Linear Logarithmic Relaxation for Phase Transitions in Statistical Field Theory

James Roscoe[1], PEL Rakow[1], P. Buividovich[1], K. Langfeld[2]

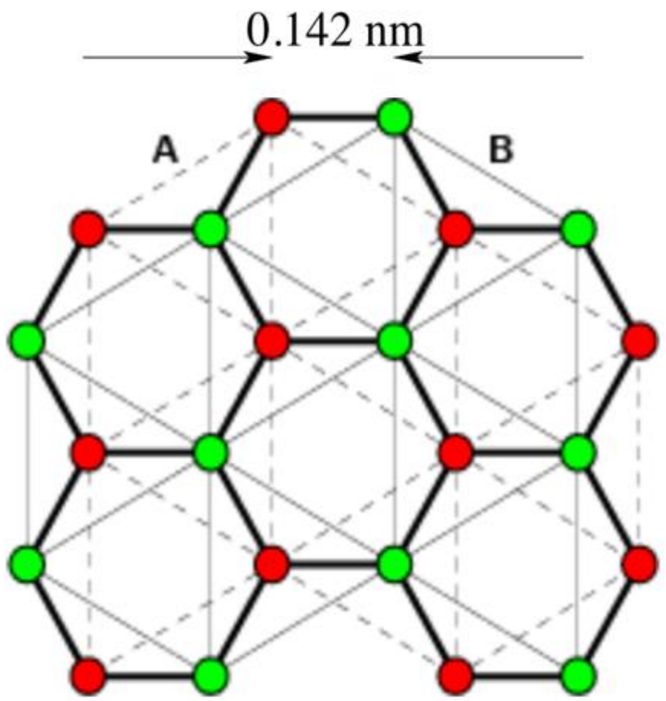
[1]University of Liverpool, [2]University of Leeds

June 2023

The Project

Goals:

- Statistical averaging over a huge configuration space.
- Test efficiency of Linear Logarithmic Relaxation.
- Use the 2D square lattice Ising model as it is a model where we know a lot of information so serves as a good testing ground.
- Forming multi-modal probability distributions.



Ising Model

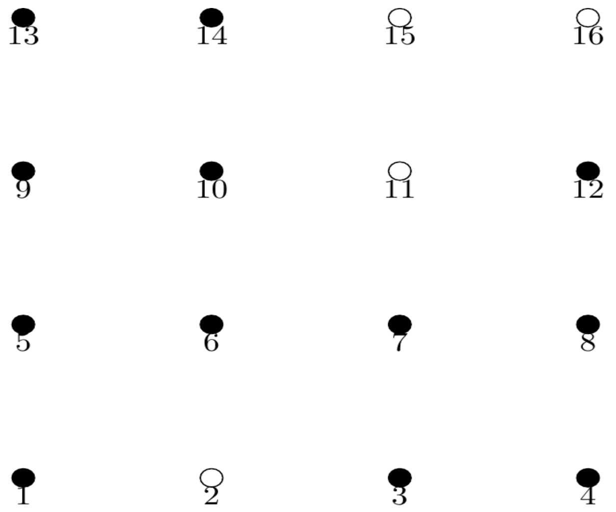


Illustration of a 4 x 4 Ising model lattice, where black circles represent up (+) spins and white represent down (-) spins.

- For Hamiltonian $\mathcal{H}$,

$$\mathcal{H} = \beta \sum_{\text{bonds}} s_i s_j - H \sum_{\text{sites}} s_i$$

- At position i, the spin value is denoted s_i .
- β refers to the inverse temperature value. High values causes nearby spins to have the same sign.
- H is the external magnetic field. High values favour positive spins.

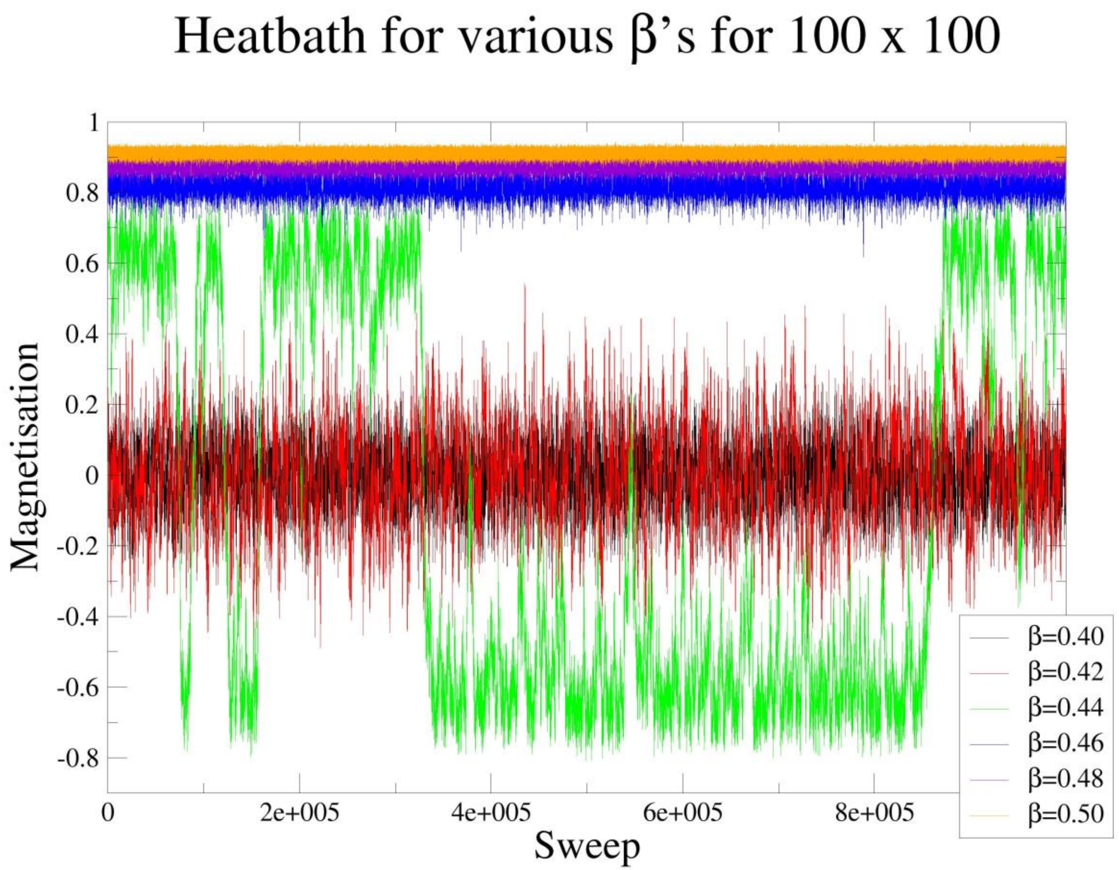
Ising Model

- Single variable distribution against magnetisation at $\beta = 0$ at any volume. Can be calculated exactly as a binomial.
- Single variable distribution against $H = 0$ in infinite volume. Derived from Onsager solution.

$$U = - \sum_{\text{bonds}} s_i s_j \qquad -2L^2 \leq U \leq 2L^2$$

$$M = - \sum_{\text{sites}} s_i \qquad -L^2 \leq M \leq L^2$$

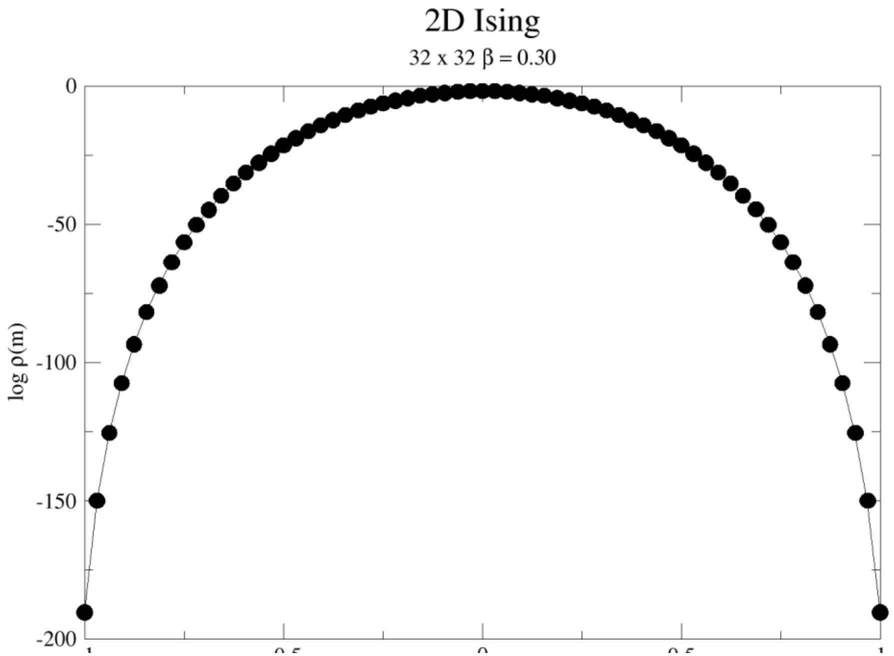
Lack of Ergodicity

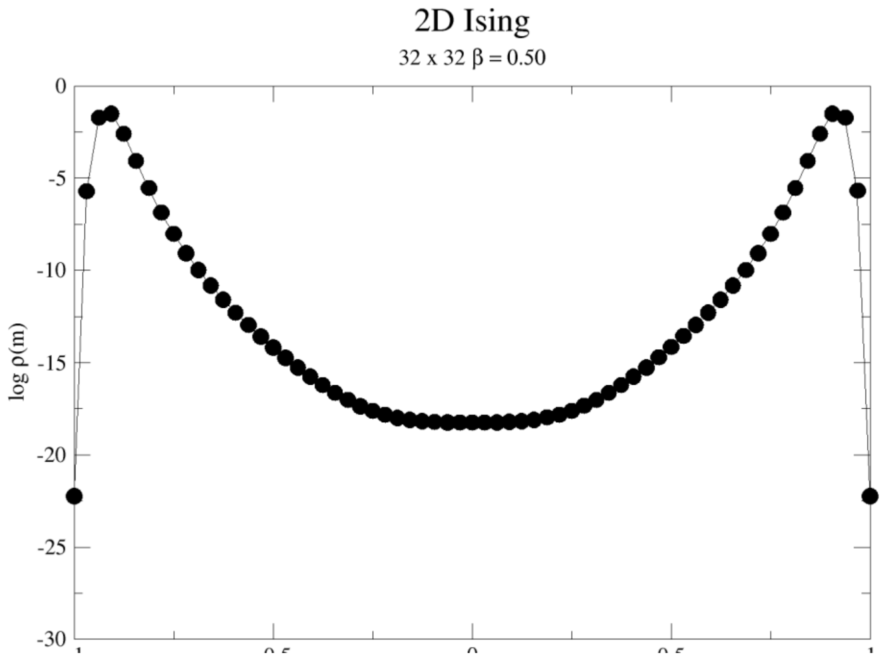


- One flaw with standard heatbath measurements of a lattice is the underestimation of error bars brought on by not measuring the full range of values.

- We can see above, at inverse temperature values (β) above the critical value of 0.44, ergodicity has rapidly decreased as the magnetisation measured is only is exclusively above 0.50, leading to underestimation of the error bars when measuring average magnetisation.

Don’t sample full configuration in broken phase





Density of states

- Probability density of the various states of a system.
- With partition function

$$Z(\beta) = \int dM \rho(M)$$

- We formulate the density of states

$$\rho(M) = \frac{1}{Z} \sum_{\{s_x\}} \delta\left(M, \sum_x s_x\right) \exp\{\beta S\}$$

- Update a spin variable based on probability

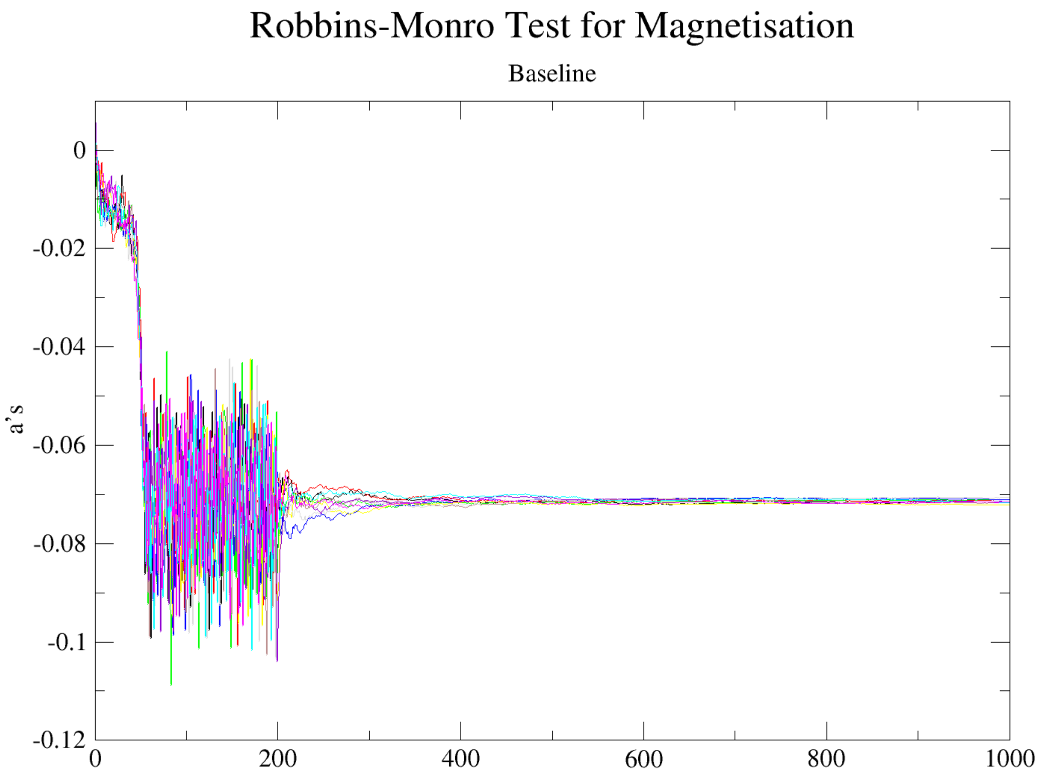
$$p = \frac{1}{1 + \exp[-2\beta b]}$$

How to get Density of states

- The LLR coefficient a, is coupled with the action, and so can be used to estimate the slope.

$$\langle\langle f \rangle\rangle(a) = \frac{1}{N} \sum_{\{s\}} f(s) \exp\left(\beta S + aM(s)\right) W_\delta(M_0, M(s))$$

$$W_\delta(M_0, M(s)) = \begin{cases} 1 \text{ for } M_0 - \delta \leq M(s) \leq M_0 + \delta \\ 0 \text{ else} \end{cases}$$



Linear Logarithmic Relaxation

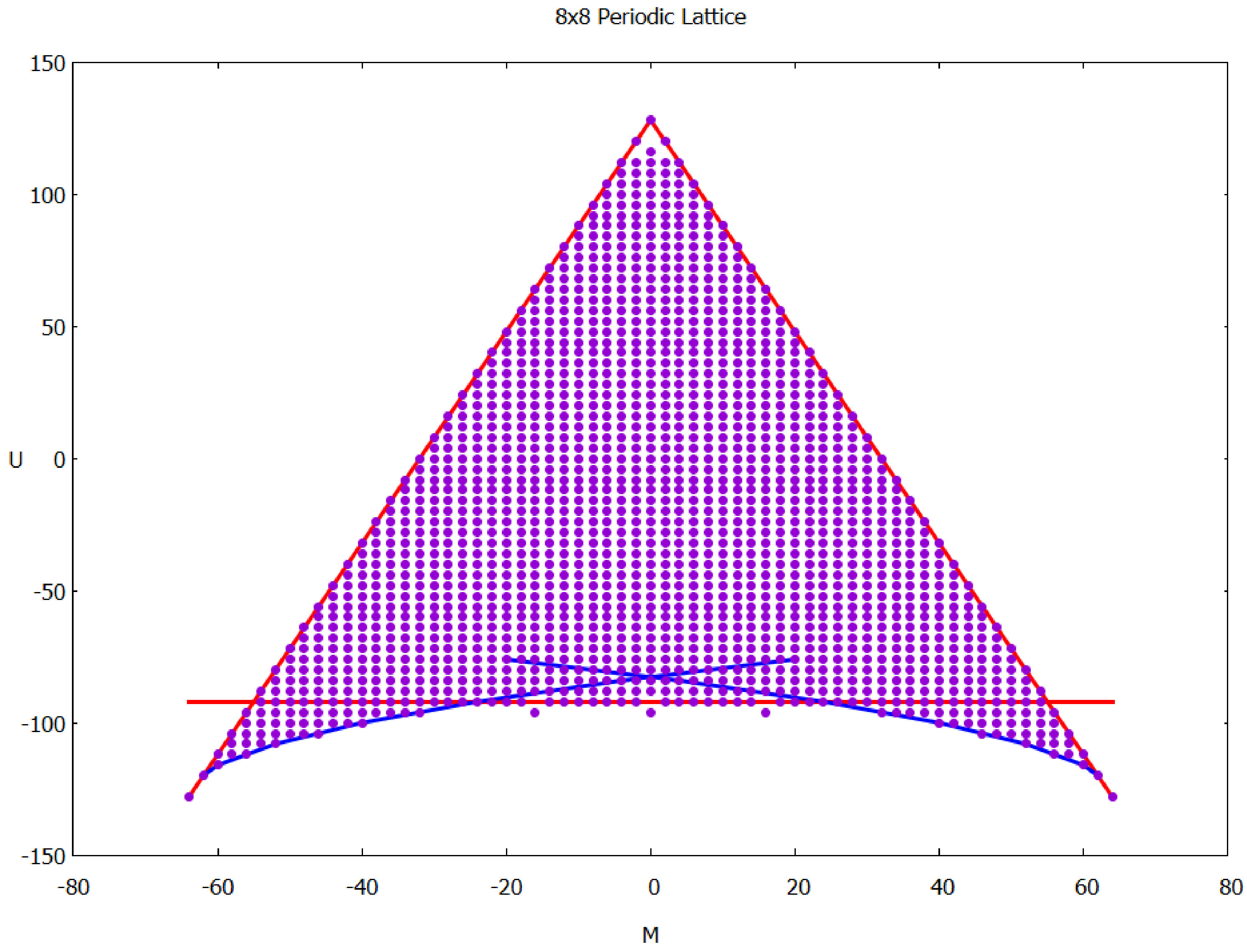
Key ingredient is the slope.

$$\Delta M(a) = 0$$

$$a(M_0) \approx \frac{\partial \ln \rho(M_0)}{\partial M_0}$$

$$a_{i+1} = a_i - \frac{3\Delta M(a_i)}{\delta^2}$$

Allowed values for magentisation and energy



Windows and boundary of the accessible region

Simulate inside each magnetic window. Tune magnetic field and temperature so within each window we acquire

$$\frac{\partial \ln \rho}{\partial U} \qquad \frac{\partial \ln \rho}{\partial M}$$

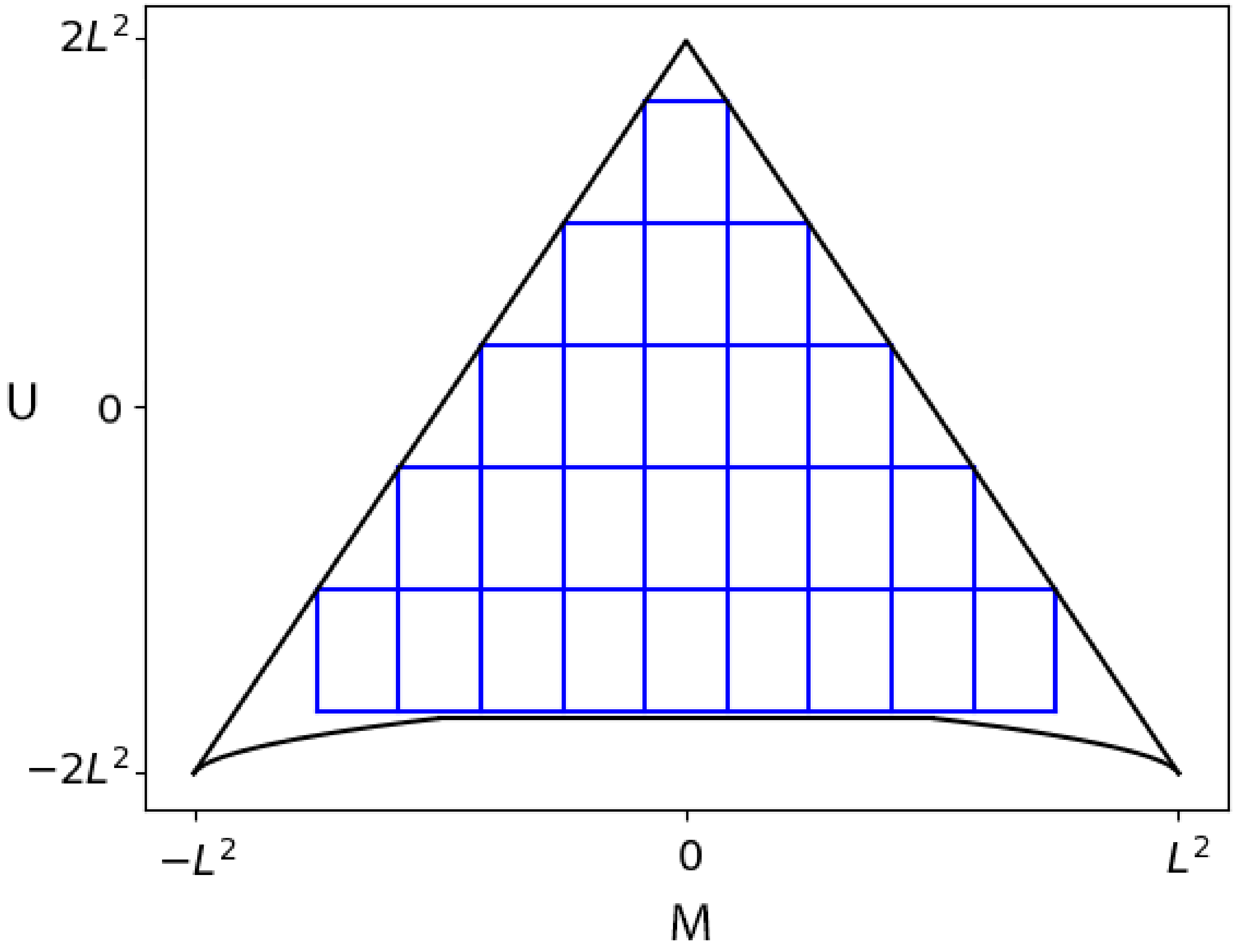
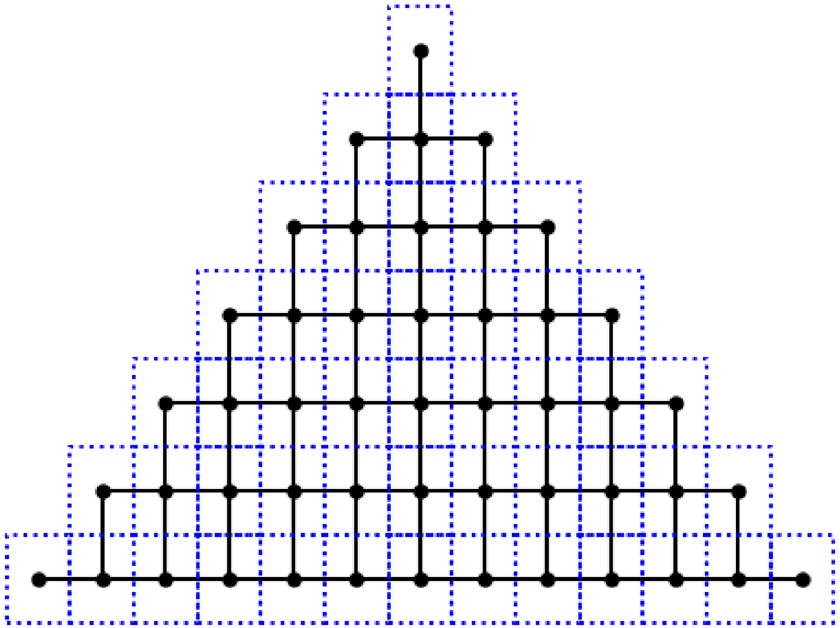


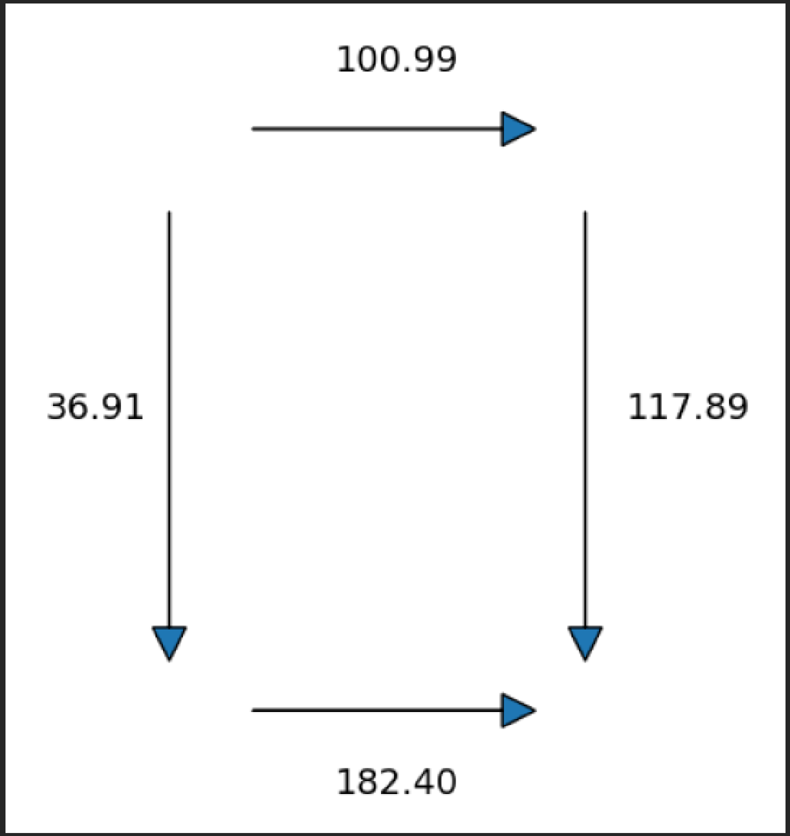
Illustration of the windows for two-variable LLR



- Both measured derivatives for the magnetisation and energy should be consistent with the change in logarithmic density.

$$\ln \rho_j - \ln \rho_i = \delta_M (a_{Mi} + a_{Mj})$$
$$\ln \rho_k - \ln \rho_i = \delta_U (a_{Ui} + a_{Uk})$$

Plaquette loop integrals

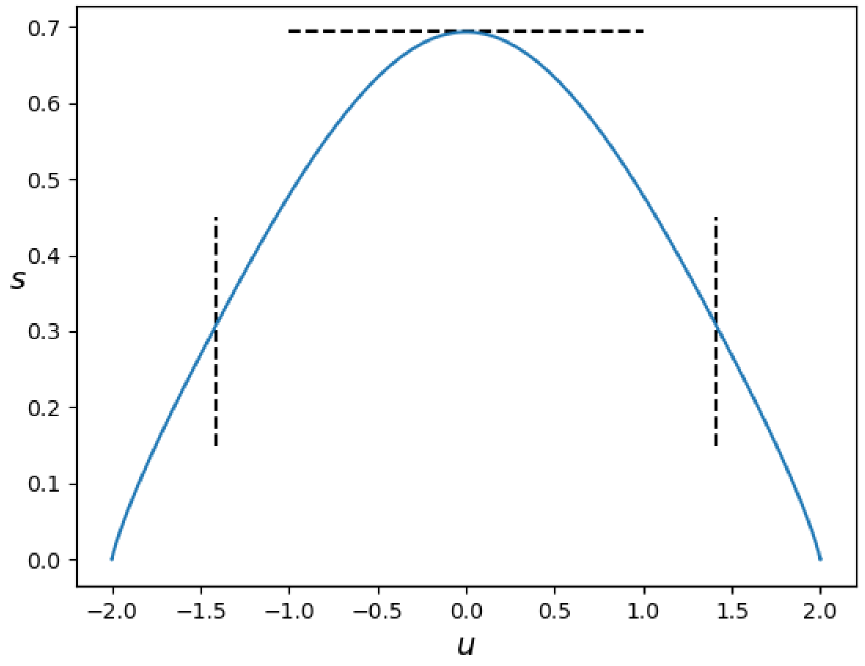


$$C \approx \frac{\partial a_U}{\partial M} - \frac{\partial a_M}{\partial U} = \frac{1}{A}\oint (a_M, a_U) \cdot (dM, dU)$$

$$C = 182.40 - 117.89 - 100.99 + 36.91 = 0.43$$

Onsager Test

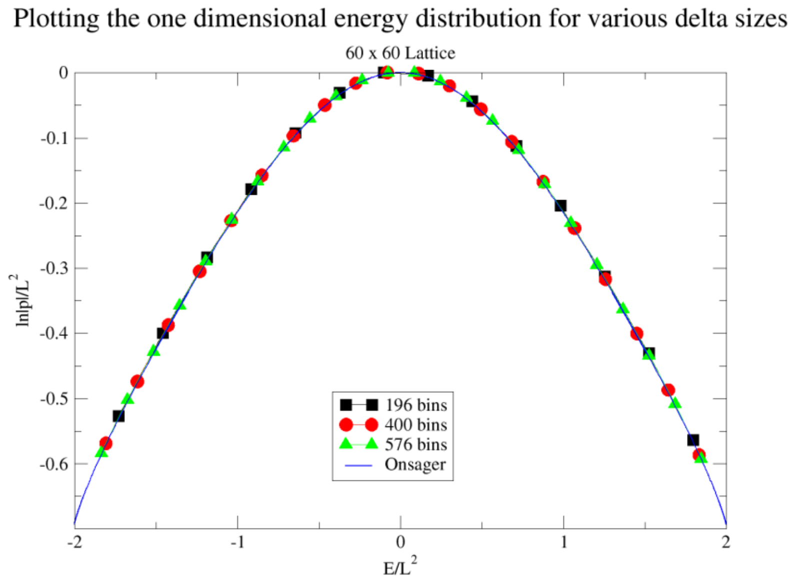
- Entropy per site in terms of energy gives us density of states.



Onsager Test

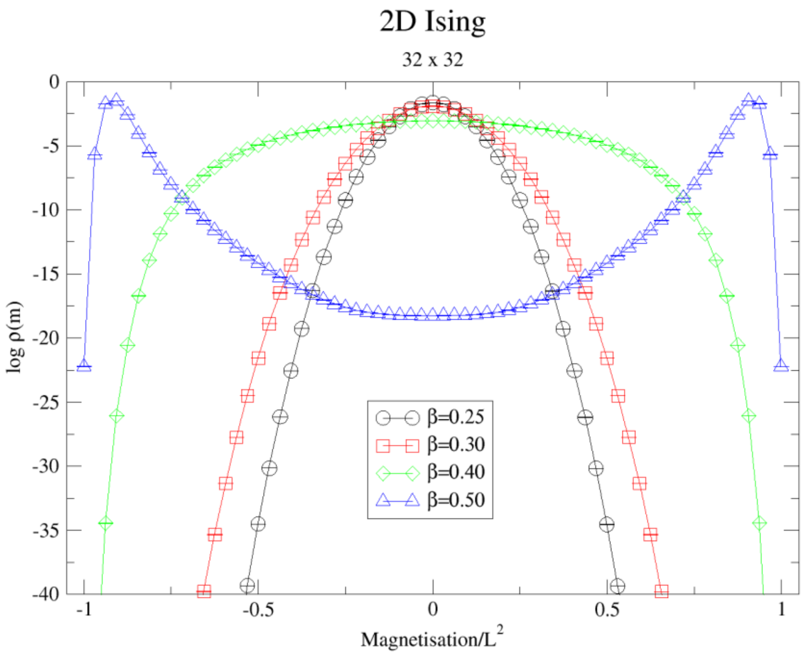
- The Onsager solution for the one-dimensional energy distribution when $H = 0$ was derived in 1944.
- It serves as a useful check that the two variable LLR is accurate.

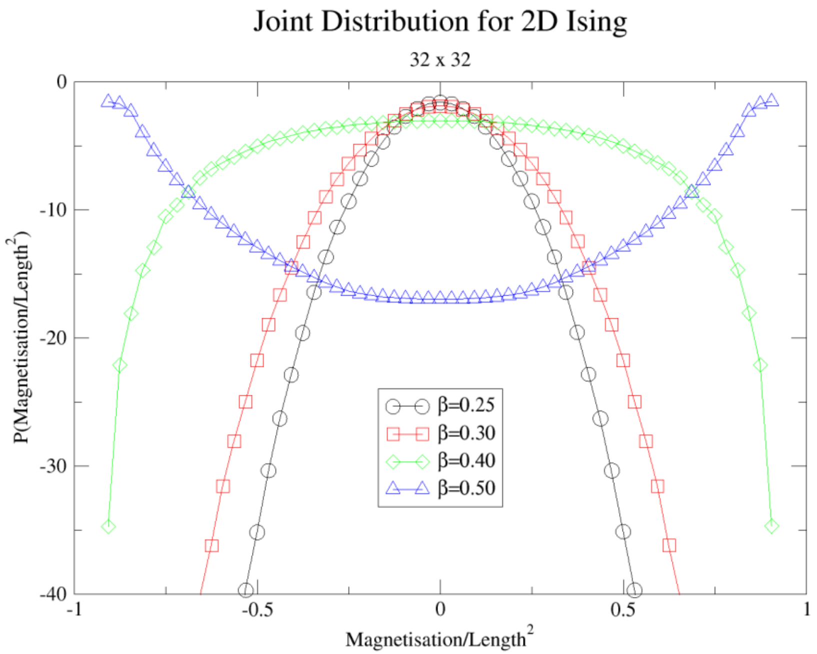
$$p(U) = \int_{(U-2L^2)/4}^{(2L^2-U)/4} \rho(M,U)dM = \frac{2\delta_M}{L^2}\sum_M \rho(M,U)$$



Comparing both distributions

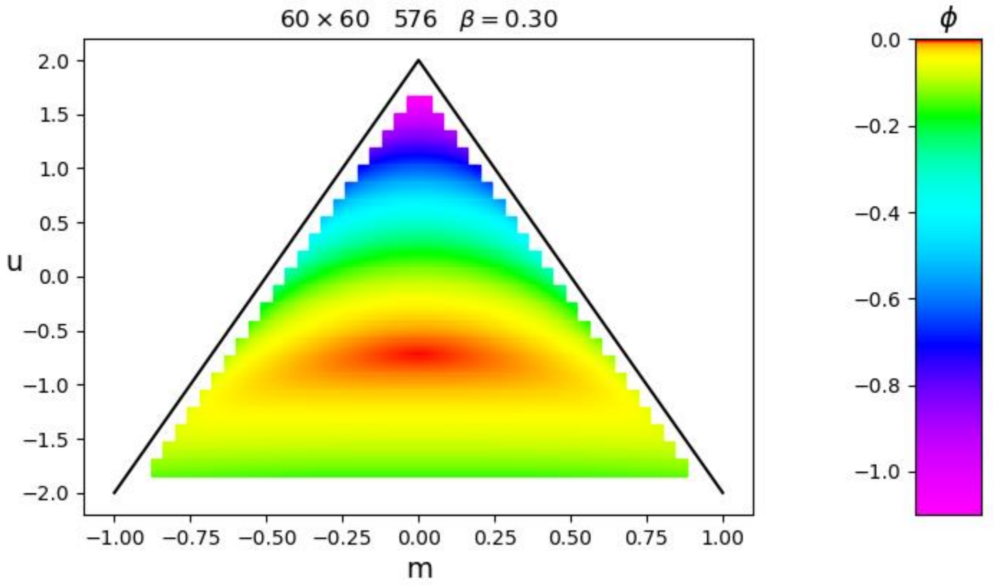
- Can recreate single variable results with two variable method.
- Good fit between both methods.
- Error bars produced using bootstrap method.

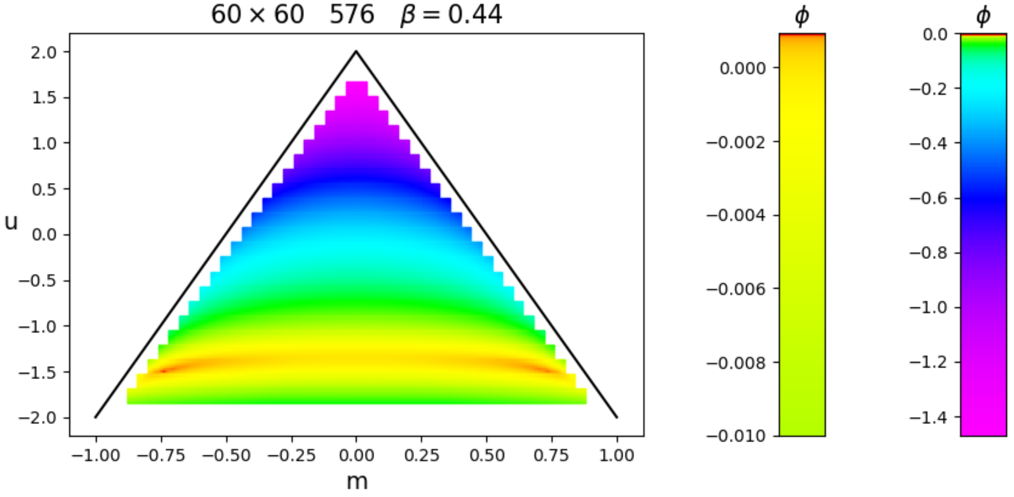




Joint Distribution Contour Plots

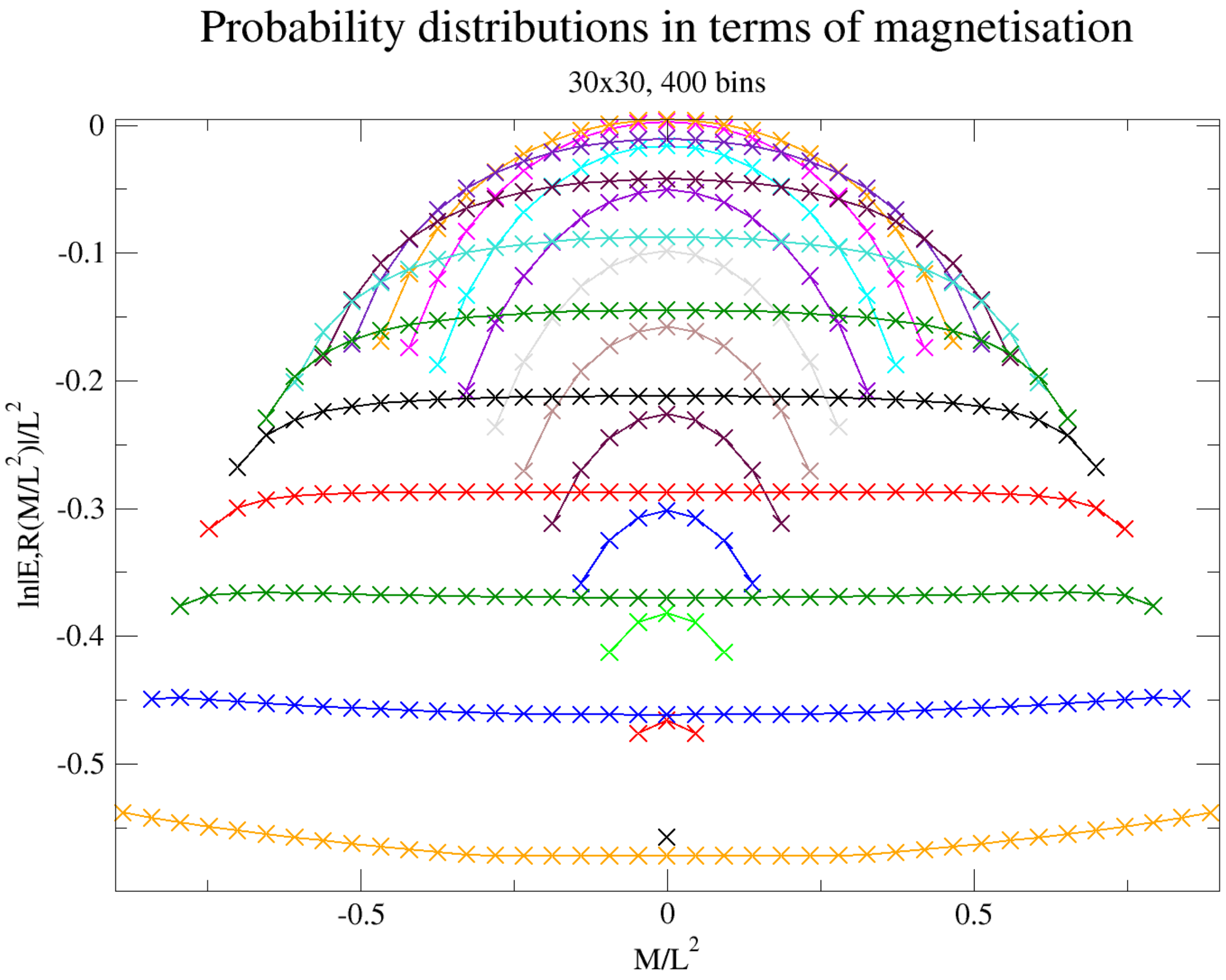
- Contour mapping has been altered so the higher densities are reached more rapidly.



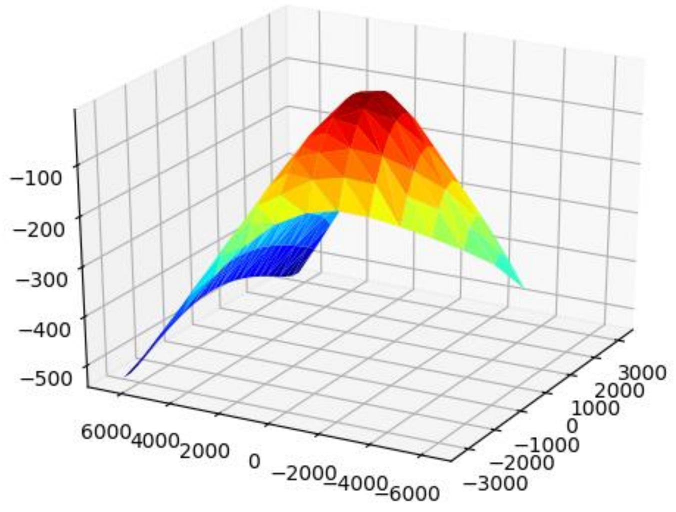


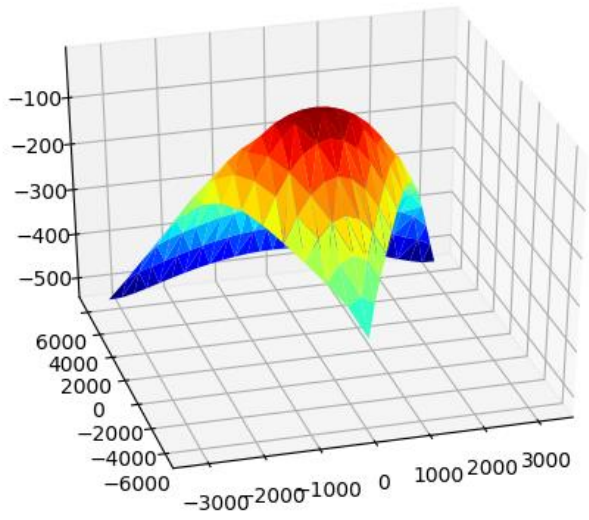
Probability Densities (Magnetisation)

- Minimum probability densities for highest and lowest fixed energy values.
- Fixed energy around zero gives us higher probability densities.
- Higher energy values have plateaued.



3D plots


−100
−200
−300
−400
−500
6000
4000
2000
0
−2000
−4000
−6000
3000
2000
1000
0
−1000
−2000
−3000


−100
−200
−300
−400
−500
6000
4000
2000
0
−2000
−4000
−6000
−3000
−2000
−1000
0
1000
2000
3000

Summary

- LLR can be extended to calculate two variable distributions.
- Could likely find critical values where the phase transitions occur without having to run multiple simulations.

- Outlook
  - Extend to other models.
  - Use this to extend to regions where we can’t simulate by Monte Carlo for example real β but imaginary H.
  - Look for Lee-Yang zeroes.
  - It may be possible to reweight the procedure into areas where we encounter sign problems (positive and negative contributions to the integral cancelling each other out), such as when applying an external imaginary magnetic field.