The 2D Ising model: para- to ferromagnetic phase transition

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Introduction: The Ising model

The Ising model [1] is a computational model to simulate the phase transition of a material from paramagnetism to ferromagnetism. By looking at a 2D system of particles in a magnetic field in either of two states, parallel or anti-parallel to the magnetic field, the system's response to different magnetic fields at different temperatures can be simulated. From a randomly initialised system, optimising each particle state in the system over a number of "thermalisation sweeps" using the Metropolis algorithm [2], it converges to a final system state dependent on these factors.

Milestone problem

For the system as described in Fig.1, two averaging methods have been explored. The first, averaging the mean spin state of the particles, M_S in the system from sweep number 100 to 150 gives a value of -0.9377. The second, using a χ^2 fit of an exponential model (eq.1) gives a value of -0.9394.

$$M_S = e^{-(a_1 \times n + a_2)} + a_3, \tag{1}$$

where n is the sweep number and a_i the parameter to be optimised. Here a_3 is the converging value.

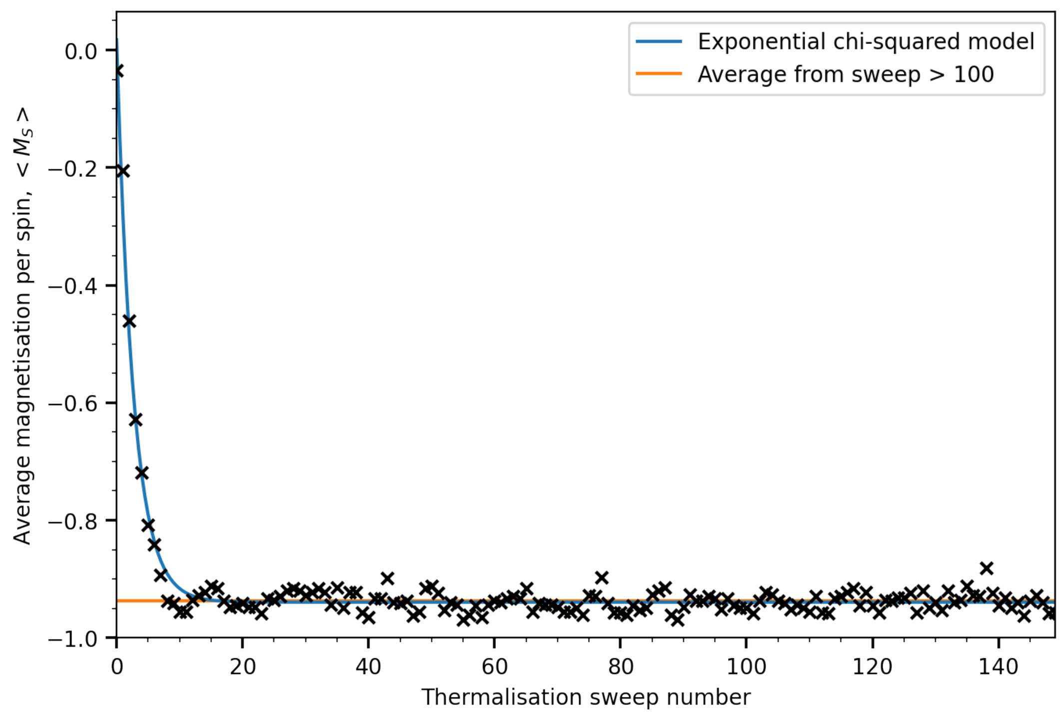

Fig. 1: The convergence to an average magnetisation per spin M_S for a 32 by 32 particle system with magnetisation $B/(k_B T)$, is -0.05 and exchange force $J/(k_B T)$ is 0.5.

To account for a magnetic field in the opposite direction or of zero value, the system may converge to a positive value. To account for this, a adjusted version of eq. 1, with adapted expectation parameters are used in the χ^2 fit. Which model to use and plot is determined by the sign of the average.

The Onsager model

The Onsager model [1] is an analytical prediction of M_S within the Ising model, dependent on the normalised exchange force, $J/(k_B T)$. It has the following form:

$$M_S = \pm \frac{(1+z^2)^{0.25}(1-6z^2+z^4)^{0.125}}{\sqrt{1-z^2}}, \tag{2}$$

where $z = e^{-2J/k_B T}$. This model predicts the behaviour of the material as it transitions to ferromagnetism at $z \geq 0.441$, which is a root of the function.

Temperature sweep

By varying the normalised exchange force $J/(k_B T)$ in the computational model, the temperature dependence of M_S can be simulated. Whilst the exponential model provides a good converging value when the magnetic field is sufficiently high, when this is not the case it is seen that M_S oscillates before reaching a final value. In this case, the exponential model does not fit well anymore (Fig. 3) and hence is not used for the temperature sweep. The results are plotted against the Onsager model in Fig. 2.

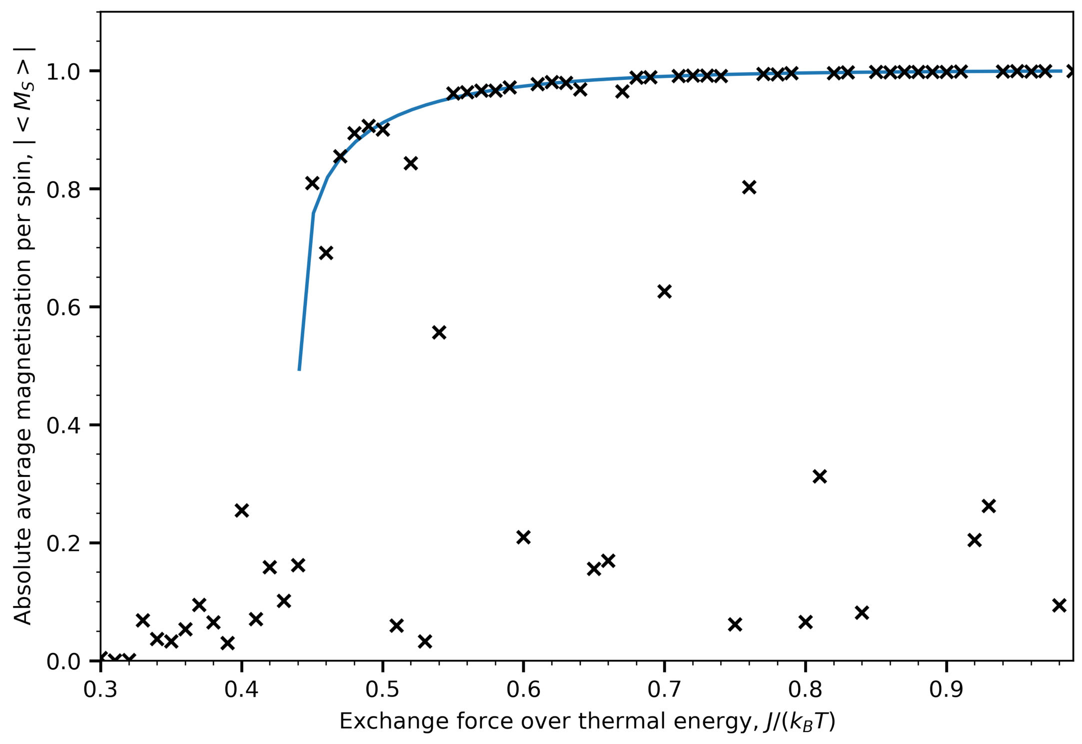

Fig. 2: The convergent absolute average spin of a 32 by 32 system for varying normalised exchange forces plotted with the analytical Onsager model in blue. The magnetic field is zero.

It can be noted that, whilst most points do follow this model well, a considerable amount lies much below it. When the graphs of all models are plotted it can be seen that these correspond to systems that have not converged to a final state yet in the Metropolis algorithm.

Adaptive thermalisation

Instead of performing the thermalisation sweeps and averaging based on a parameter given in advance, an adaptive model can be devised. This model uses the standard deviation, σ of the values of M_S between the last sweep and the one from which they are being averaged. σ is then compared to a predetermined value, set at $0.25/\sqrt{\Delta n - 1}$, where Δn is the number of sweeps M_S is averaged over. The factor of 0.25 is determined empirically. When σ is found to be too big, an extra number of sweeps is performed in steps of Δn, until σ is smaller and the system thus has converged to a final state. The average is then taken over the final Δn points.

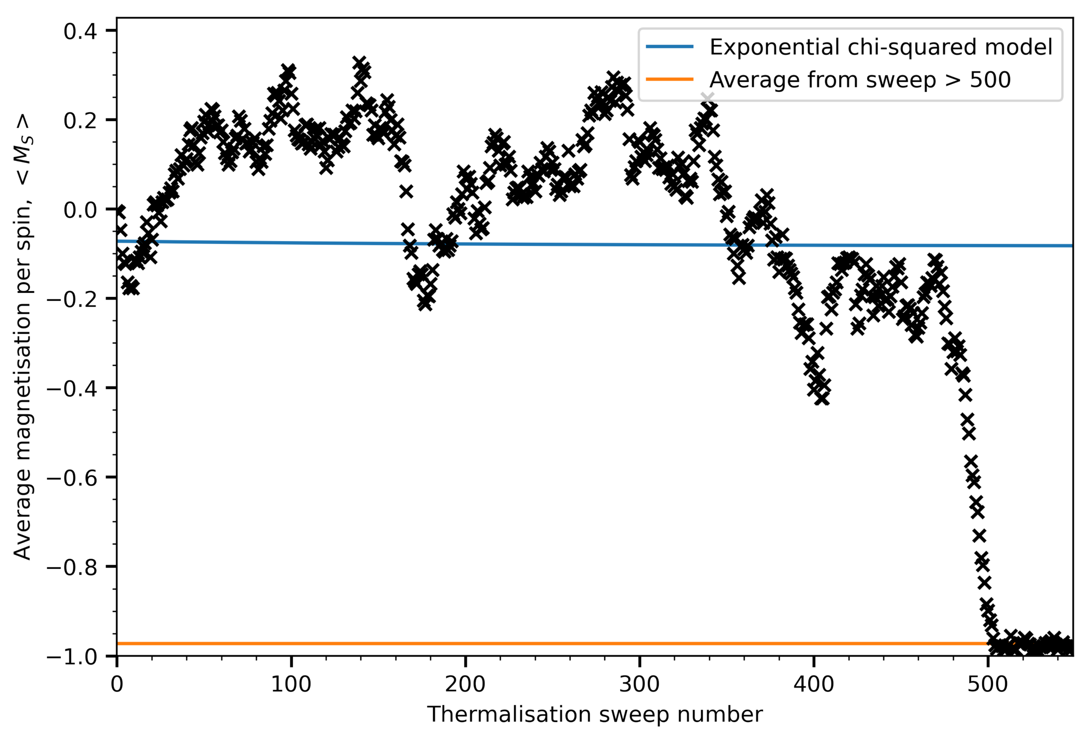

Fig. 3: The convergence to an average magnetisation per spin M_S for a 32 by 32 particle system with a 0 B-field and exchange force $J/(k_B T)$ of 0.6.

Adaptive temperature sweep

Using the adaptive thermalisation model, the temperature sweep can be performed and is plotted in Fig. 4. A limit has been introduced on the amount of times a jump in number of thermalisation sweeps can be performed, at 20 jumps of 50 thermalisations. This is done to work with the paramagnetic values (low $J/(k_B T)$), as their $< M_S >$ value is close to zero and does not appear to converge with the values of M_S varying more notably. Error bars have been introduced in Fig. 4 on $| < M_S > |$, as the standard error of $< M_S >$.

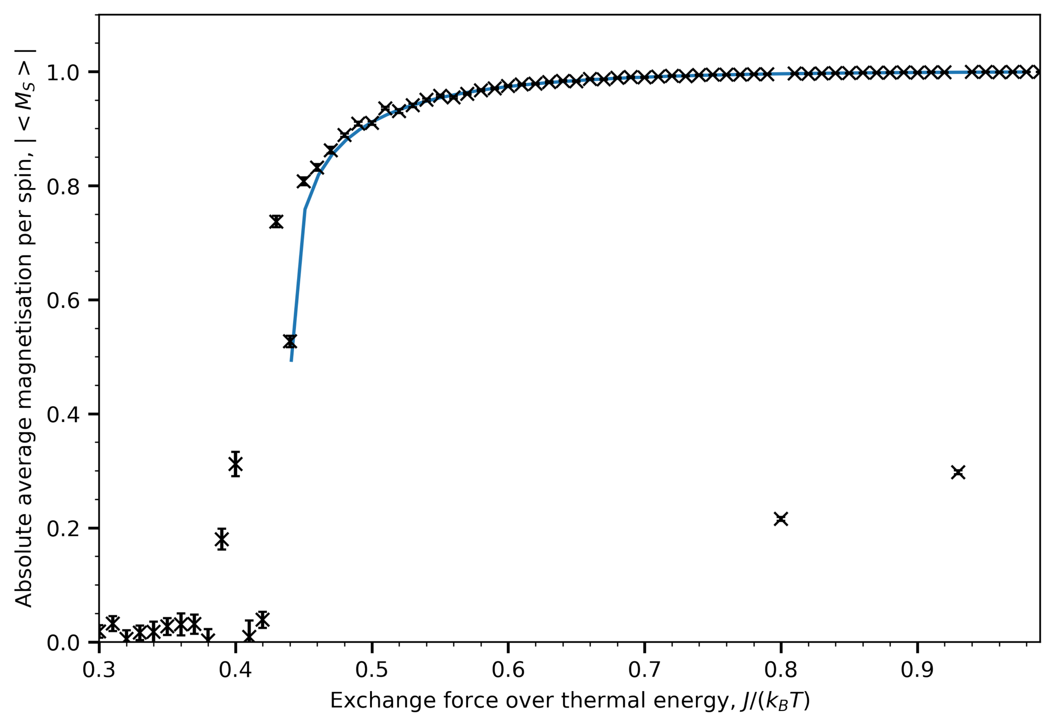

Fig. 4: Using adaptive thermalisation, the convergent absolute average spin of a 32 by 32 system for varying normalised exchange forces. Plotted with the analytical Onsager model in blue. The magnetic field is zero.

The reason for this adaptive thermalisation is to ensure as many points as possible represent a converged value, without having to run a 1000 thermalisation sweeps on each point, thus saving processing time. Instead of σ, other methods to determine convergence have been tested. These contained the difference between consequent groups of M_S values or the difference between certain groups of values and a group of values from the last thermalisation sweeps. These empirically proved not to be as reliable.

Conclusions

It can be seen that the use of adaptive thermalisation, using σ as a indication of thermalisation provides more consistently converged $< M_S >$ values and therewith align better with the analytical model. Whilst the exponential model gives an accurate value when the system converges quickly, it does not when any form of oscillation is present. Averaging over all converged values thus provides a better value for $< M_S >$.

Further work

Another important model to simulate magnetic phase transition is the Heisenberg model [3], where the spin states are treated as operators. This model comes in a classical and quantum mechanical form, which both can be explored. This can be developed and compared against the Ising model. Additionally, the 2D systems can be expanded to 3D or higher rank systems.

References

[1] Barry M. McCoy and Tai Tsun Wu. *The Two-Dimensional Ising Model.* Harvard University Press. 2013.

[2] I. Beichl and F. Sullivan. The Metropolis Algorithm. *Computing in Science Engineering*, 2(1):65–69, 2000.

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