Kiril Panayotov Blagoev 3753135
Homework 1

1 1. Exact solution to the 1D Ising Model

The 1D Ising Model has analytic solutions, and they can be derived for several different cases, such as the Non-Interacting case, the Zero-field case, and so on. As it wasn't specified in the problem sheet which one should be approached, here two of them will be tackled - the Zero-field case and the General case.

1.1 Zero-field case

To find any physical properties inside an Ising Model, all we need is the partition function Z. In the case of zero magnetic field, the Hamiltonian is

$$H(\{s_i\}) = -J \sum_{<i,j>} s_i s_j = -J \sum_i s_i s_{i+1}$$

, where J is the strength of interaction between spins.
To implement the free boundary conditions on it, we would have to use a coordinate transformation

$$\{s_1, s_2, ..., s_N\} \to \{s_1, p_2, ..., p_N\}$$

, where $p_N = s_{N-1}s_N$

The inverse transform can be written as

$$s_2 = s_1 p_2, s_3 = s_1 p_2 p_3, s_N = s_1 p_2 ... p_N$$

so, the one to one correspondence between the two coordinate systems can be seen.
It's worth mentioning the the free boundary conditions carry big finite size effects, but they should vanish as the thermodynamic limit $N \longrightarrow \infty$ is reached. After the transformation the partition function Z is

$$Z = \sum_{s_1, p_2, \ldots, p_N} e^{\beta J(p_2 + p_3 + \ldots + p_N)}$$

$$= 2 \prod_{i=2}^{N} \sum_{p_i = \pm 1} e^{\beta J p_i}$$

$$Z = 2(2cosh(\beta J))^{N-1}$$

To derive the exact energy and heat capacity of the function, one takes the derivatives mentioned in the problem sheet and gets

$$< E >= J(1-N)tanh(\beta J)$$
$$C = \frac{J(N-1)}{k_B T^2}\frac{1}{cosh^2(\beta)}$$

At the limit of $N \longrightarrow \infty$ u and c get the following forms

$$u = -Jtanh(\beta J)$$
$$c = \frac{J}{cosh^2(\beta)kT^2}$$

They stop depending on the number of spins in the system, and start behaving like macroscopic systems.

1.2 General case

In the general case the Hamiltonian is

$$H(\{s_i\}) = -J\sum_{<i,j>} s_i s_j - B\sum_i s_i$$

In this case the partition function is expressed as the trace of a matrix.
We define a matrix such as

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

and then the partition function is

$$Z = sum_{\{s_1 s_2\}} e^{-\beta H} = Tr(P \cdot P)$$

Or in general, with N spins

$$Z = Tr(P^N)$$

Taking into consideration the properties of the trace, we can diagonalise the matrix P using eingenvalues λ and get

$$\lambda_{\pm} = e^{\beta J}\left(cosh(\beta B) \pm \sqrt{sinh^2(\beta B) + e^{-4\beta J}}\right)$$

$$Z = Tr(P^N) = \lambda_+^N + \lambda_-^N$$

$$Z = e^{N\beta J}\left[\left(cosh(\beta B) + \sqrt{sinh^2(\beta B) + e^{-4\beta J}}\right)^N + \left(cosh(\beta B) - \sqrt{sinh^2(\beta B) + e^{-4\beta J}}\right)^N\right]$$

Finding the energy and specific heat from this expression seems like a computational nightmare, but for the thermodynamic limit we can notice that $\lambda_+ > \lambda_-$, and use that to get

$$lnZ \approx Nln\lambda_+ = N\beta J + Nln\left(cosh(\beta B) + \sqrt{sinh^2(\beta B) + e^{-4\beta J}}\right)$$

and from that we can find the required derivatives to derive the energy and specific heat expressions at the thermodynamic limit $N \longrightarrow \infty$

2 Graphical representations of the exact solution to the 1D Ising Model

As a disclaimer, the calculations were made by assuming that the strength of interaction J and the Boltzmann constant k_B are both equal to one
Here follow the plots of the computed values of u and c.

First is the internal energy per spin, which varies a little around the absolute zero temperature, depending on the number of spins in the system, but quickly becomes uniform for higher temperatures.

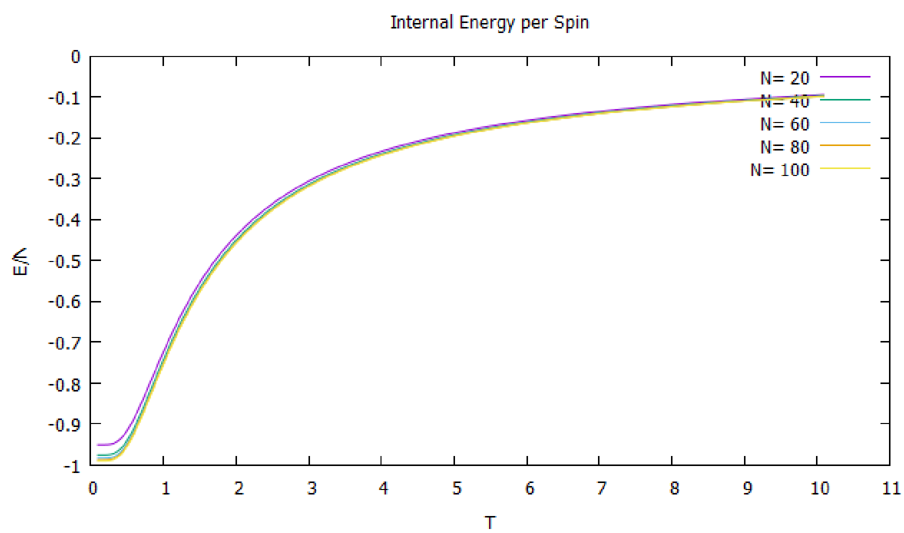

Figure 1: Energy per spin for temperatures between 0 and 10K. After that the plot flattens significantly, following the tanh function

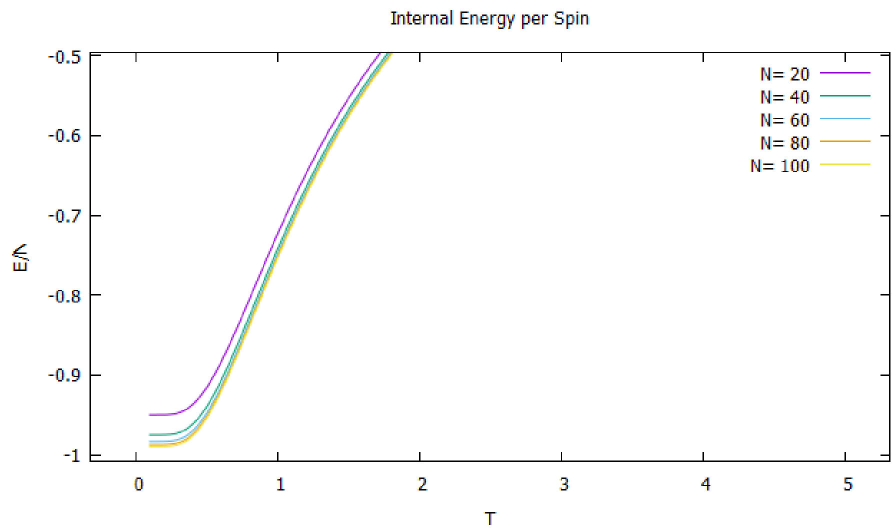

Figure 2: Zoomed in the region where the energy per spin differs for different N

Next comes the heat capacity per spin. It does indeed have a maximum, somewhere around $0.83K$, same for all N. The maximum itself does differ slightly for different N, increasing slowly together with N. The correlation with the energy plot is visible, since at the maximum of the specific heat (which is a derivative of the energy), the energy function slope is at its maximum.

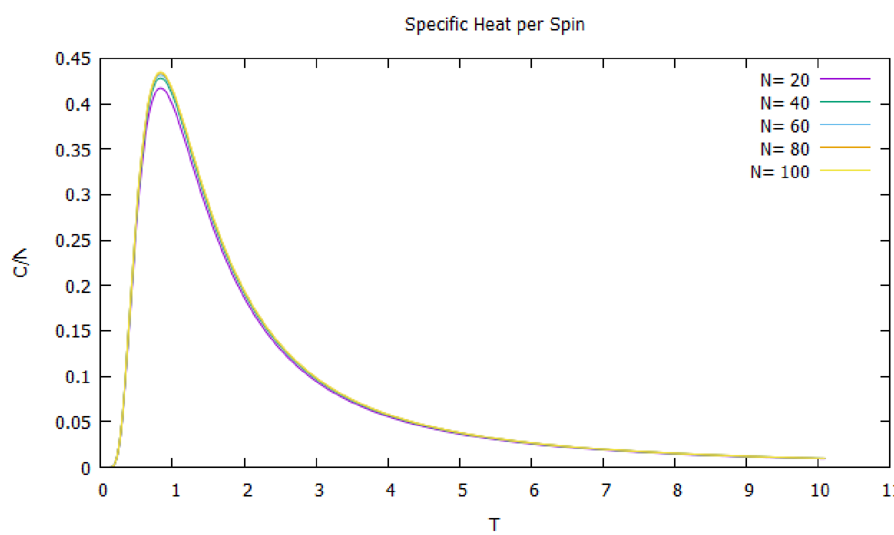

Figure 3: The specific heat per spin, a first derivative of the internal energy

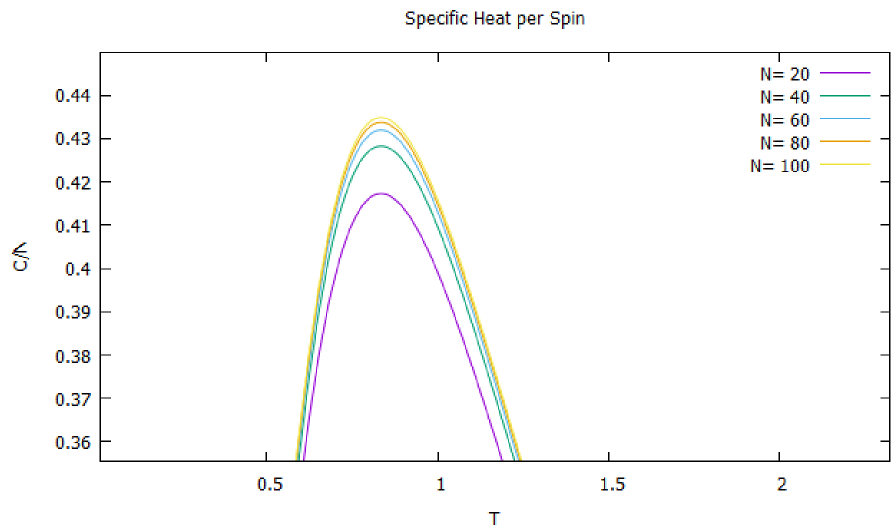

Figure 4: Zoomed in into the region of the maximum, corresponding to the maximal slope of the internal energy function

Next is encapsulated the base class of the code for calculating these values, with the purpose of error checking.

```
using System.Collections;
using System;

public class ExactIsingModel {

        // NOTE: The strength of interaction J and the k_B are defaulted to 1

        public double InternalEnergy(int n, double temperature)
        {
                double energy = (1 - n) * (Math.Tanh (1 / (temperature)));
                return energy;
        }

        public double energyPerSpin(int n, double temperature)
        {
                double totalEnergy = InternalEnergy (n, temperature);
                return totalEnergy / n;
```

```
        }

        public double specificHeat(int n, double temperature)
        {
                double specificHeat = (n - 1) / (Math.Pow(Math.Cosh (1 / (temperature)), 2) * temperature * temperature);
                return specificHeat;
        }

        public double specificHeatPerSpin(int n, double temperature)
        {
                double specHeat = specificHeat (n, temperature);
                return specHeat / n;
        }
}
```

And finally, for a bit of amusement, a screenshot of an 1D Ising Model Monte Carlo simulation I wrote using the Unity game engine, in a futile attempt to understand more about the model :) (The spins are organised in a grid for easier viewing, they are only interacting in one dimension). Simulation running at 0.6 degrees with 5000 spins.