Laboratório de Computação e Visualização Científica

Visualizing Monte-Carlo sampling of the Ising model phase space

João Amaral (jamaral@ua.pt)

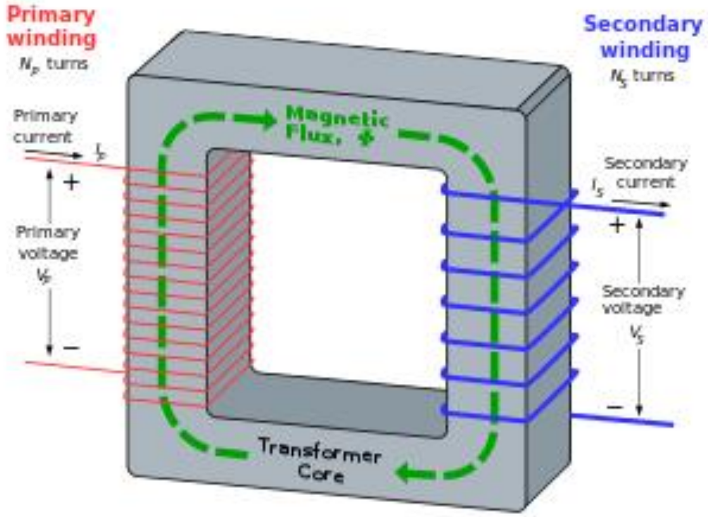
14/3/2022

Ferromagnetic materials for energy applications

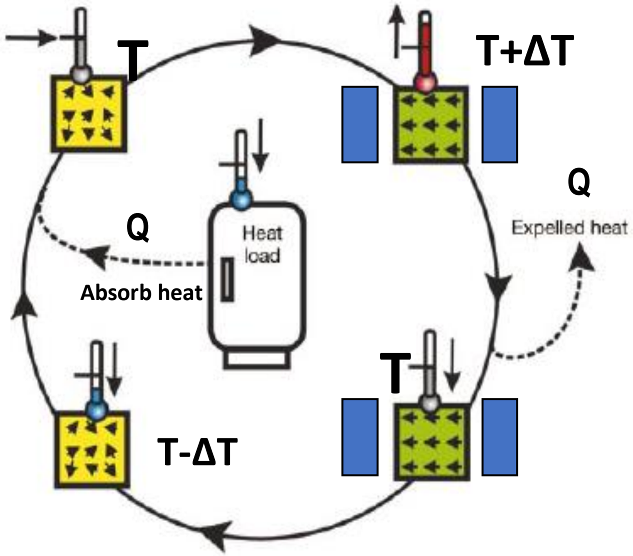
Ferromagnetic materials have three main applications in energy [1]:

- Hard magnets: magnetic motors and generators
- Soft magnets: power transformers
- Magnetocalorics: power generation and heat management

A wind turbine can have up to 3 tons of hard ferromagnetic material



All transformers, big and small, employ a "ferrous core" which is a soft ferromagnet



A ferromagnetic material has a phase transition, which can be used for cooling

[1] O. Gutfleisch et al., "Magnetic Materials and Devices for the 21st Century: Stronger, Lighter, and More Energy Efficient". Adv. Mat. 23, 821, 2011

Modeling the performance of a ferromagnet

- For these three major applications, the material's applicability depends on the temperature at which the ferromagnet transforms into a paramagnet: its **Curie temperature (Tc)**

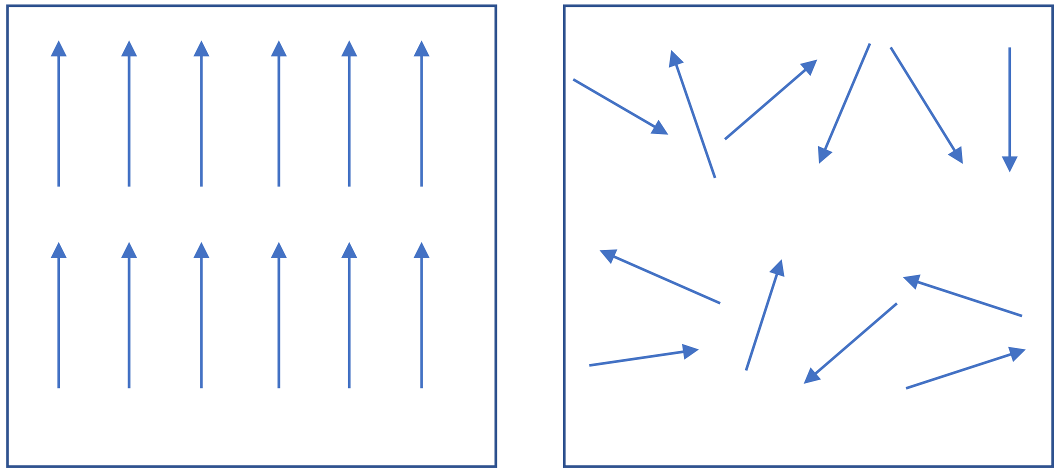
- A ferromagnet's Curie temperature establishes its working temperature limit, below which it is useful in motors and transformers. In the case of magnetocalorics, it defines the operational temperature.

- Materials currently used for these applications have been found through extensive experimental studies. With modern computational tools, it is possible to computationally search for new ferromagnetic materials for applications: **Computational materials design**

- To predict the Curie temperature of an atomic structure, we need a model that describes magnetic interactions, and their thermodynamic properties.

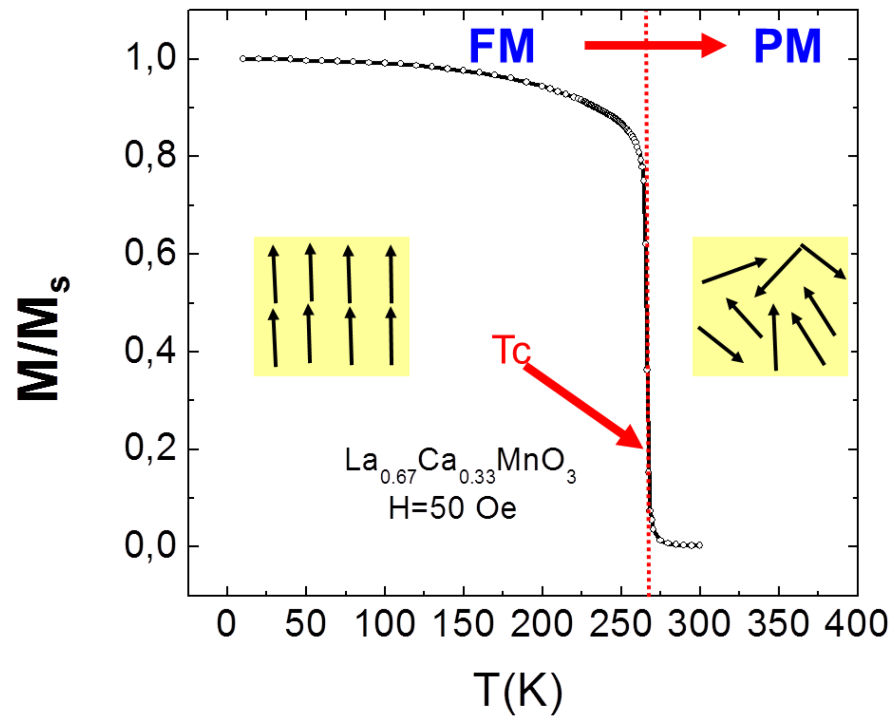
Ferromagnets – a simplified view

M = 1 (saturation) | M ~ 0 (disordered)



T < Tc (low entropy) | T > Tc (high entropy)

(experimental data)



- If we consider a free energy F = E – T.S, the energy term dominates for low T, while the entropy term dominates for high temperature
- Build the simplest model to reproduce this behavior

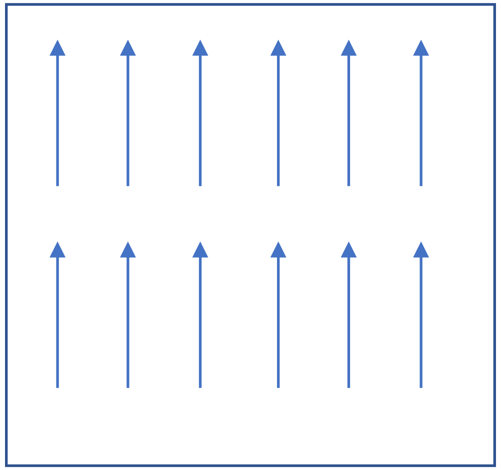
The Ising model

$$H = -\sum_{i\neq j}\frac{1}{2}J\hat{S}_i\cdot\hat{S}_j$$

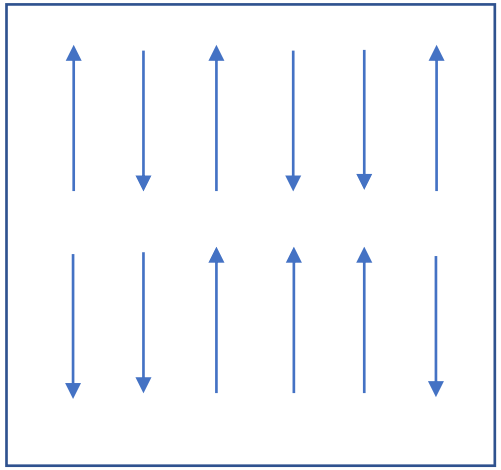
Sum over
Pairs of spins

Interaction
strength

Magnetic
moment



T < Tc
(low entropy)



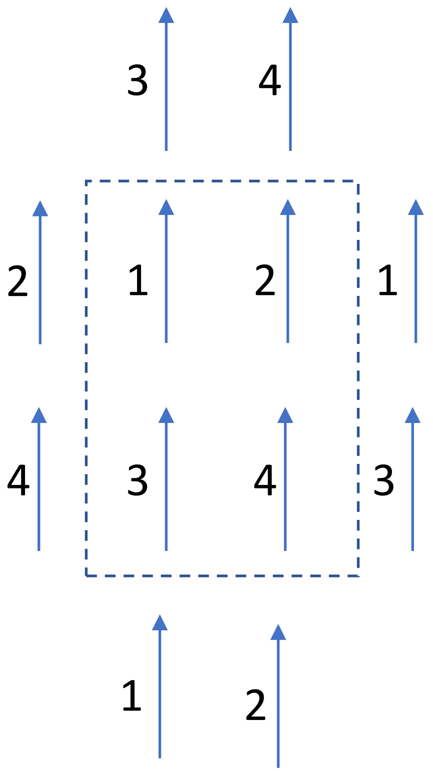
T > Tc
(high entropy)

- For each spin pair, an interaction energy is defined
- If J > 0, the system will be ferromagnetic for T = 0
- To model large systems, a lattice should be as large as possible, and use periodic boundary conditions (PBC).
- Nearest neighbor interactions should be dominant
- Does this work for a VERY small 2x2 lattice with PBC?

2x2 simple square with periodic boundary conditions

$$H = -\sum_{i \neq j} \frac{1}{2} J \hat{S}_i \cdot \hat{S}_j \qquad Z = \sum_{\eta} e^{-\frac{E_\eta}{k_B T}}$$

$$F(M,T) = -k_B T log Z(M,T)$$



The joint density of states, JDOS

M	E	Ω	Z	F
4	-8J	1	$e^{8J/kBT}$	-8J
2	0	4	4	-kB.T.log(4)
0	0	4	$4 + 2*e^{-8J/kBT}$	-kB.T.log(4 + 2*$e^{-8J/kBT}$)
	8J	2		
-2	0	4	4	-kB.T.log(4)
-4	-8J	1	$e^{8J/kBT}$	-8J
		16 total	$12 + 2*e^{-8J/kBT}+2*e^{8J/kBT}$	

Pen-and-paper JDOS calculation of a 2x2 Ising lattice with periodic boundary conditions

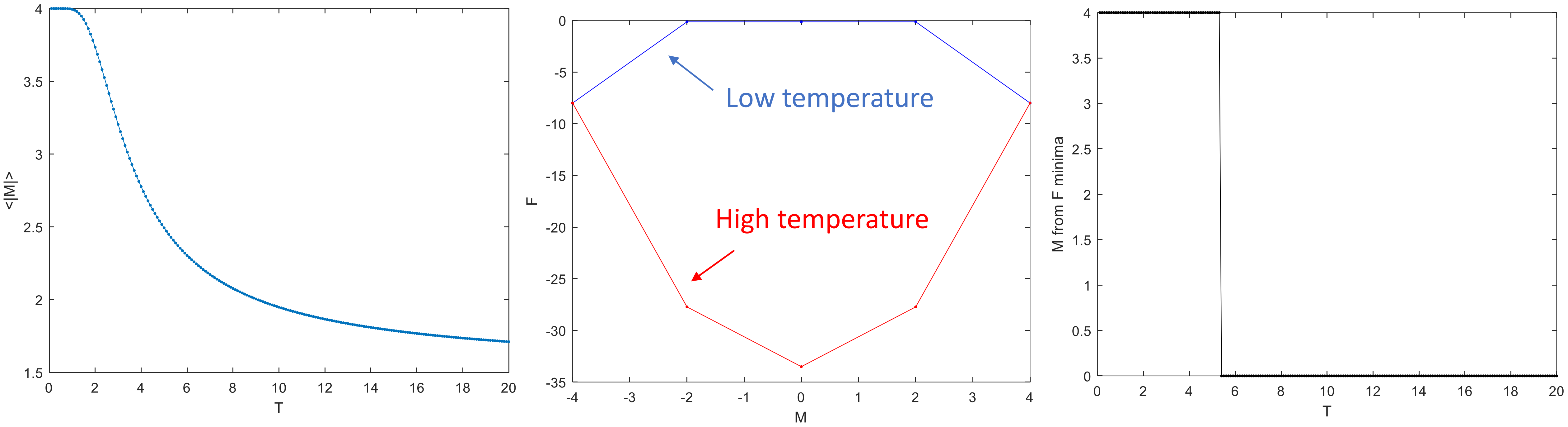
configurations		bonds	Energy (from $\sum_{i \neq j}^{NN} -\frac{1}{2} J \hat{S}_i \hat{S}_j$)	
+ + + +	M = 4	+ + + + + + + + + + + + + + + +	$-8J$	(M = 4)
− + + +	M = 2	− − − − + + − − − − + + + + + +	0	4x degenerate (M = 2)
equivalent to		+ − + + + + − + + + + −		
− − + +	M = 0	+ + − − + + − − + + − − + + − −	0	4x degenerate (M = 0)
equivalent to		+ + − − − + − + + − + −		
+ − − +	M = 0	− − − − − − − − − − − − − − − −	$+8J$	2x degenerate (M = 0)
equivalent to		− + + −		

- For such a small system, it is possible to explore by hand all possible (2^4 = 16) spin configurations
- Energy is estimated from the Hamiltonian formula
- Degeneracy is the sum of configurations with the same M and E value

M	E	Ω
4	$-8J$	1
2	0	4
0	0	4
0	$8J$	2
−2	0	4
−4	$-8J$	1

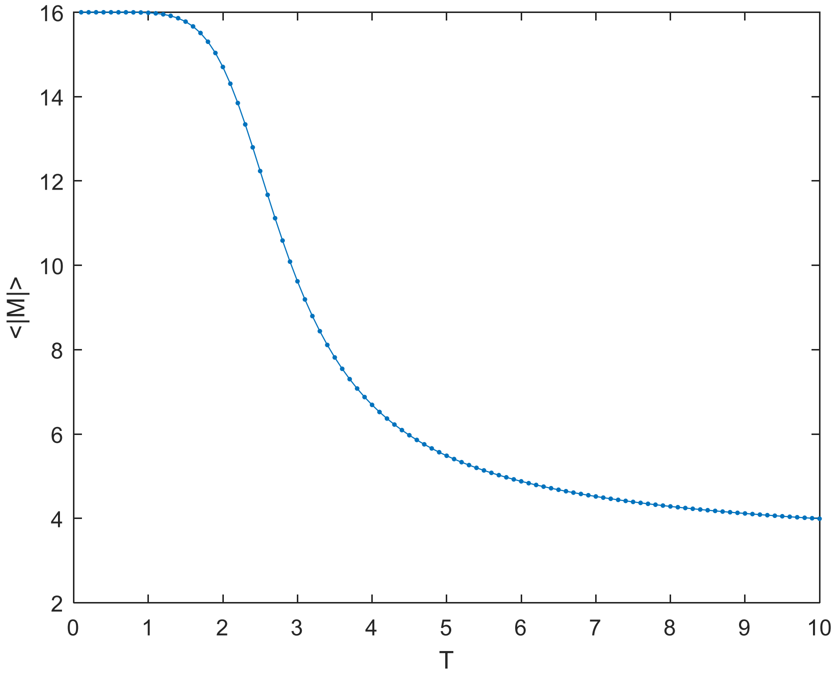
(symmetry)

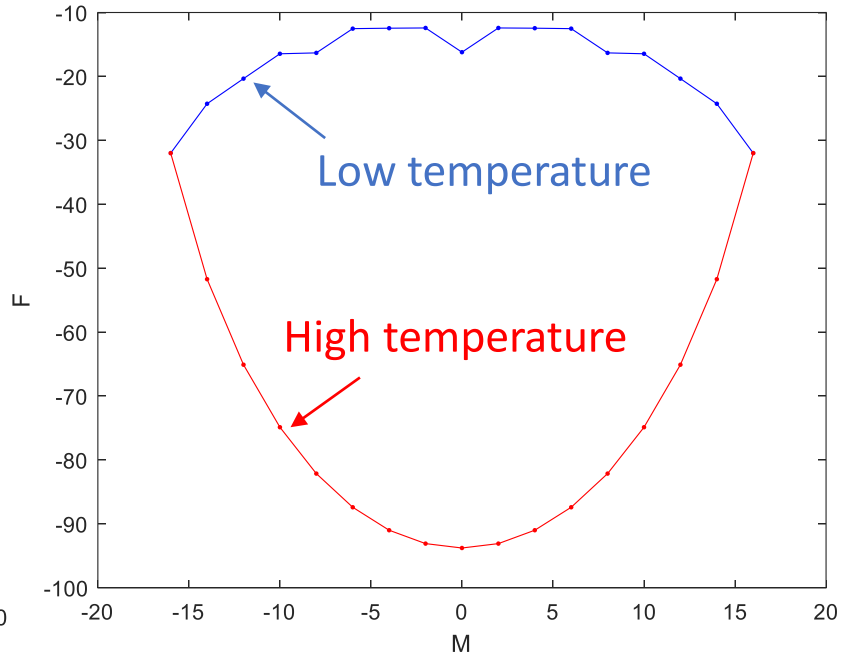
Thermodynamic properties from JDOS (2x2)

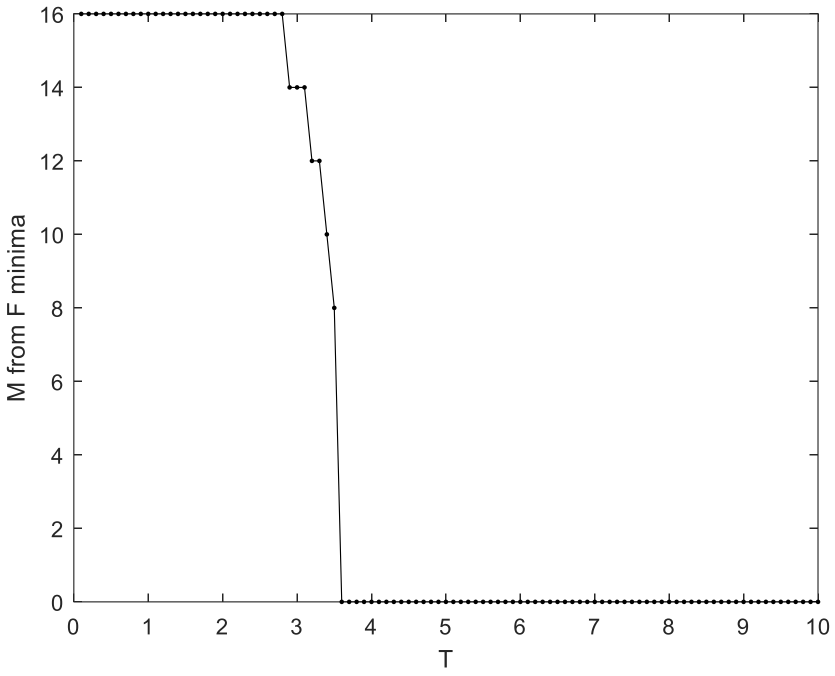


- The transition is observed in both calculations of average absolute magnetization and magnetization from free energy minima
- Larger system?

Thermodynamic properties from JDOS (4x4)

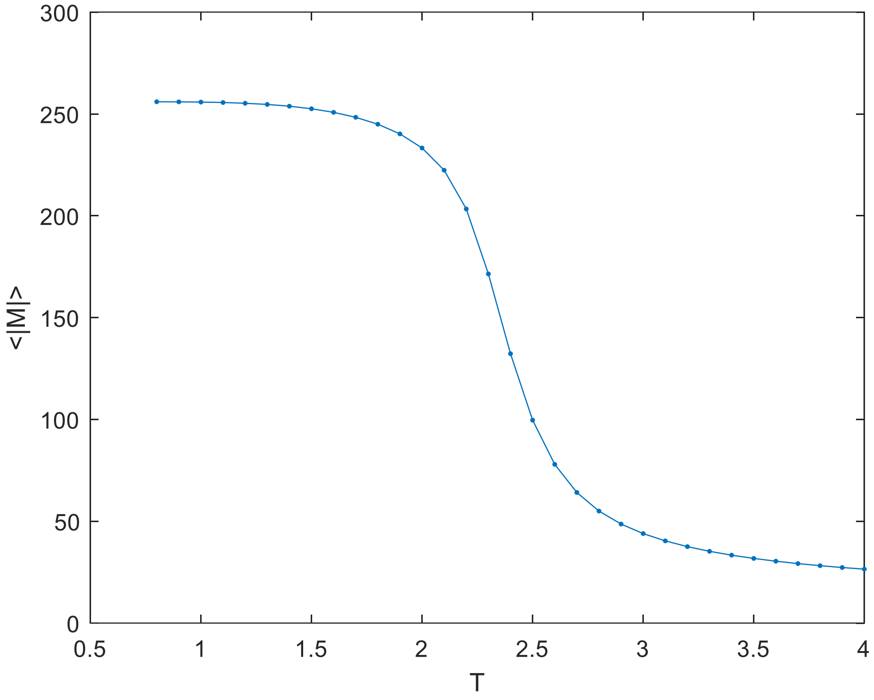


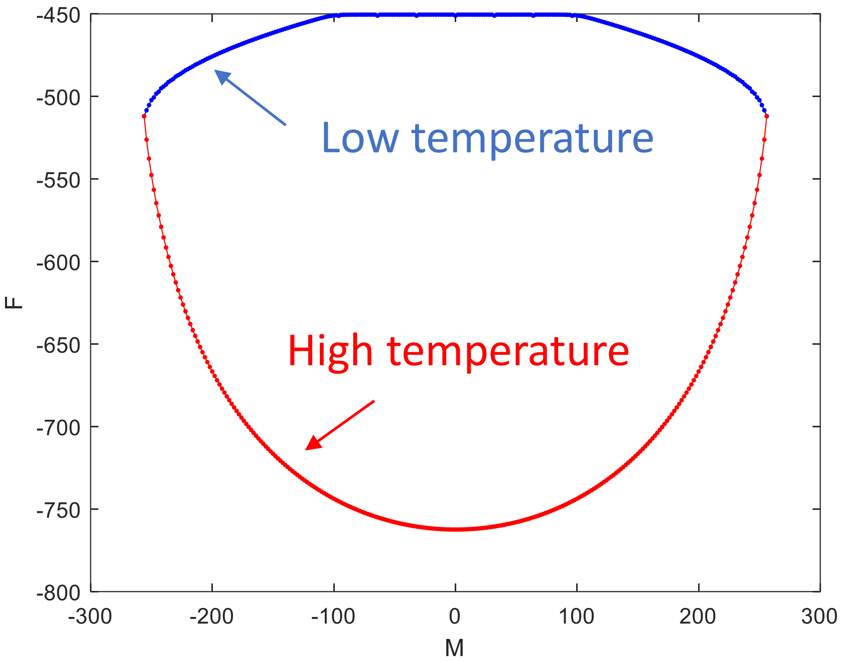


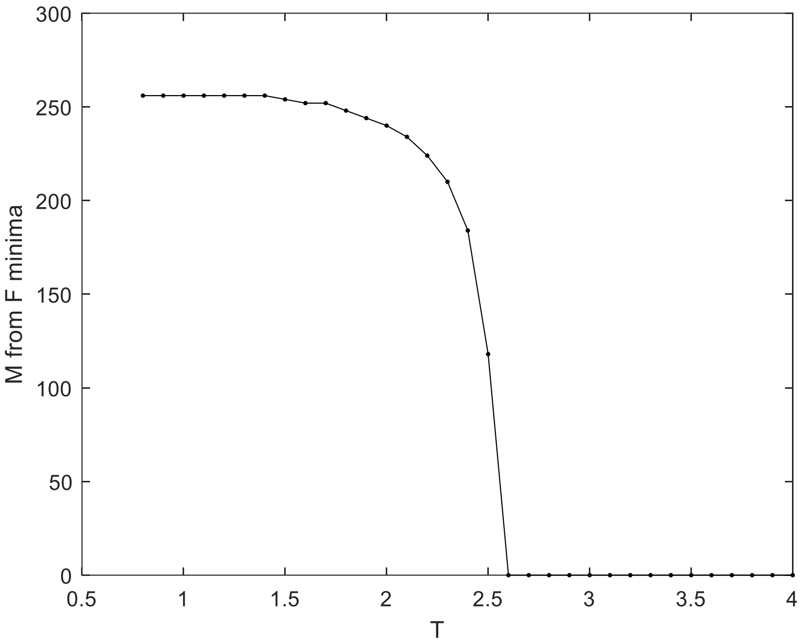


- For a 4x4 system of 16 spins, there are ~65k possible spin configurations
- Still tractable exactly (in a computer)
- Larger system?

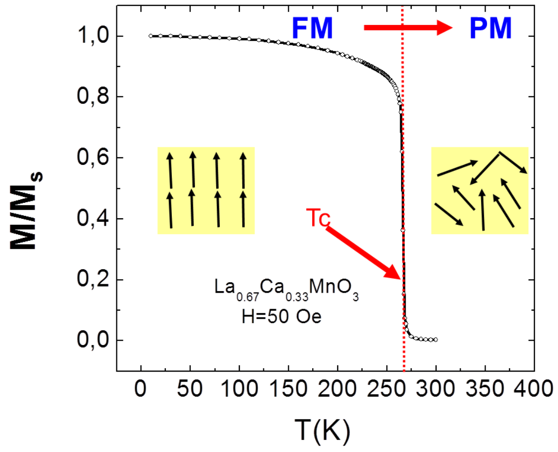
Thermodynamic properties from JDOS (16x16)







- This system has 1E77 possible configurations
- The JDOS cannot be computed exactly
- The simulations start to behave similarly to a real ferromagnet

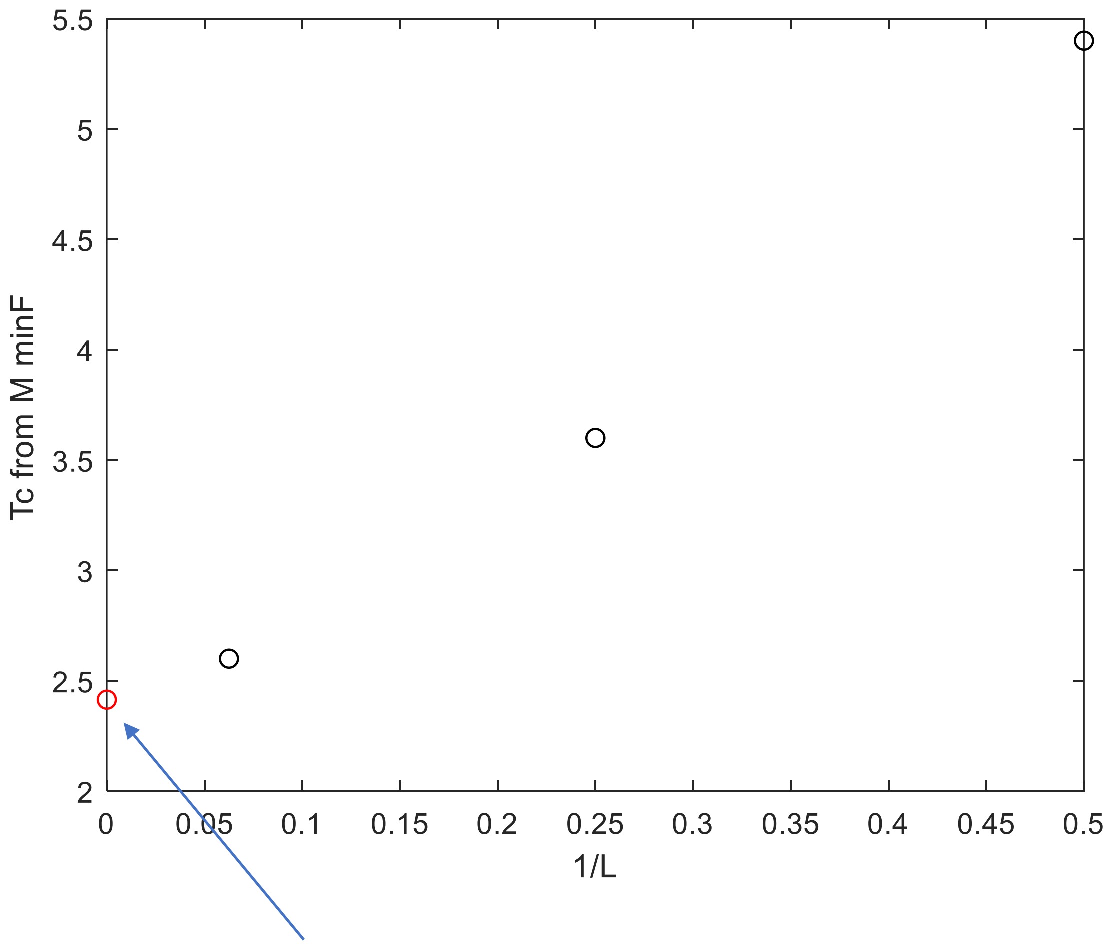


Finite size effects

- While we were not considering "large" systems, the results appear to be aiming at the right (exact) Tc result for an infinite lattice

- So, by having the JDOS (table of possible magnetization, energy and degeneracy) thermodynamic properties can be calculated

- Is it easy to estimate the JDOS of larger systems?



Exact solution (Onsager)

Estimating JDOS

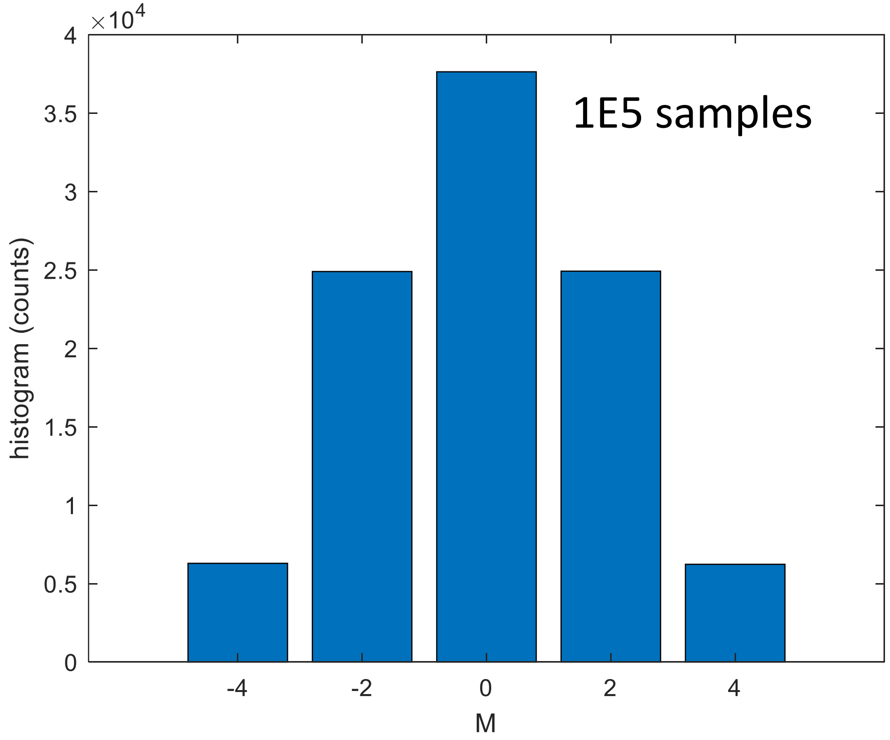
- It is actually quite difficult, due to the large number of possible configurations when the system size increases:
  - 4x4 (16 spins) : 65x10^3 <- still doable exactly
  - 16x16 (256 spins) : 1E77 configurations <- too big for listing exactly

- Even a Monte-Carlo sampling approach is not trivial
  - If random spin configurations are generated, they will be biased to low magnetization states, as these are the most probable

MC sampling 2x2

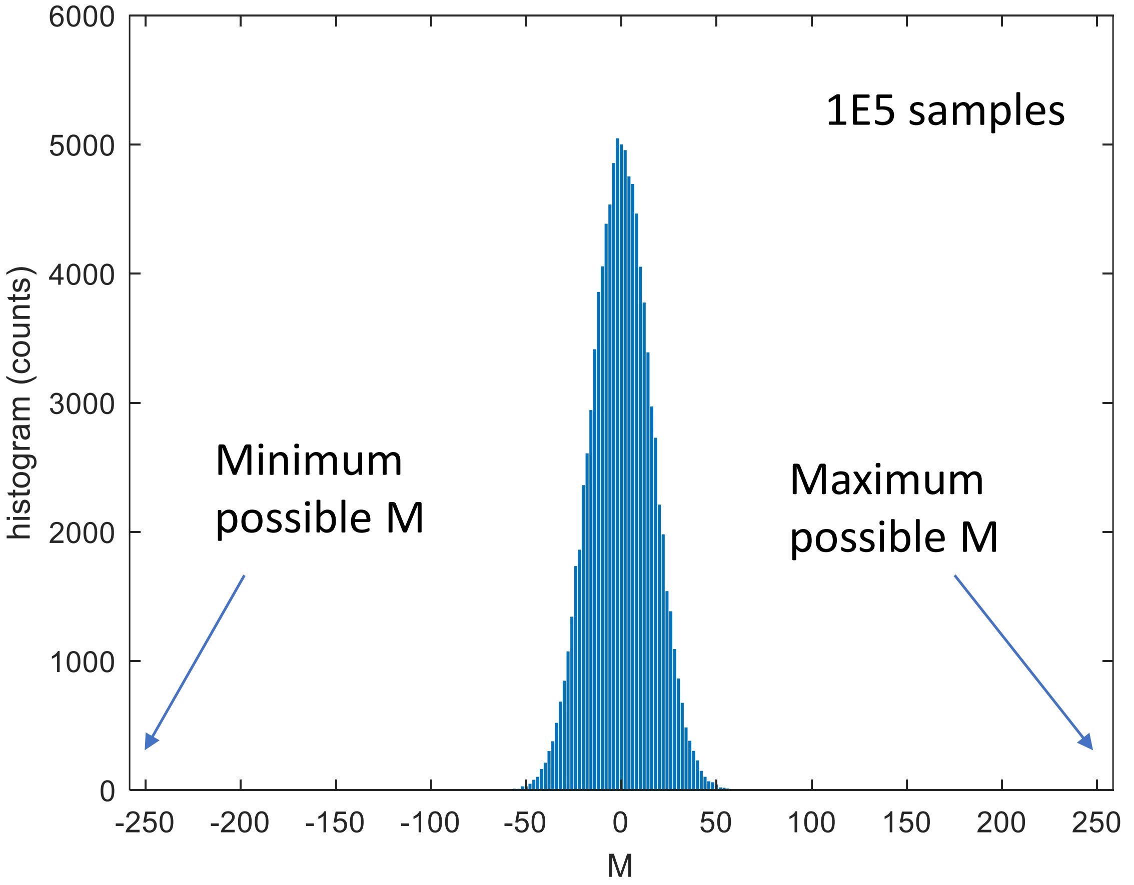
- For a system with just 16 configurations, over 1E4 samples need to be taken for a good JDOS
- Slow energy calculations (global versus local updates)
- Sampling is biased in magnetization
  - For larger systems, this type of sampling will not “see” ordered (high |M| states)

M	E	Ω exact	Ω 1E4 samples	Ω 1E5 samples
4	-8J	1	1.03	0.99
2	0	4	3.99	4
0	0	4	4.04	4
	8J	2	1.95	1.98
-2	0	4	4.02	4.02
-4	-8J	1	0.97	1



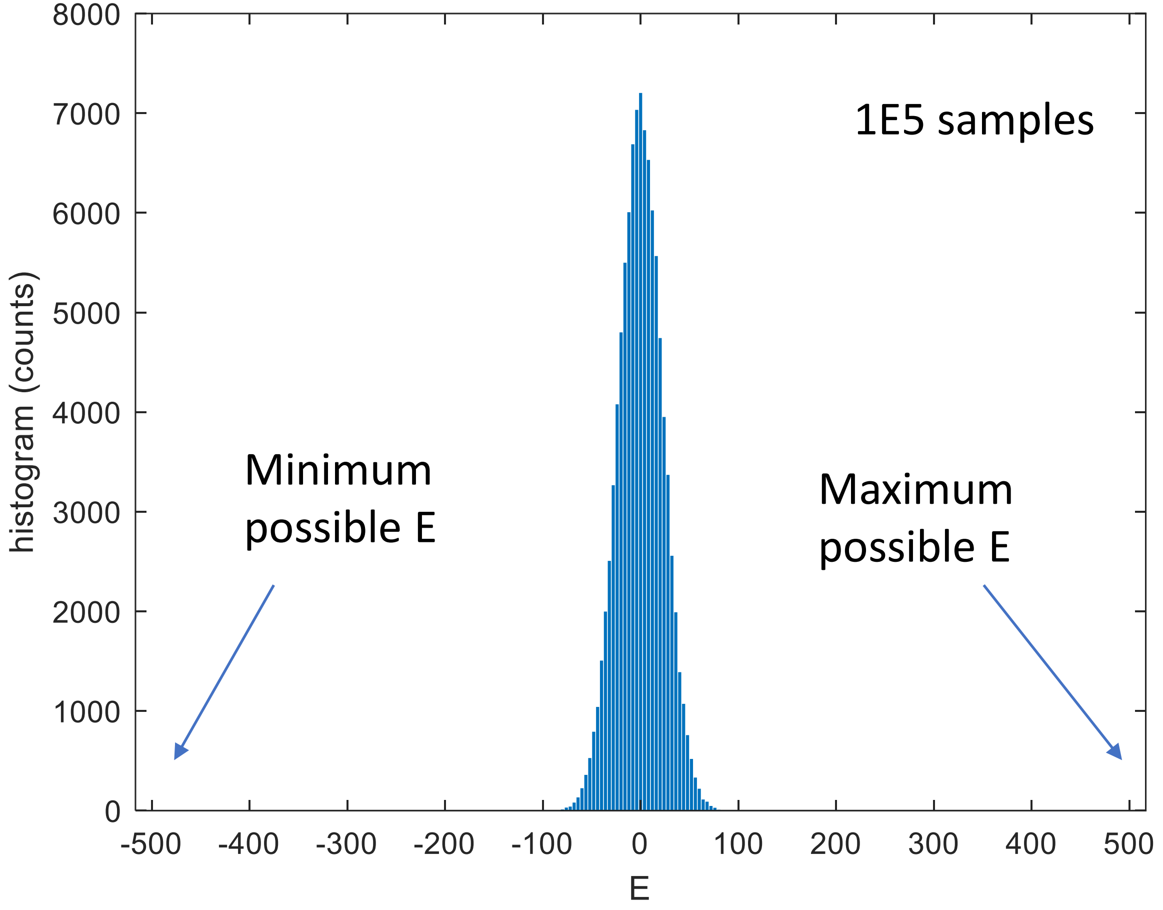
Random sampling for a 2D 16x16 Ising system

- 1E5 random samples for this system do not observe |M| values above 20% the possible value
- Many configurations are not seen by the random sampling, including two very important configurations (all spins up, and all spins down)
- The magnetization range (phase space) is not adequately explored



Random sampling for a 2D 16x16 Ising system

- Much like magnetization, 1E5 random samples for this system is not enough to observe E values near the positive and negative limits
- Both energy and magnetization phase space are not adequately sampled
  - E = -512 all spins parallel
  - E = 512 all spins anti-parallel (checkerboard)
- A JDOS estimated from these histograms would not accurately describe the system



Random spin configuration sampling of a 2D, simple square with PBC Ising lattice JDOS

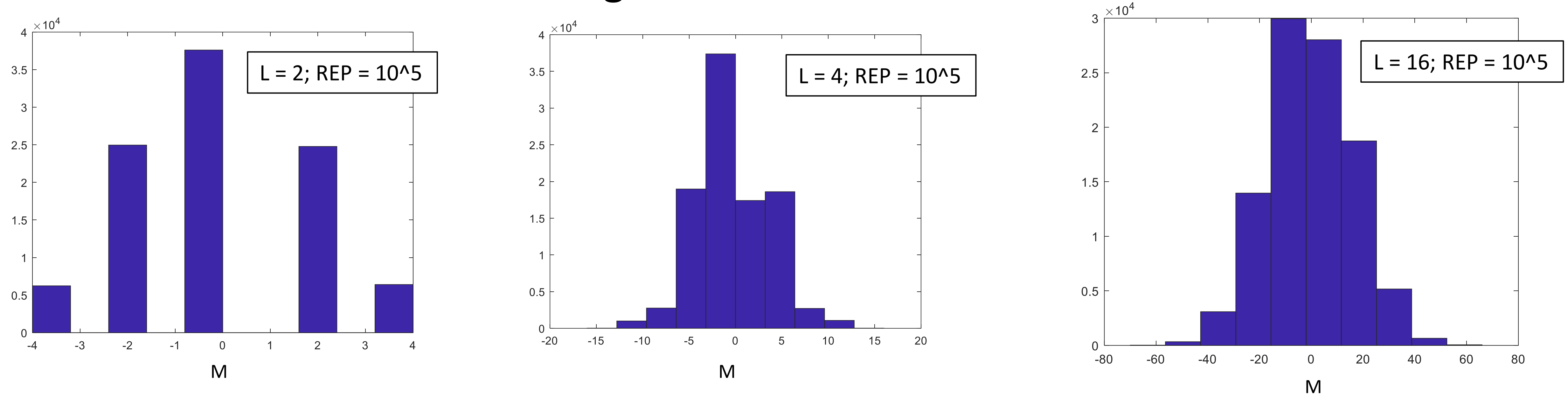
- First Matlab script: MC_sampling_Ising_2D_SS_no_vis.m
  - Input: linear system size (L) and sampling repetitions (REP)
  - Subfunction: function_Energy_Ising_2D_SS(L, S_vector): calculates energy of a spin configuration given by a [-1, 1, 1, -1, …] vector for a system size of L
  - Main outputs:
    - All observed E values (E) and M values (M)
    - Energy histogram (hist_E)
    - Magnetization histogram (hist_M)
    - Energy-Magnetization histogram (hist_EM), rows = Energy, columns = Magnetization
      - Energy value list (E_list)
      - Magnetization value list (M_list)
    - The normalized Joint Density of States (JDOS)

- Use this script to replicate the histogram figures from the three previous slides [hint: explore Matlab functions hist, histogram and bar]
- Plot the Energy-Magnetization histogram of the 2x2, 4x4 and 8x8 lattices [hint: explore contour, surf and bar3]. Is the phase space fully explored with 1E5 samples?

WORK!

Visualizing the magnetization histogram I

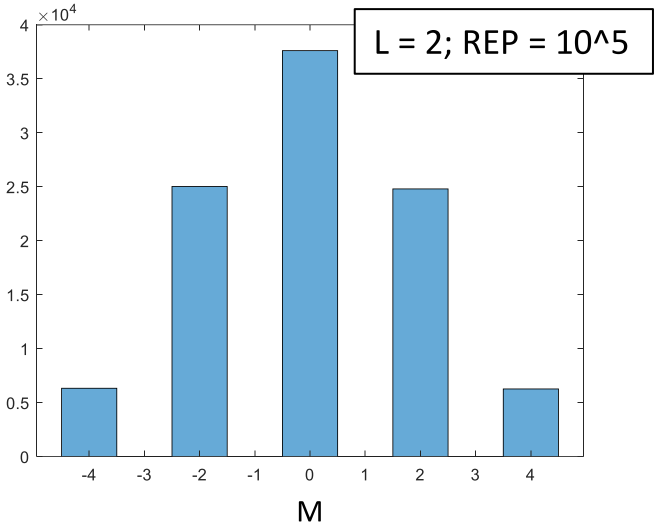
- The Matlab in-built function “hist” shows a histogram, as it should, but the automatic binning choice is not the best.

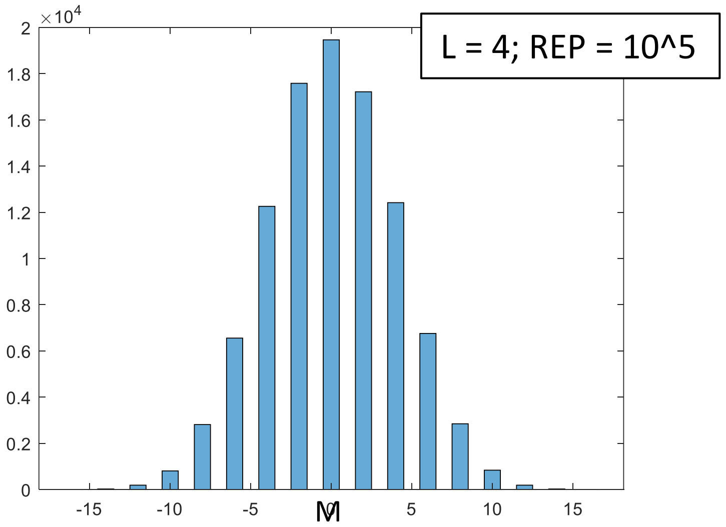


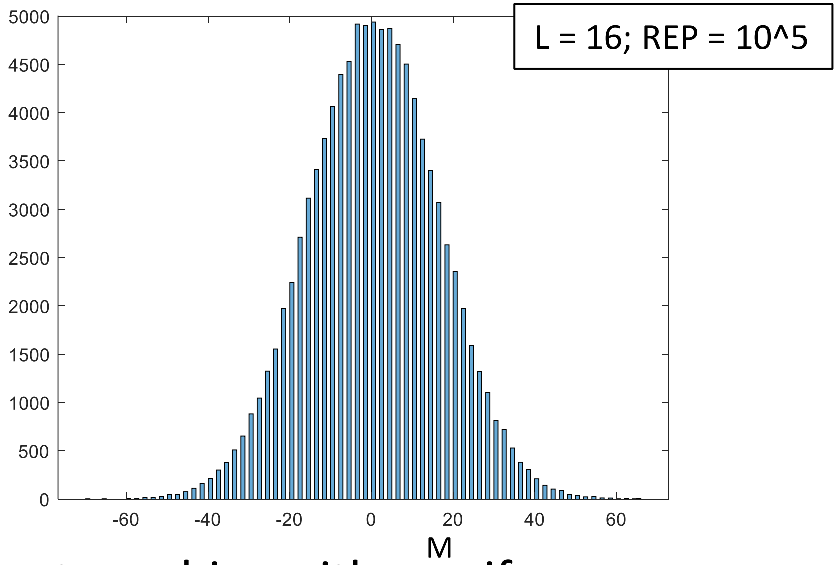
- “The elements in x are sorted into 10 equally spaced bins along the x-axis between the minimum and maximum values of x.”
- This automatic binning does not work well, even for the smallest lattice, the histogram is not centered, with a maximum at the wrong M value

Visualizing the magnetization histogram II

- The Matlab in-built function “histogram” works well for small systems, but its simple use is not enough for larger systems



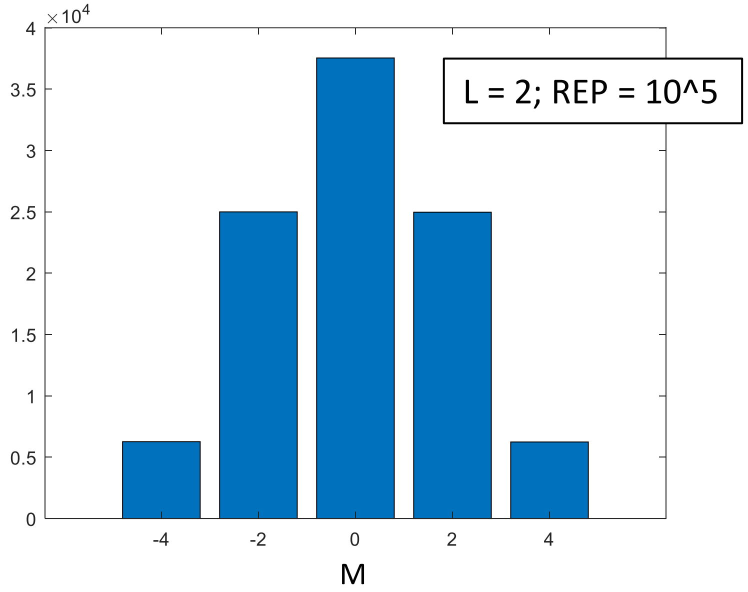


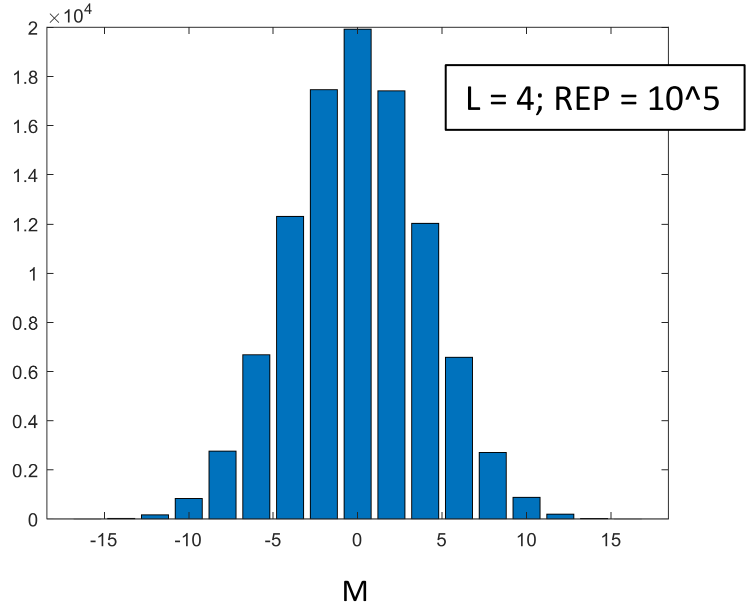


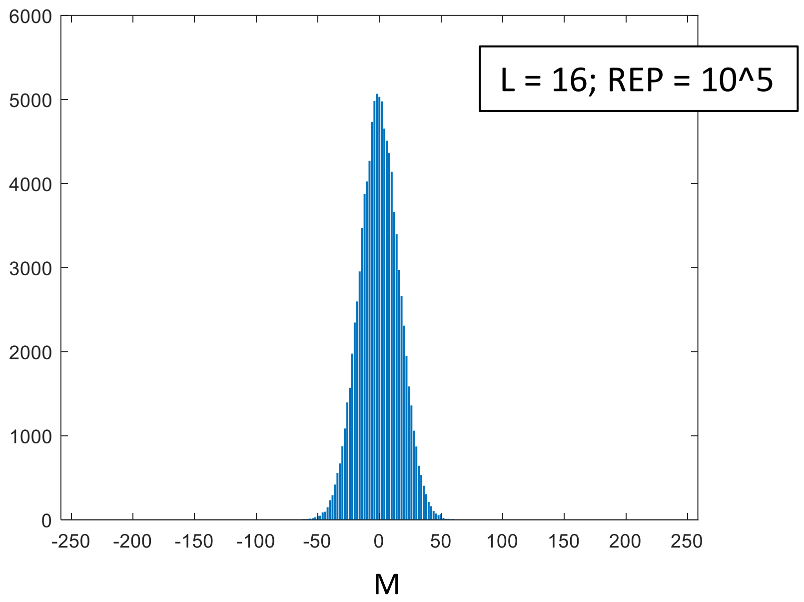
- “The histogram function uses an automatic binning algorithm that returns bins with a uniform width, chosen to cover the range of elements in X and reveal the underlying shape of the distribution.”
- This automatic binning may not work well, and may need tweaking to accurately show what we want to show
- The third plot is the magnetization histogram for L=16 and REP = 10^5, and zooming in for M=0, we can see it is not centered

Visualizing the magnetization histogram III

- Instead of letting Matlab choose the binning for the histogram, we can instead use a simple bar plot, and the calculated hist_M







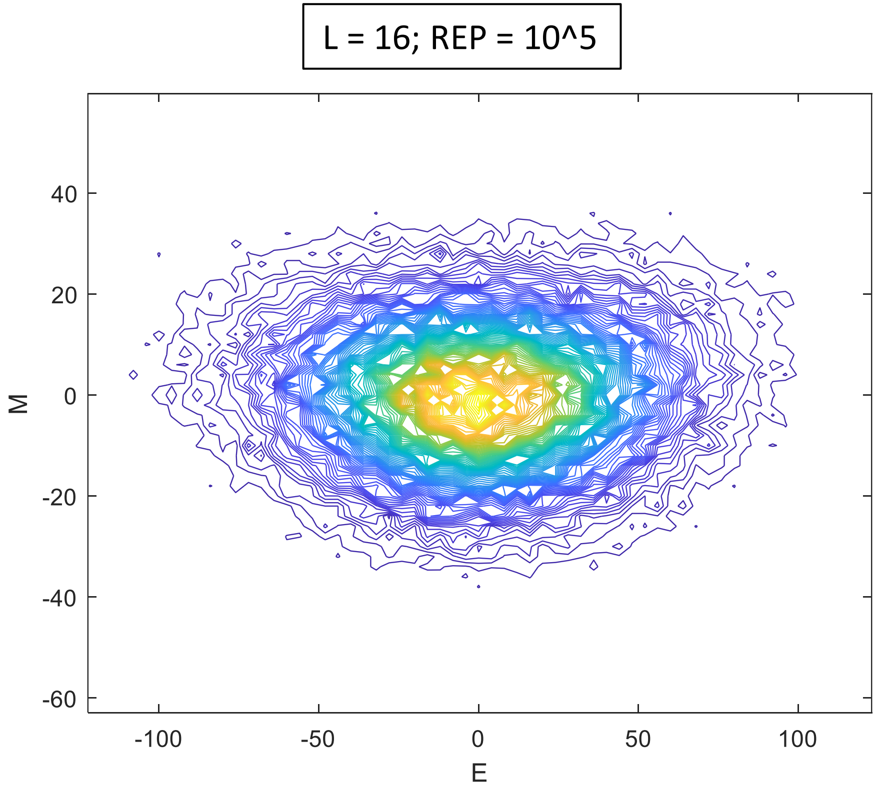
- The bar plot forces the x axis binning (or lack of it), preserving the accuracy and symmetry of the data.
- This should also be the best approach for plotting the energy histograms

Visualizing the joint energy-magnetization histogram (I)

- While looking independently at the magnetization and energy histograms will tell us if the phase space is being accurately sampled, the joint E-M histogram should show this clearly
- Now we are dealing with a 3D plot, and that brings added difficulties. Let's try the Matlab function contour.

- The plots looks nice, using increased plot detail:
  - contour(-E_list,M_list,hist_EM,100)

- Still, the data seems odd, and it would be nice to see this in 3D…

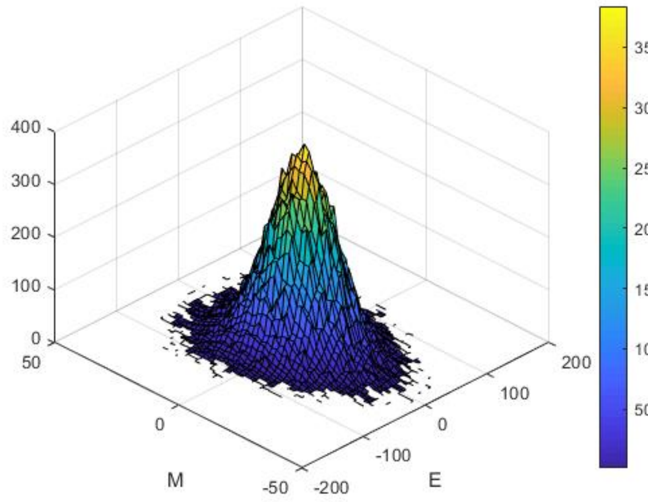


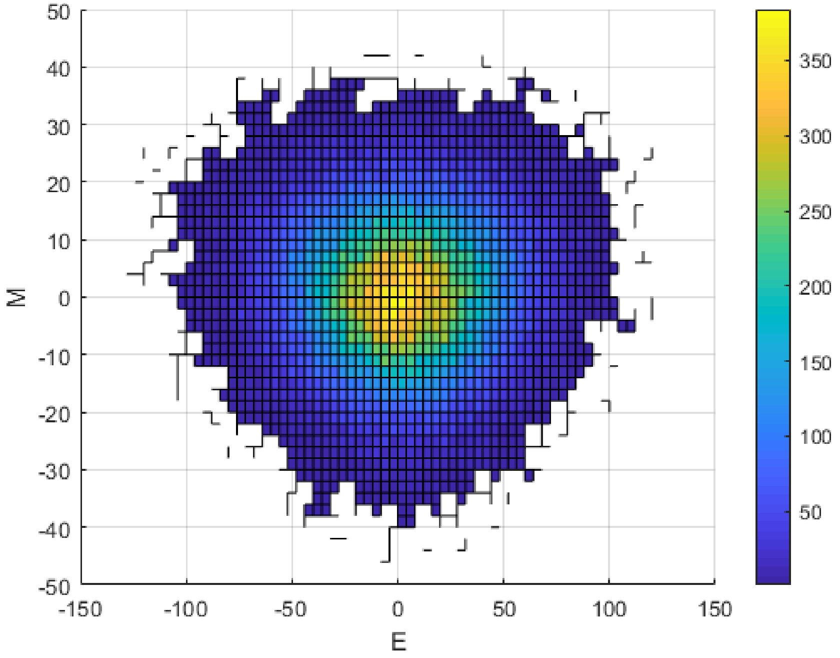
Visualizing the joint energy-magnetization histogram (II)

- Now let’s try the Matlab function surf. This is a “real” 3D plot, which allows side views

- The plots look colorful and nice, with some tricks:
  - hist_EM(hist_EM==0)= nan;
  - Colorbar
  - View(2)
  - view(-45,45)
- The plot is not centered, and what are those squiggly lines?

L = 16; REP = 10^5



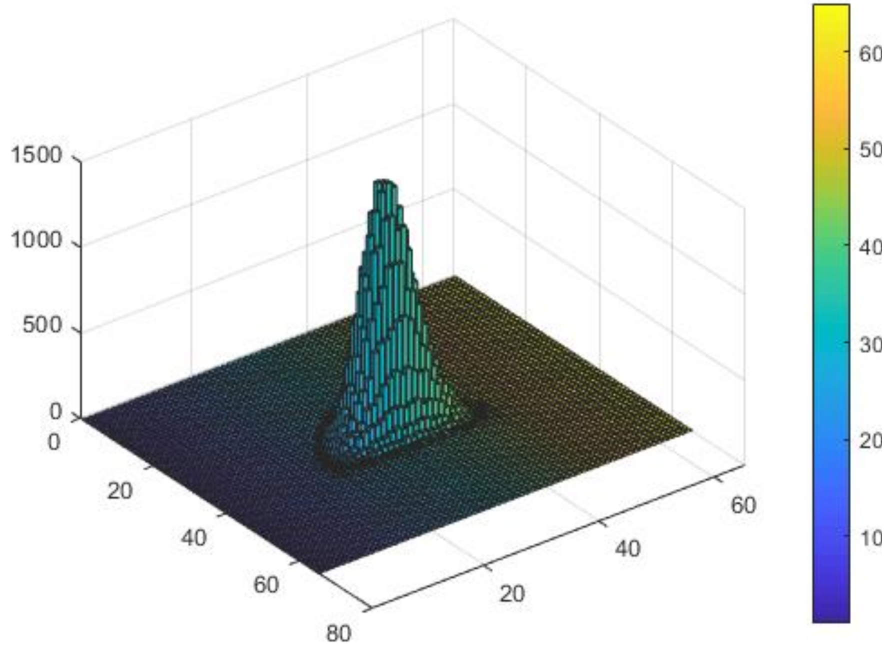


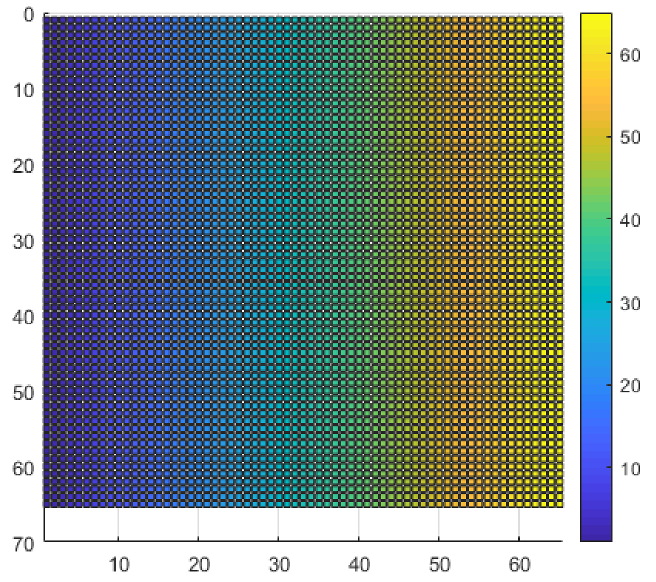
Visualizing the joint energy-magnetization histogram (III)

- It seems we still don't have the kind of plot we want. What about bar3?

L = 8; REP = 10^5

- Using bar3 directly will not work
  - You cannot define the axis tick values via input
  - The color bar shows the wrong axis
  - Even with NaNs, the plot color is not good
  - The 2D (top view) does not show any information

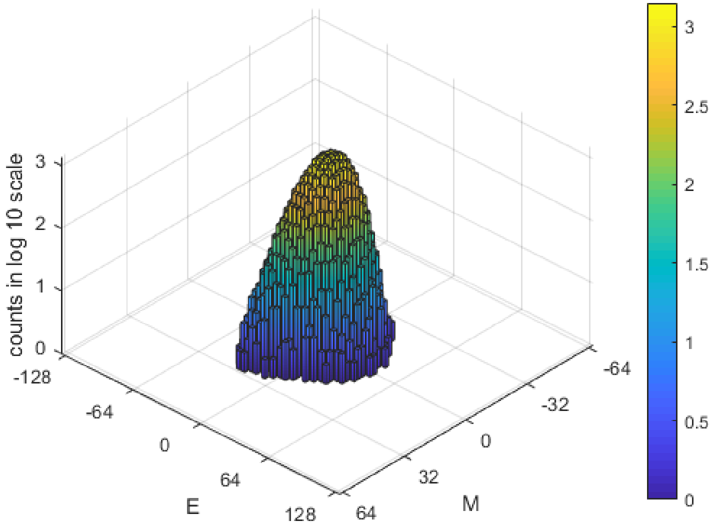


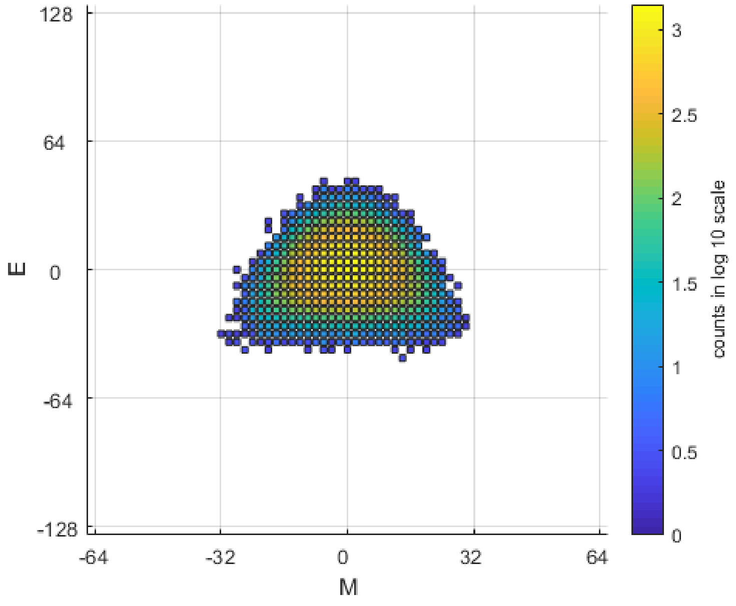


Visualizing the joint energy-magnetization histogram (IV)

- The bar plots were the best solution for the 2D histograms, so we dig a little deeper.

- These look better, the plots are centered, without any weird artifacts
- Tricks:
  - Log scale for better color visibility
  - White color for 0 z value
  - Manually defined scales and tick values
  - 50 lines of code!





L = 8; REP = 10^5

Valuable lessons

- Automatic plot types are excellent when they do exactly what you want
- For more complex data plots, you will invariably need to start looking “under the hood”
- Most of the times, someone else already solved your technical issue, and looking for the solutions online (instead of working them out by yourself) is the pragmatic approach

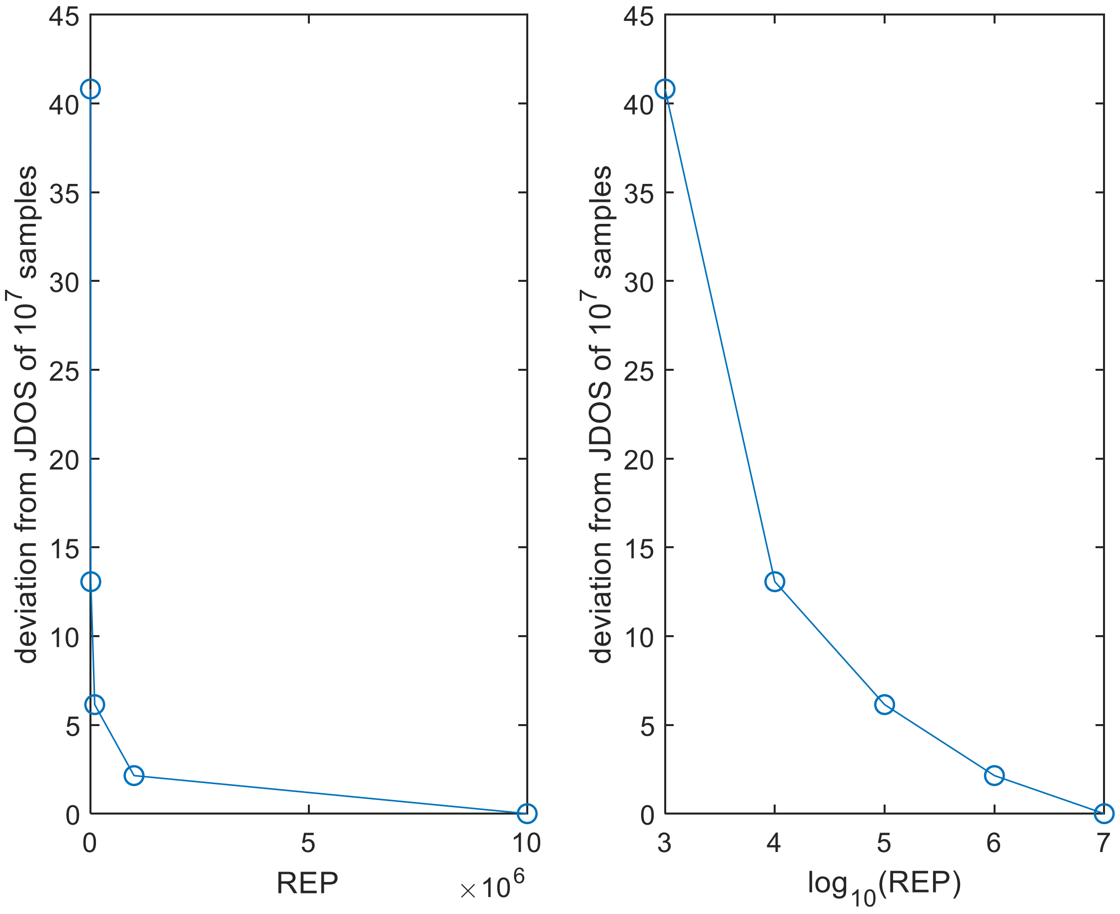
Numerical convergence and accuracy of random configuration sampling

- Using the small 2x2 lattice as an example, we previously saw how the random configuration sampling converged to the correct value for high sampling counts
- When we don't know the exact value, how can we show the method is converging?

M	E	Ω exact	Ω 1E4 samples	Ω 1E5 samples
4	-8J	1	1.03	0.99
2	0	4	3.99	4
0	0	4	4.04	4
	8J	2	1.95	1.98
-2	0	4	4.02	4.02
-4	-8J	1	0.97	1

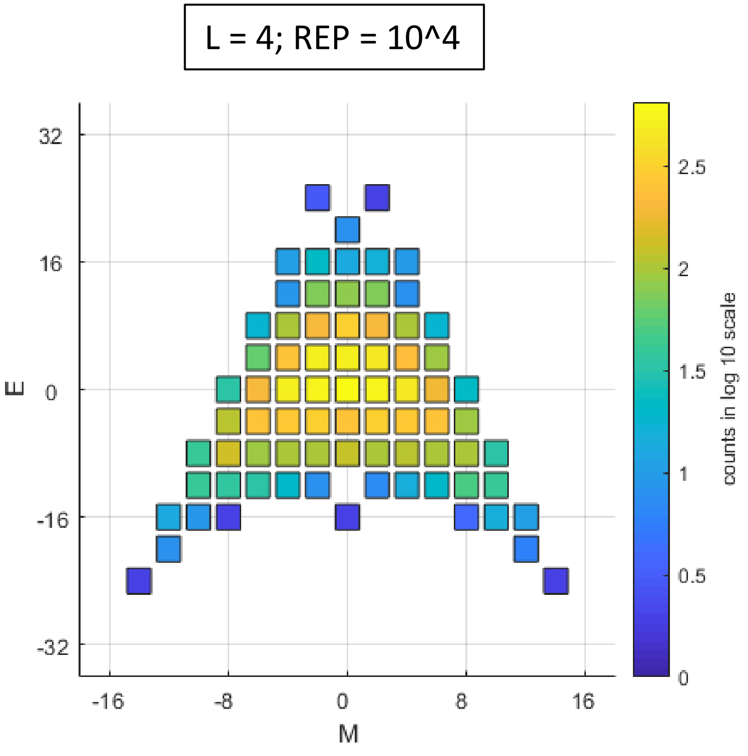
Convergence for the 4x4 lattice

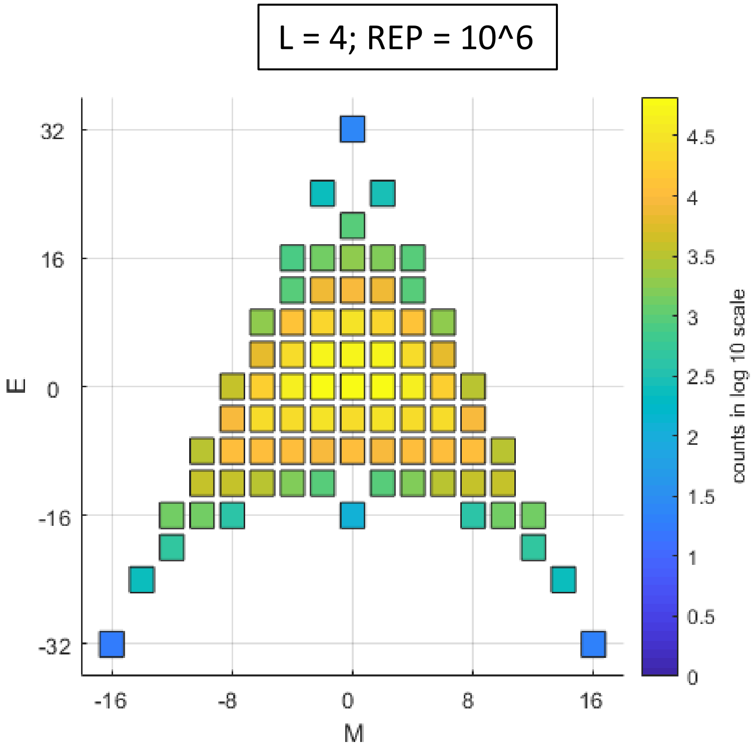
- We can take as reference the simulation with the highest number of samplings we can reasonably do, and check the trend of deviations
  - Deviation = abs(JDOS - JDOS[1E7])/JDOS[1E7]
- Logarithmic scale is useful as convergence is slow



Is the phase space properly sampled?

- As we have seen from the simulation of larger systems using this Monte-Carlo approach, the phase space sampling is denser near M=0 and E=0
- Only with large sampling it is possible to get data for the following states/configurations
  - All spins up (M=16,E=-32)
  - All spins down (M=-16, E=-32)
  - Checkerboard (M=0, E=32)
- This evolution of phase space sampling would be nice to see in a video





If a picture is worth a thousand words…

- Visualizing the histograms at the end of the sampling run allows us to assess the final result, but a video would allow us to visualize the dynamics of the phase space exploration

- Videos can be easily made in Matlab via the 'getframe' command

- We can start by making simple videos of the 2D magnetization and energy histograms, which highlight the biased sampling of both values

- We then move on to making videos of the 3D energy-magnetization histogram

WORK!

Main conclusions

- The simple Monte-Carlo approach of generating random spin configurations to explore the phase space works, since
  - It can sample the whole Energy-Magnetization phase space
  - It smoothly converges to an accurate value
- But…
  - The number of samples must be larger than the number of possible states, which is not efficient, and makes this approach worse than just listing all the spin configurations/states sequentially
  - There are, thankfully, much more efficient Monte-Carlo approaches for estimating the JDOS of the Ising model, which we will discuss in the next class