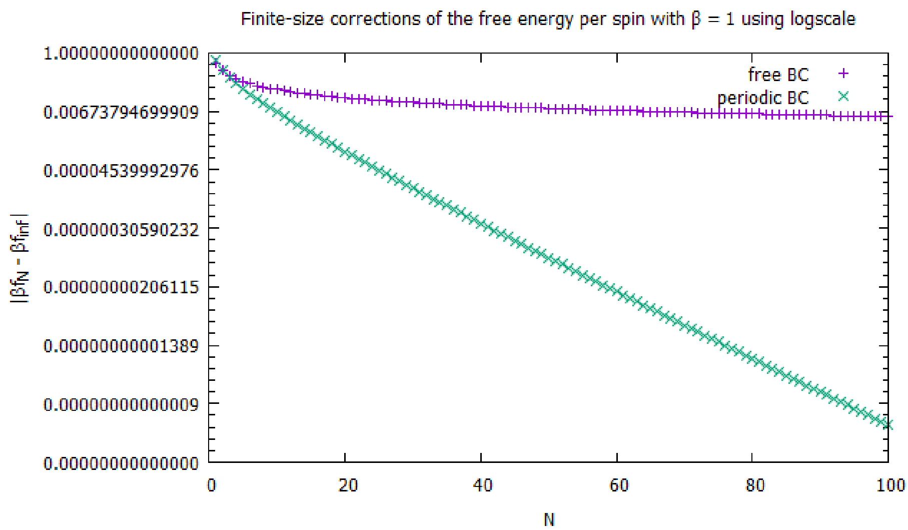

Figure 4: Free boundary conditions vs periodic boundary conditions for $\beta = 1$ with logscale

Now we look at the results for $\beta = 10$. We see that, even though the absolute value of the correction for free boundary conditions is significantly bigger than that for periodic boundary conditions, both values decrease at a very similar rate. The rate of decrease under periodic boundary conditions is no longer exponential.

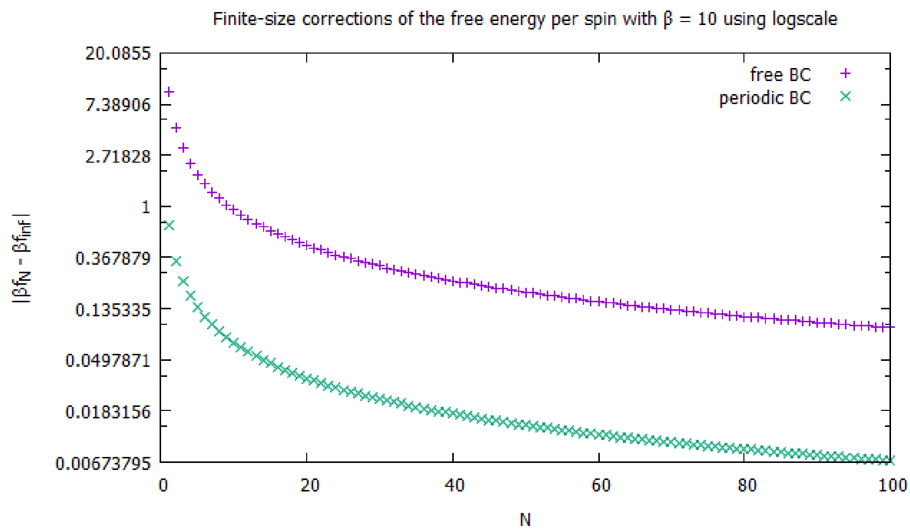

Figure 5: Free boundary conditions vs periodic boundary conditions for $\beta = 10$ with logscale

In fact we can compare the rates of decrease of the correction for periodic boundary conditions with the two different βs, to show that the decrease of the correction for $\beta = 10$ for periodic boundary conditions is very similar to that under free boundary conditions, and much slower than the exponential decrease of the correction under periodic boundary conditions for $\beta = 1$.

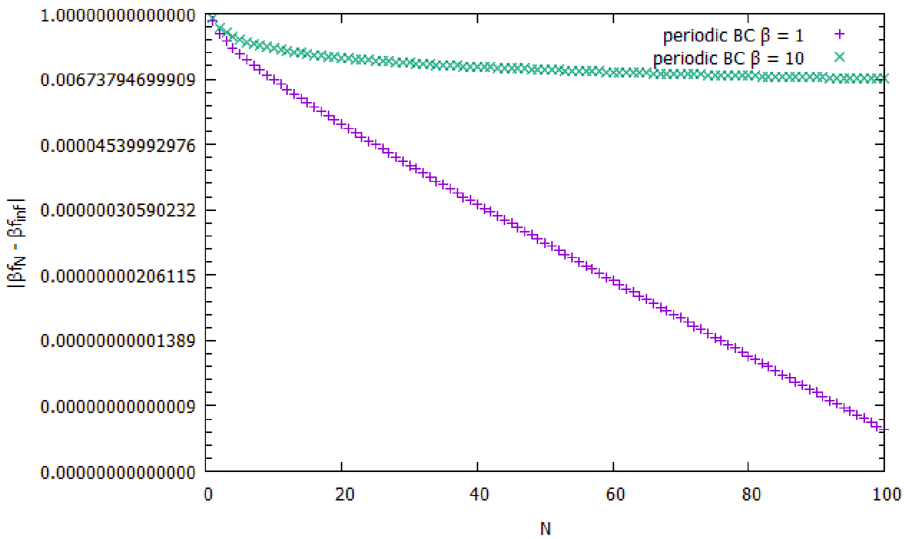

Figure 6: Periodic boundary conditions for $\beta = 1$ and $\beta = 10$ with logscale