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Computational Physics – Exercise 1

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1 What is J?

For the 1-D Ising Hamiltonian,

$$\mathcal{H}(s) = -J \sum_{\langle x,y \rangle} s_x s_y - h \sum_x s_x \tag{1}$$

Where $\langle x, y \rangle$ denotes a sum over the nearest spins and h is the external coupling. J is a coupling constant that models the interaction between neighbouring spins. For $J > 0$, the similar nearest neighbour pairs are favoured as this minimizes the total energy. In this context of magnets, this corresponds to having ferromagnetic order (see figure 1) [6].

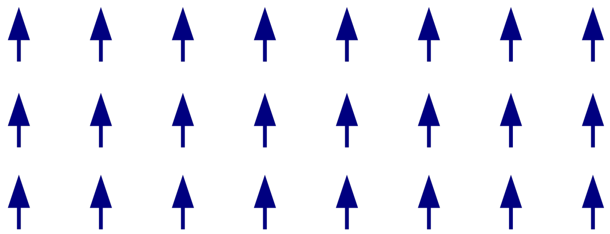

Figure 1: Ferromagnetic ordering in $d = 2$. Taken from [3]

For $J < 0$, opposite nearest neighbour pairs are favoured. In this context of magnets, this corresponds to having anti-ferromagnetic order (see figure 2).

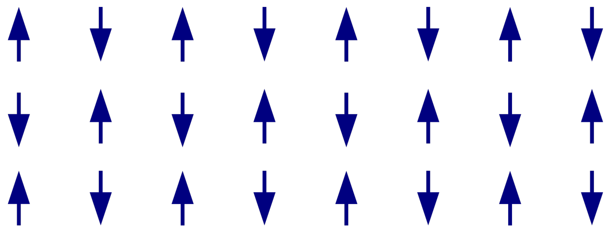

Figure 2: Antiferromagnetic ordering in $d = 2$. Taken from [2]

2 Periodic boundary conditions

Having periodic boundary conditions implies that all sites have the same number of nearest neighbours [5].

3 Simulating the Ising model in $d = 1$

The average magnetization is given by:

$$\langle m \rangle = \frac{T}{N} \frac{\partial}{\partial h} \ln Z \tag{2}$$

Where the partition function Z is given by,

$$Z = \lambda_+^N + \lambda_-^N \tag{3}$$

for

$$\lambda_\pm = \mathrm{e}^{\frac{J}{T}} \left(\cosh\left(\frac{h}{T}\right) \pm \sqrt{\sinh\left(\frac{h}{T}\right)^2 + \mathrm{e}^{-4\frac{J}{T}}} \right) \tag{4}$$

In this problem the relevant dimensionless ratios are as follows:

- $\frac{J}{T}$
- $\frac{h}{T}$

In order to calculate the average magnetization numerically, we use the formula

$$\langle m \rangle = \frac{1}{N} \sum_i S_i \tag{5}$$

We shall now simulate the Ising model in $d = 1$, the python code for that can be found at [1].

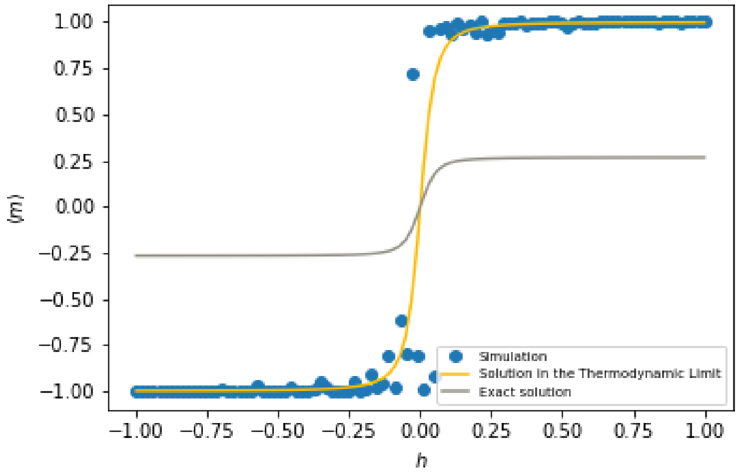

Figure 3: A plot of the $\langle m \rangle$ versus external field h for a fixed $J = 1$, $T = 0.75$ and $N = 20$.

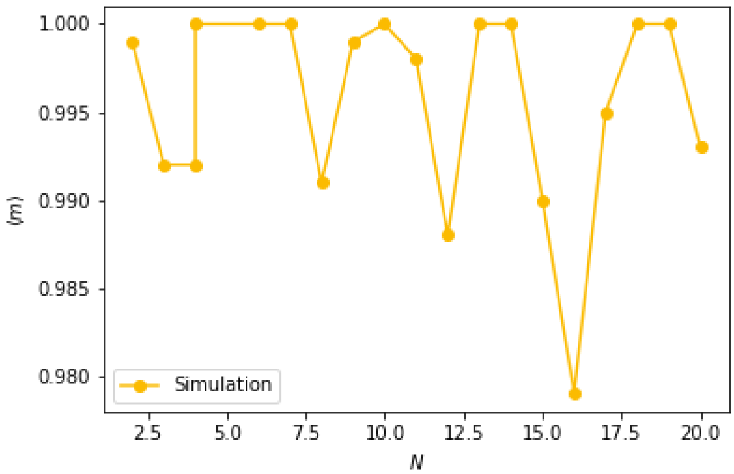

Figure 4: A plot of the $\langle m \rangle$ versus external field N for a fixed $J = 1$, $T = 0.75$ and $h = 0.5$.

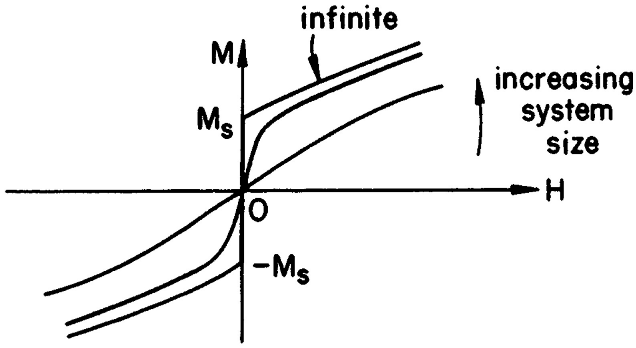

Figure 5: A plot of magnetisation M versus the external coupling parameter H. Taken from [4].

Numerically we were able to approximate $\langle m \rangle$ close enough to the value we observe at the thermodynamic limit as shown in figure 3. We can compare this to a plot from the literature in figure 5, we find these to be in close agreement. We find that the value of $\langle m \rangle$ is constrained heavily by the couplings h and J, however it does it does vary a little depending on the number of sites for $d = 1$ i.e. if it is even or odd and so on (see figure 4).

We computed the error for simulation via the residual standard deviation, which came to about 0.0004.

References

[1] P. Anancia Devaneyan and R. K. Senthilkumar. Exercises for the Physics 760: Computational Phyics course during the WS 22/23 Term.

[2] W. Commons. File:antiferromagnetic ordering.svg — wikimedia commons, the free media repository, 2020. Online; accessed 23-October-2022.

[3] W. Commons. File:ferromagnetic ordering.svg — wikimedia commons, the free media repository, 2020. [Online; accessed 24-October-2022].

[4] N. Goldenfeld. *Lectures On Phase Transitions And The Renormalization Group.* CRC Press.

[5] M. E. J. Newman, G. T. Barkema, M. E. J. Newman, and G. T. Barkema. *Monte Carlo Methods in Statistical Physics.* Oxford University Press.

[6] J. Thijssen. *Computational Physics.* Cambridge University Press, 2 edition.