Spring 2022 - PHYCS426

INVESTIGATING MAGNETISM WITH THE ISING MODEL

Instructor

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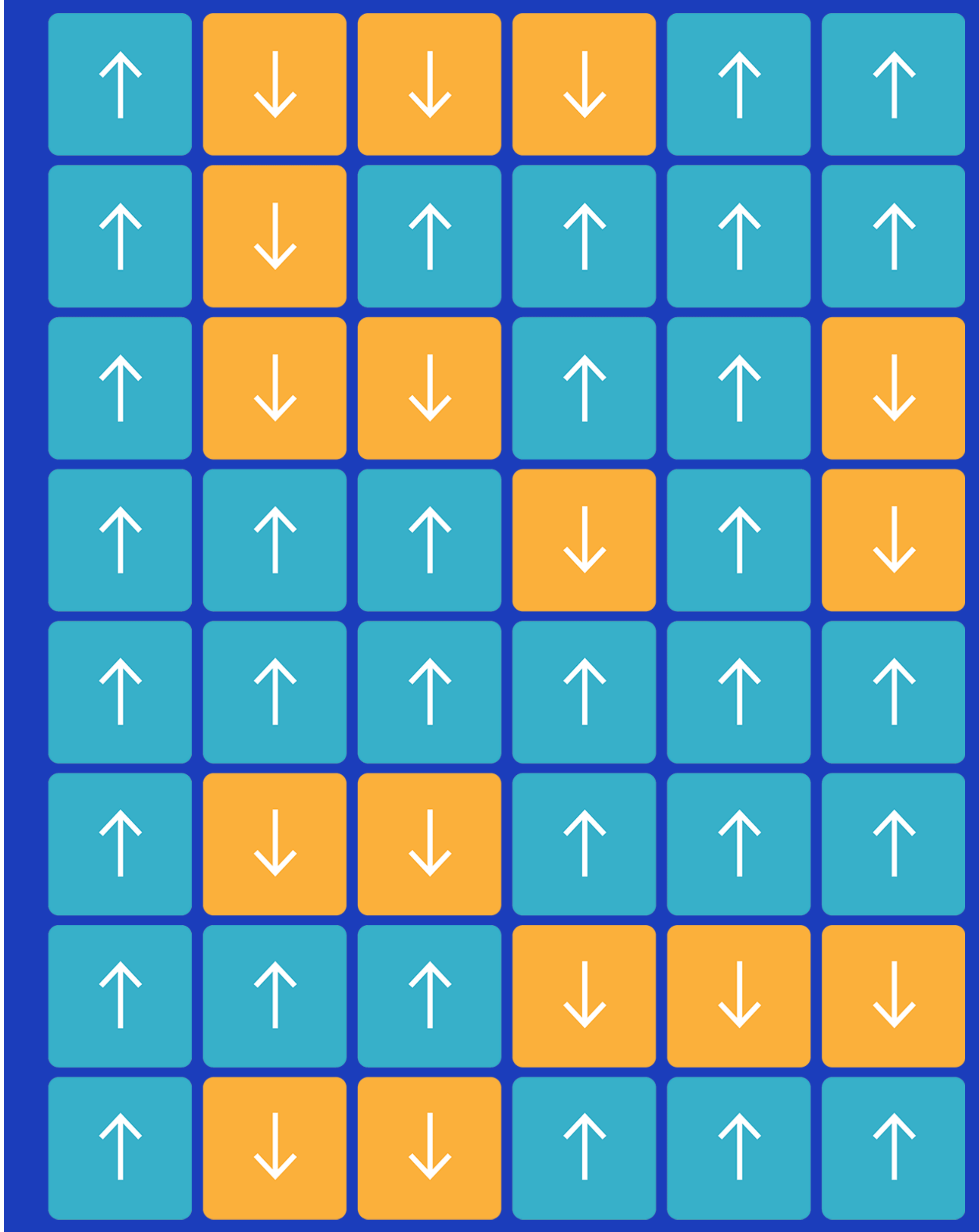

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INTRODUCTION

- The Enduring Mystery of Magnets
- Types of Magnetisms
- The Ising Model
- Monte Carlo Metropolis Method

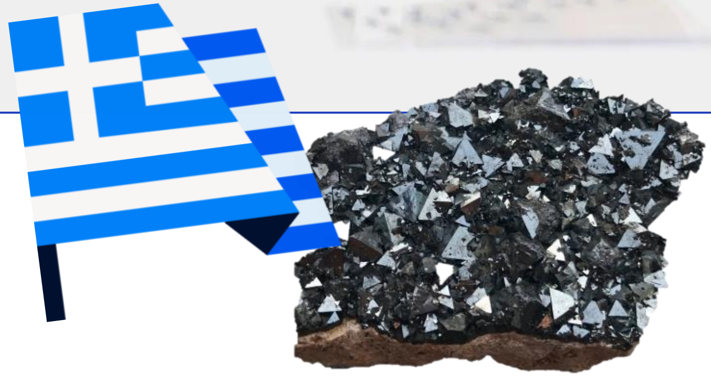
The Enduring Mystery of Magnets

How do magnets work?

It turns out we need quantum mechanics to fully explain it.

Ancient Greeks found that certain stones attracted pieces of iron.

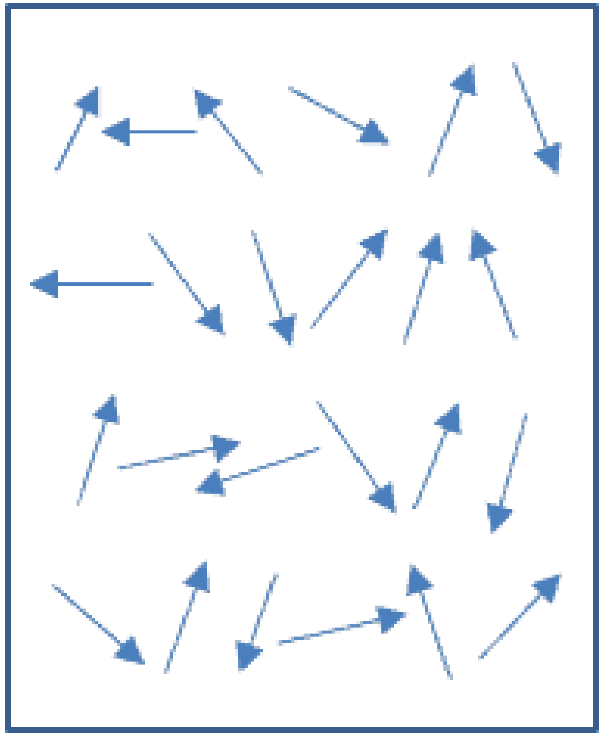
In fact, the word “magnet” comes from the Greek region of Magnesia, where these stones were observed.



Types of Magnetisms

Paramagnetic Materials:

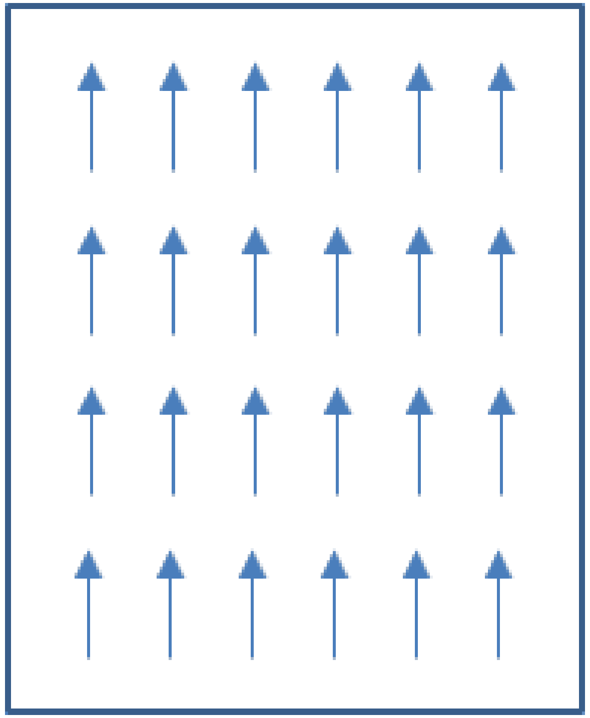
- Composed of atoms/ions that have a permanent atomic dipole.
- Aligns in the direction of external magnetic field. No permanent magnetization without external field.
- Susceptibility X is small and greater than 0.



Paramagnetic ordering

Ferromagnetic Materials:

- Possess a permanent magnetization (via domains), even in the absence of external field.
- Strongly aligns with external magnetic field.
- Possess very large positive susceptibility.
- Characterized by a critical Temperature called Curie Temperature above which they exhibit paramagnetism.



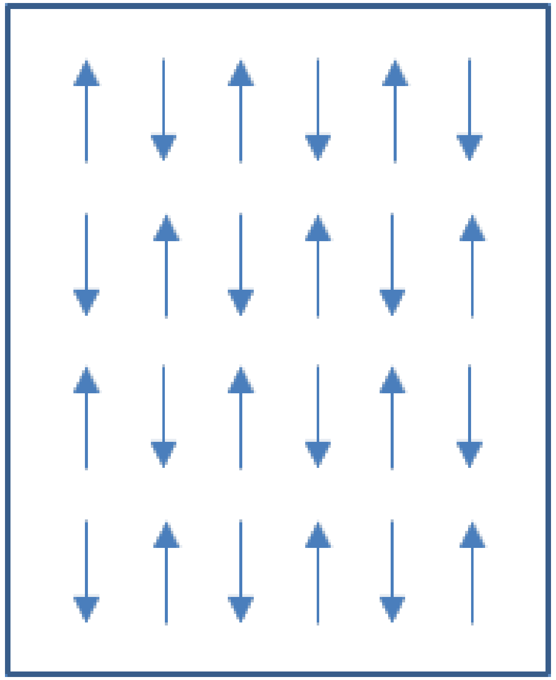
Ferromagnetic ordering

Anti-ferromagnetic Materials:

- Unlike ferromagnets, the intrinsic magnetic moments tend to cancel each other out. (Due to neighboring unpaired electrons having opposite spins)

- Characterized by the Néel temperature, above which the material exhibits paramagnetic behavior.

- Usually not attracted by external field, with small susceptibility.

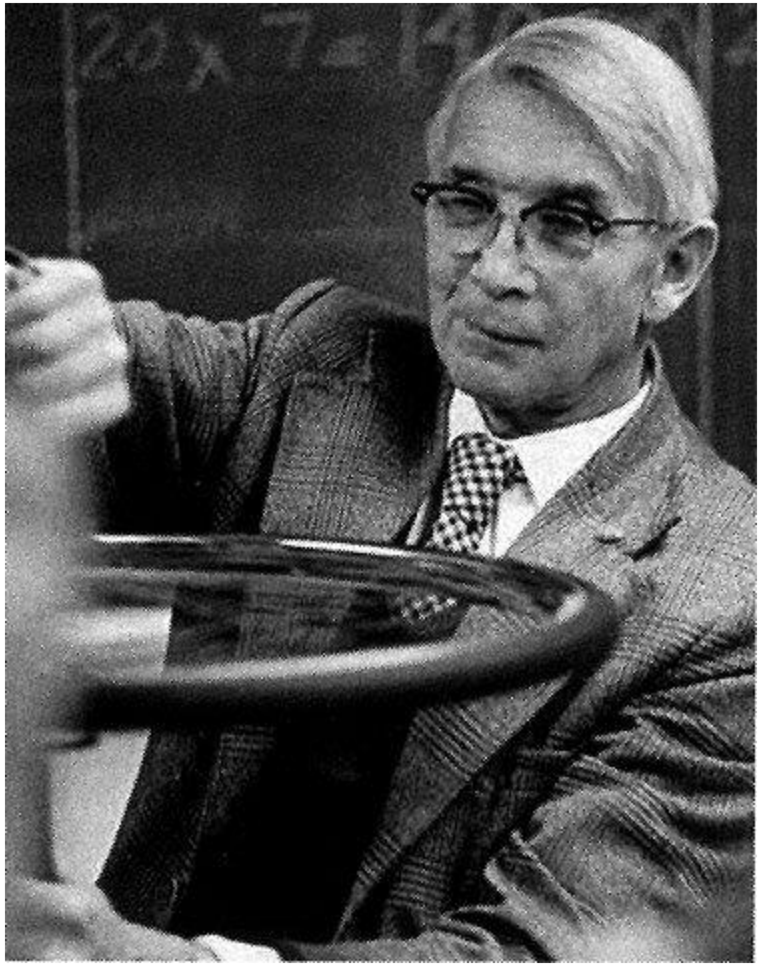


Antiferromagnetic ordering

The Ising Model

The Ising model is a toy model of magnetism that simplifies the picture of magnetism at the atomic level.

It models the interaction of atoms by treating them as small magnets ("Spins") that point either up/down.

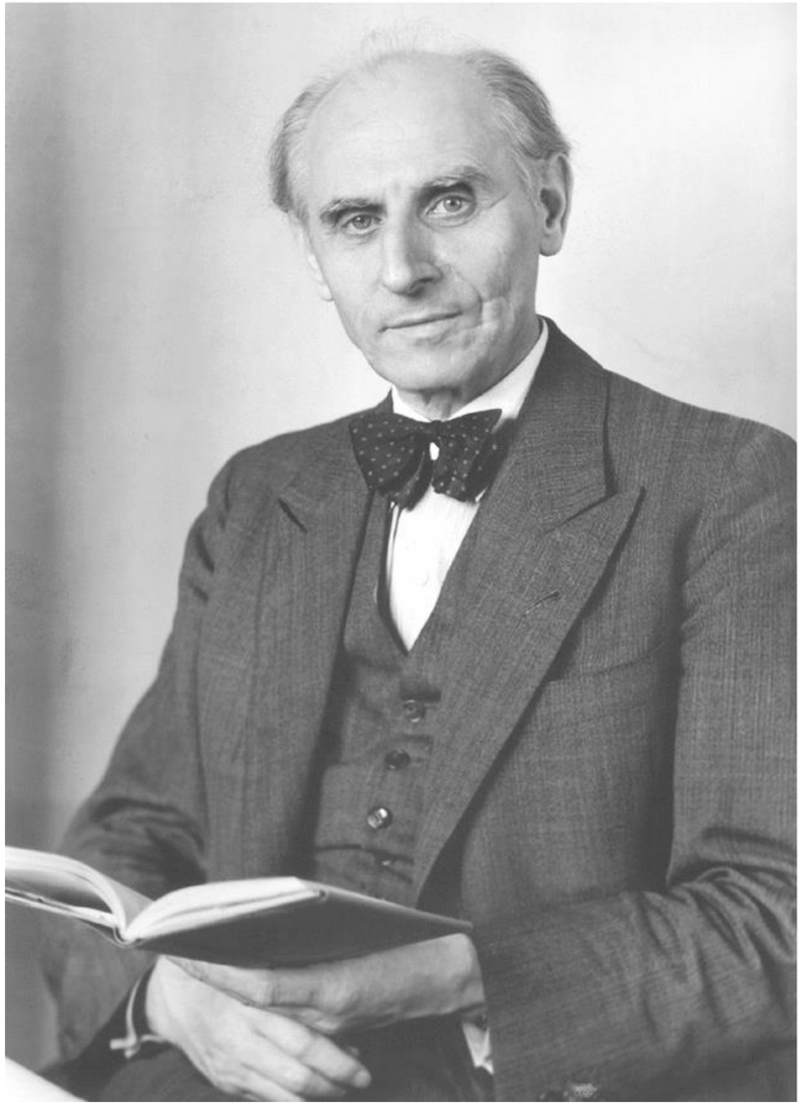


There are 2 competing "forces" at play:

1) The interaction of magnetic moments/"spins" of the atoms with each other and external magnetic field. (This tends to align them).

2) The tendency of external temperature to induce random fluctuations in the system.

$$H = -\sum_{i,j} J_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i$$



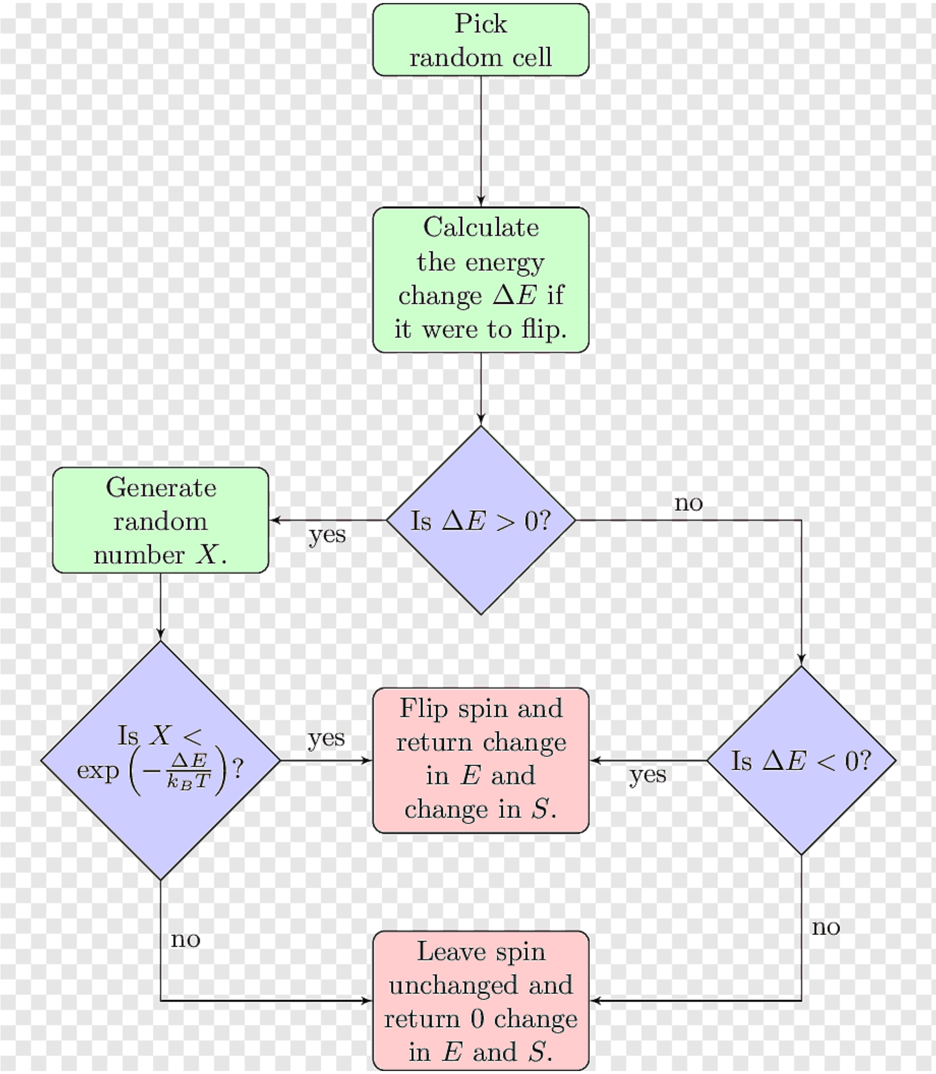
Monte Carlo Metropolis Method

- Take a grid of spins and assign them an initial spin. Use periodic boundaries

- Go over the grid, and decide to flip/leave the spin unchanged based on "Metropolis-Hastings" Algorithm (Figure on right)

- Do the same for all spins in the grid

- Repeat this for specified "Monte Carlo Steps"



MAGNETIC PROPERTIES

- Magnetic Moment and Magnetization
- Magnetic Susceptibility
- Curie and Néel Temperature
- Coercive Field

Magnetic Moment and Magnetization

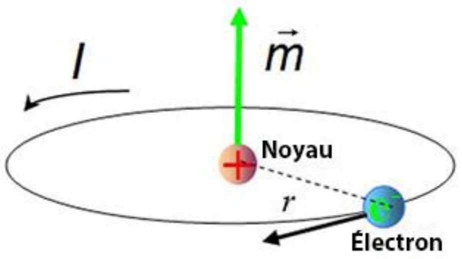
Magnetic moment is a measurement of magnetic dipole strength.

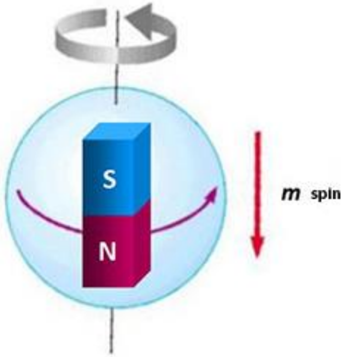
Magnetization is the density of magnetic dipoles, which are induced in a magnetic material by an external magnetic field.

Different materials react differently to external field, which allows us to classify them (ferro,para etc.).

$$\mu = IA \qquad M = \frac{\mu}{V}$$

$$M = \Sigma\, S_{ij}$$

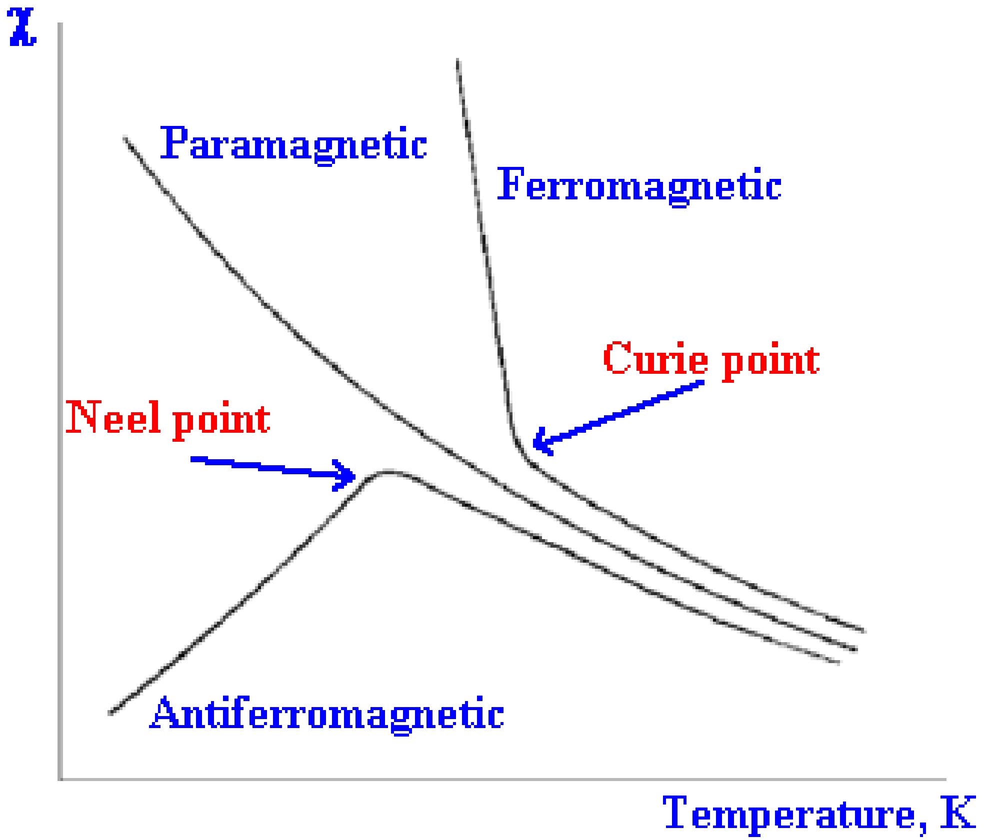




Magnetic Susceptibility

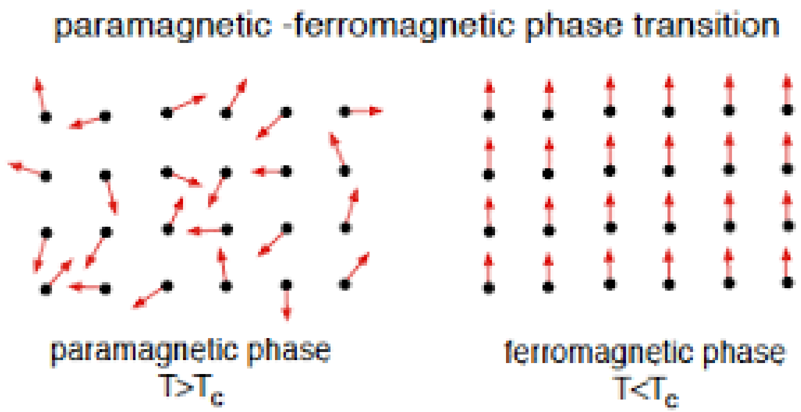
Magnetic susceptibility $M=\chi H$

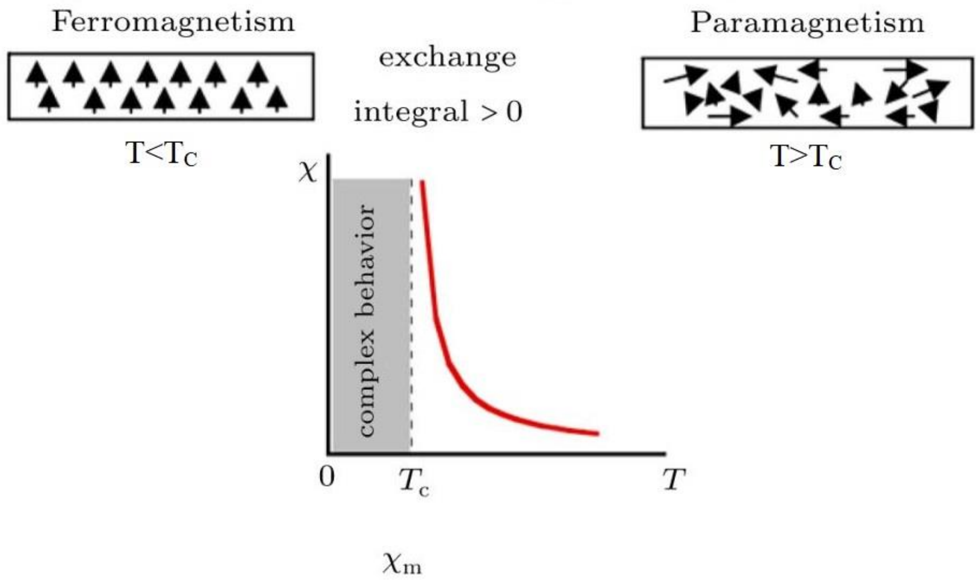
- Indicates the extent of magnetization in response to an external field H.
- Studying Susceptibility behavior allows us to classify magnetic materials.
- The sign indicates whether a substance is attracted/repelled.
- Susceptibility is usually a function of the temperature and indicates nature of magnetism.



Curie Temperature (Tc)

- It is the temperature at which a ferromagnetic material transitions into a Paramagnetic one.
- Below Curie temperature, the material is said to have "spontaneous magnetization“
- Curie Law is accompanied by first/second order phase transitions in several properties of the magnet: <M>,X & C



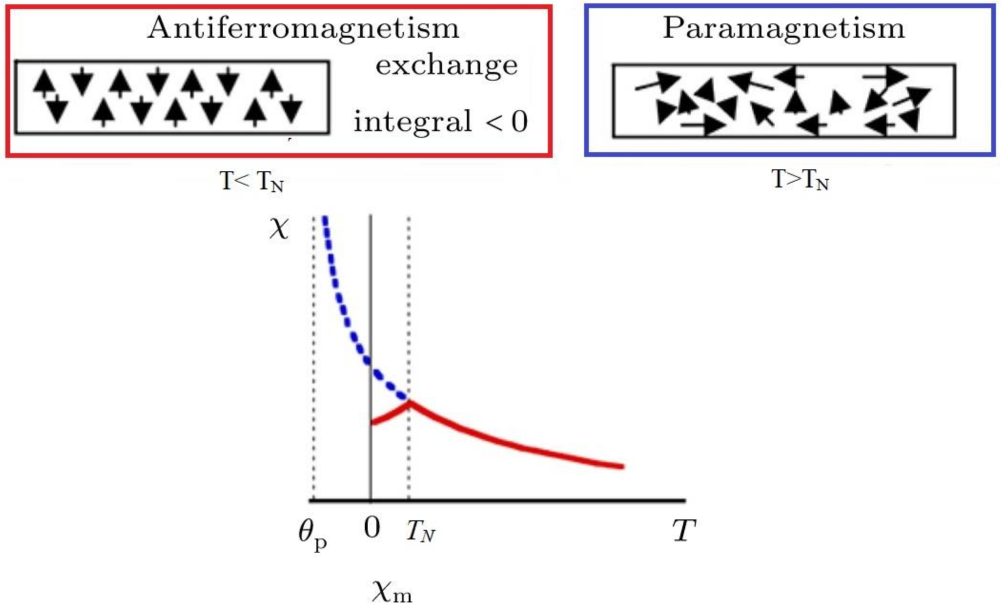


Néel Temperature (Tn)

- It is the temperature at which an antiferromagnetic material transitions to paramagnetism.

- At Néel temperature, the anti-parallel alignment of the material is destroyed.

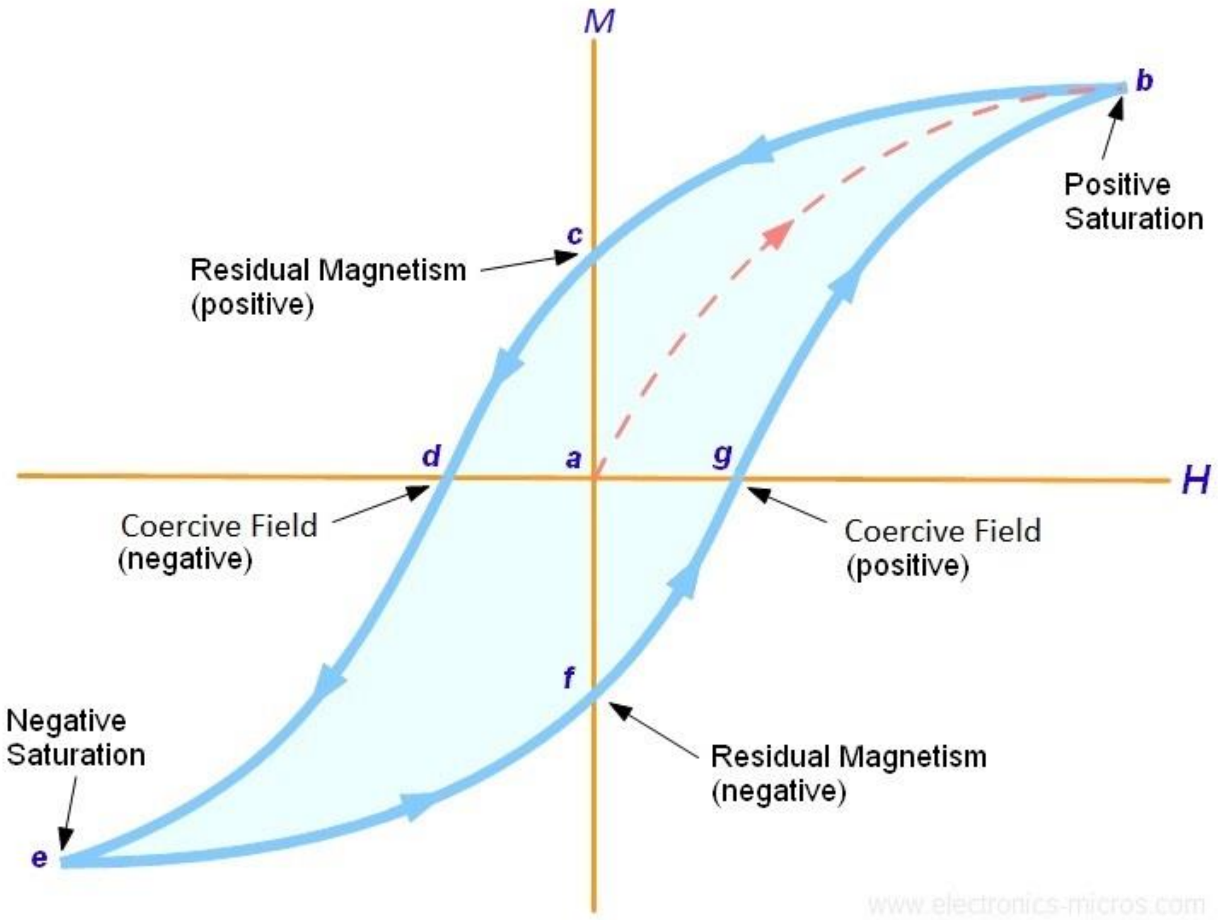
- Similar to Curie temperature, Néel temperature accompanies phase transitions in the magnetic properties of the substance.



Coercive field

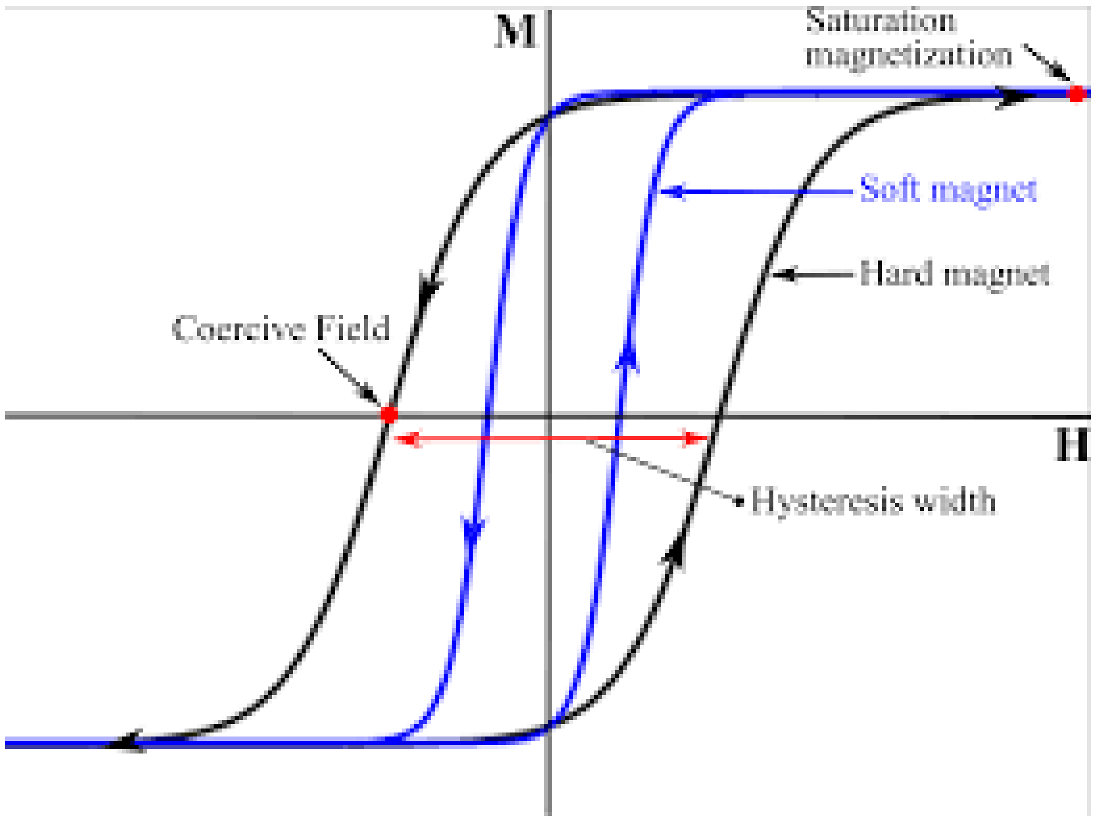
- It is the strength of applied magnetic field (H) required to demagnetize a ferromagnetic material.

- For a permanent magnet, we want the coercive field to be large.



- Coercivity depends on how fast we change the magnetic field (annealing time).

- The coercive field reduces as we increase the temperature, going to 0 as the material transitions to paramagnetism.



RESULTS & DISCUSSION

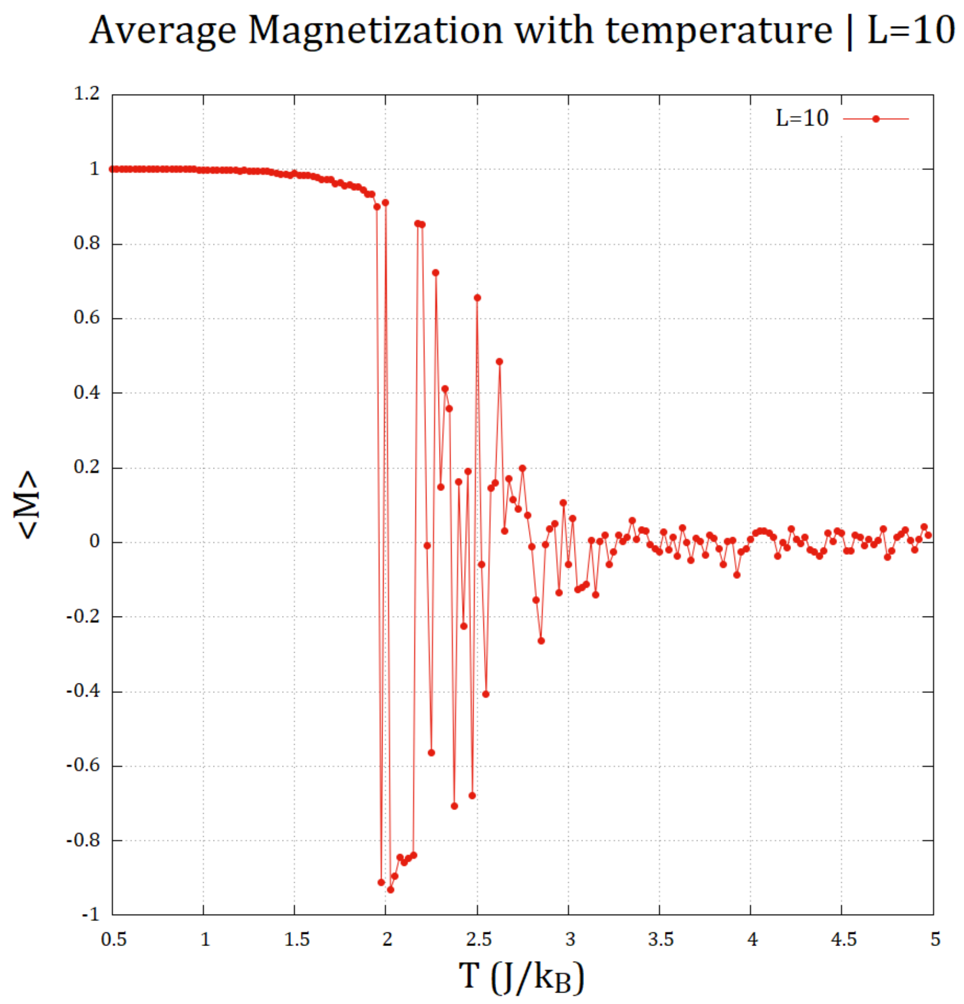
- System Size, 2D and 3D Analysis
- Coupling Constant Analysis
- Anti-ferromagnetism
- Arbitrary Spin Direction in 2D

System Size and 2D Analysis

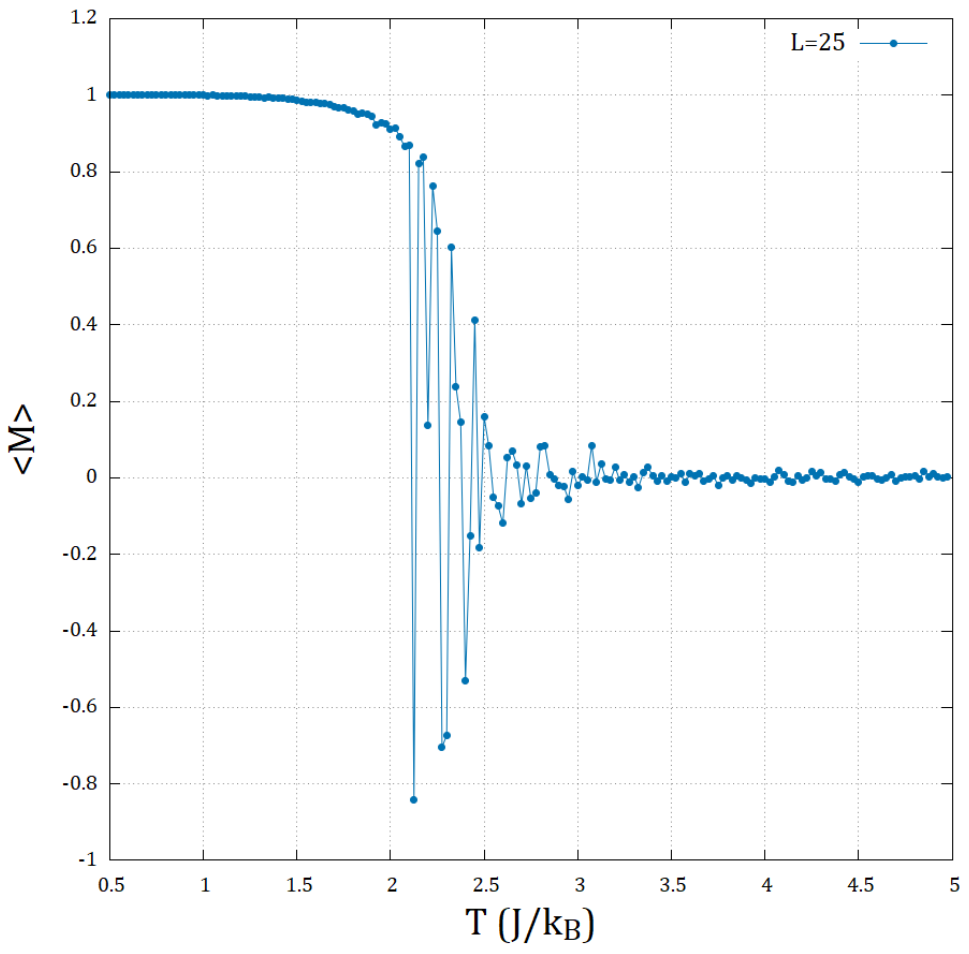
As we increase the system size the fluctuation near the Curie temperature (Tc) decreases.

That let's get more precise value of Curie temperature (Tc).

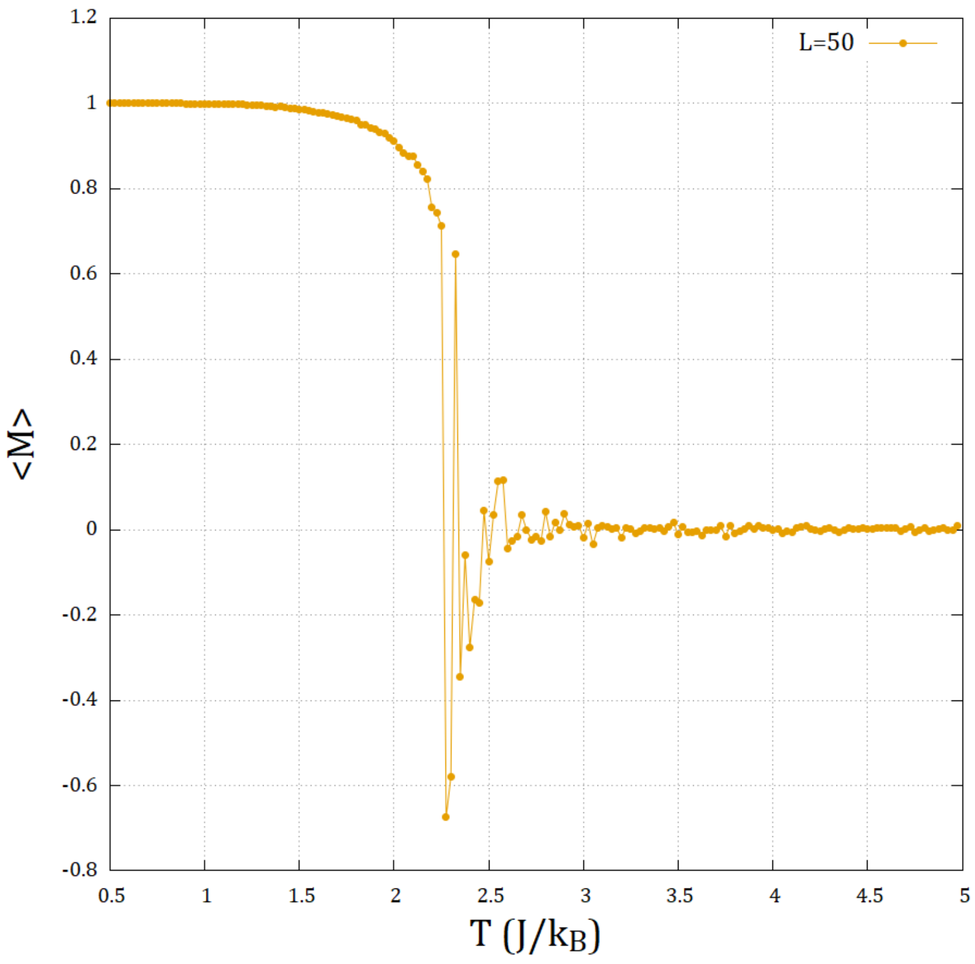
Another way to find Curie temperature (Tc) when M goes to zero is by interpolation.



Average Magnetization with temperature | L=25



Average Magnetization with temperature | L=50



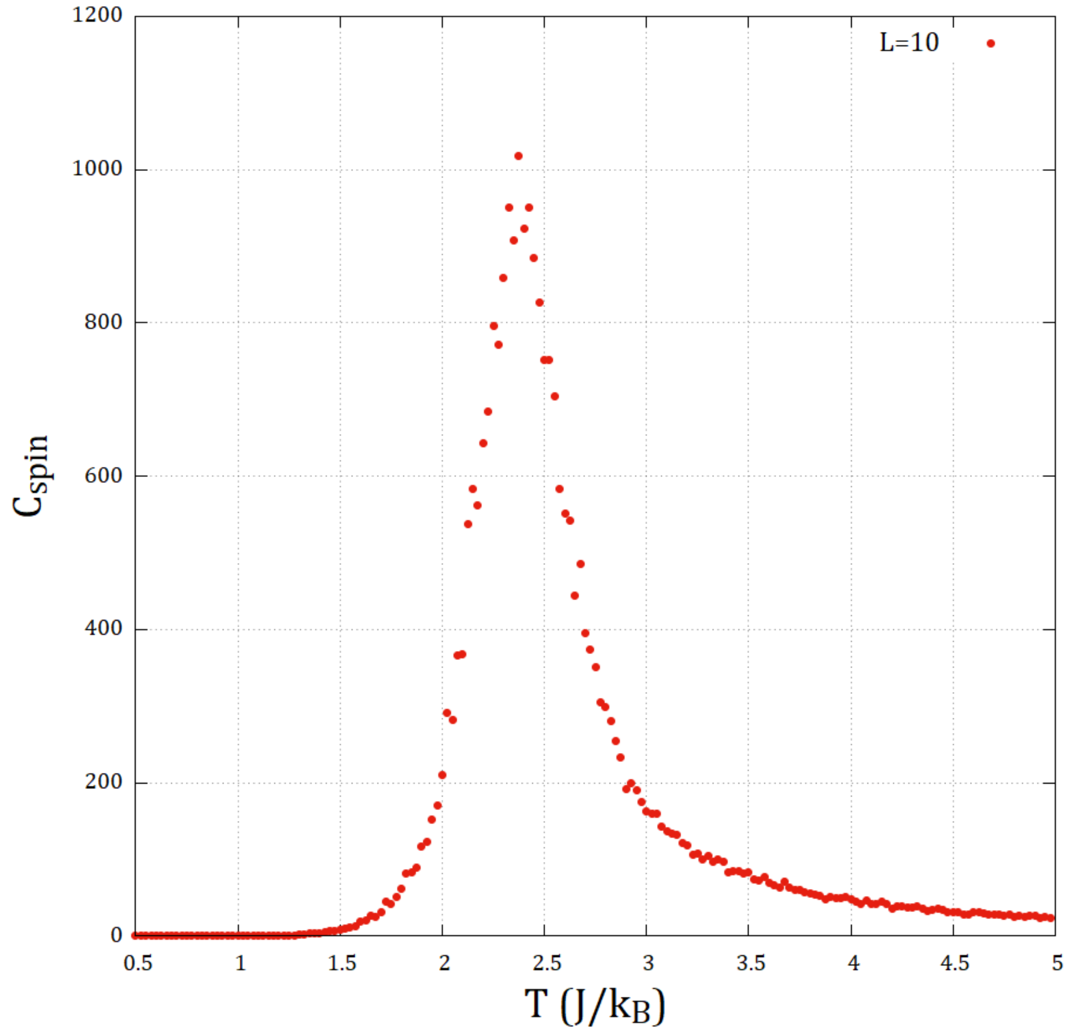
System Size and 2D Analysis

HEAT CAPACITY vs TEMPERATURE
C vs. T

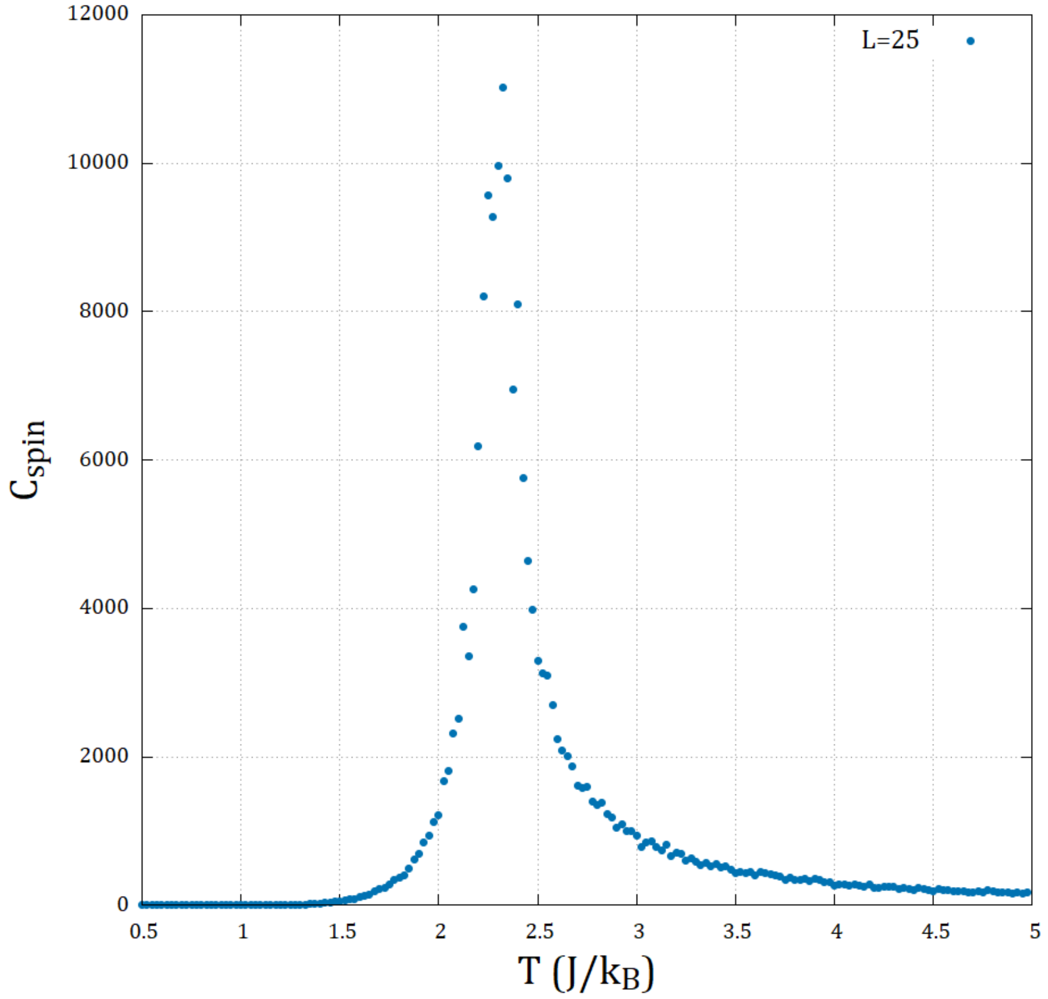
In Ising model, Specific heat capacity per spin is given by:

$$C_{spin} = \frac{(\Delta E)^2}{k_B T^2} = \frac{C}{L^2}$$

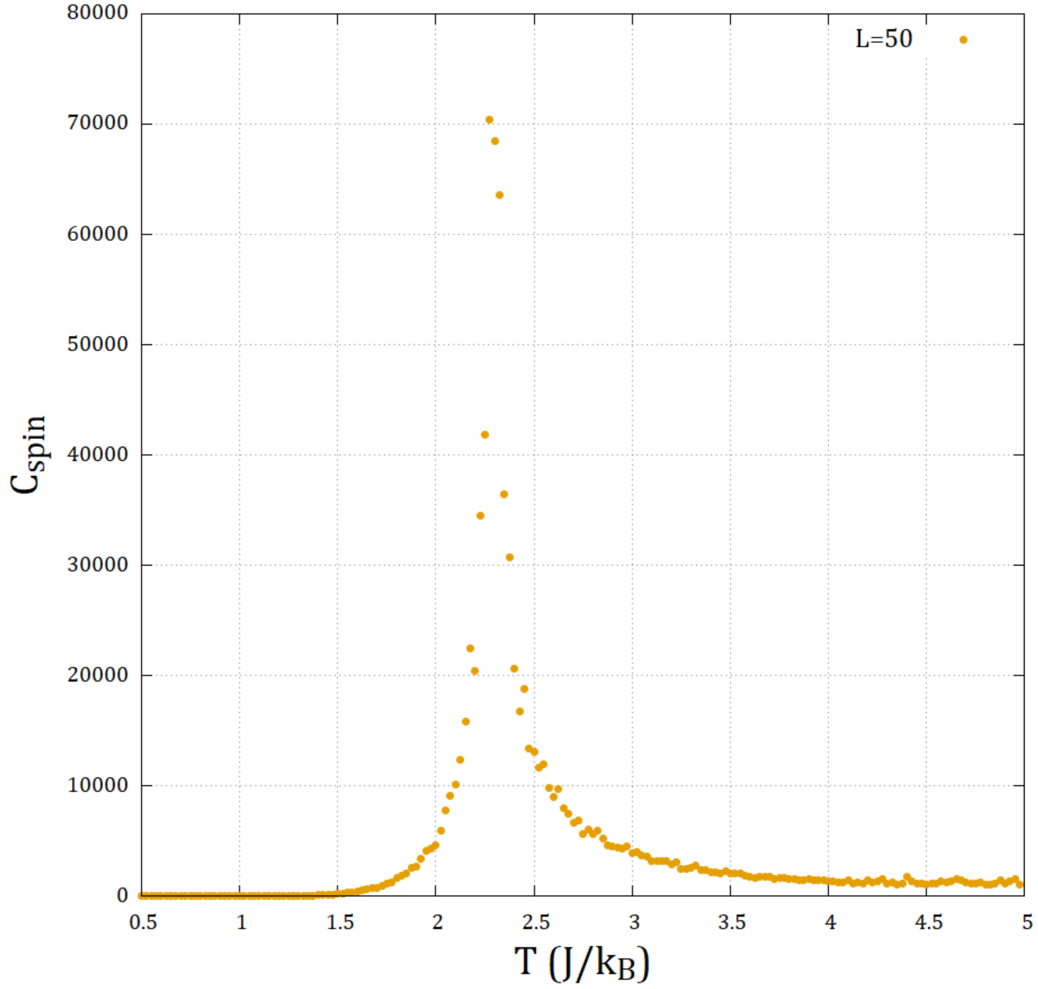
Specific heat per spin with temperature



Specific heat per spin with temperature



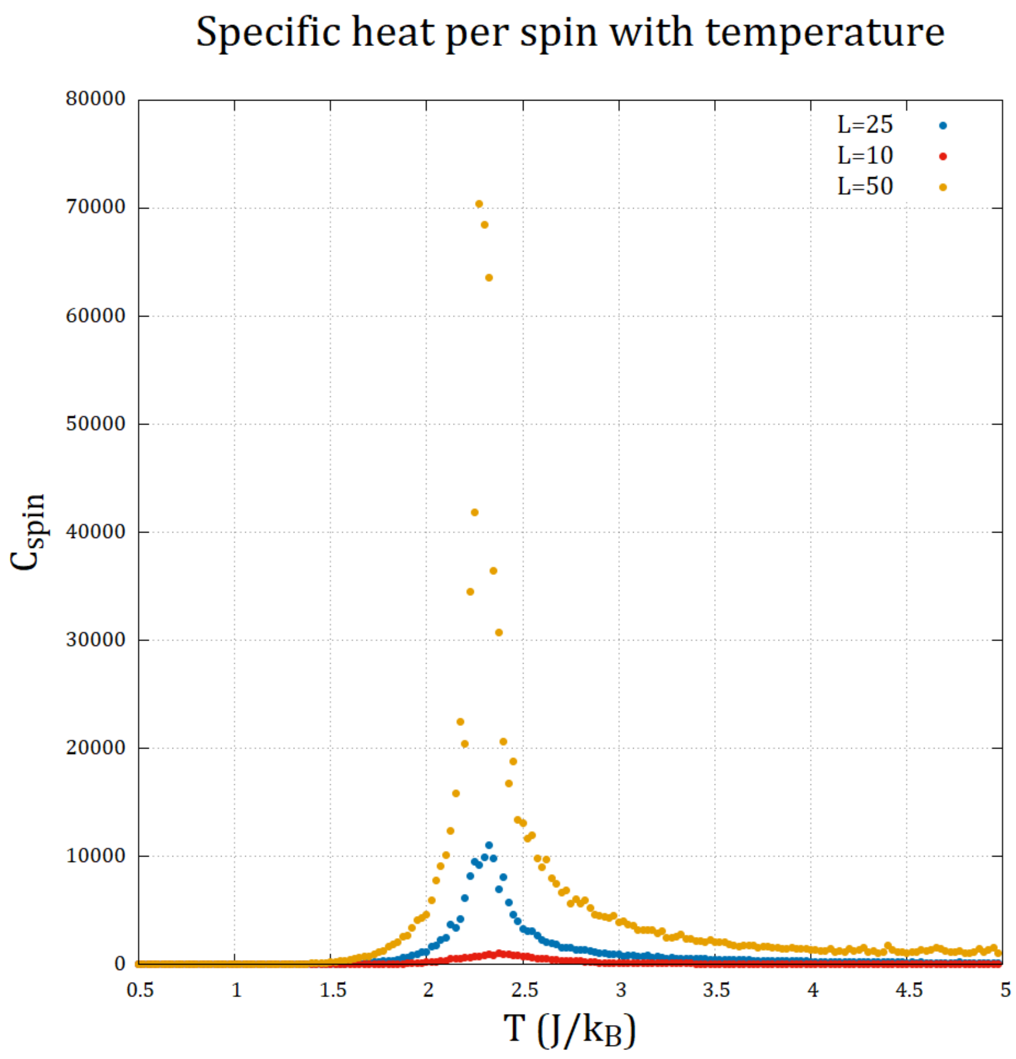
Specific heat per spin with temperature



System Size and 2D Analysis

As we increase the system size (L) the specific heat capacity diverges to infinity at the Curie temperature (Tc).

And the fluctuations decreases with increasing system size (L).

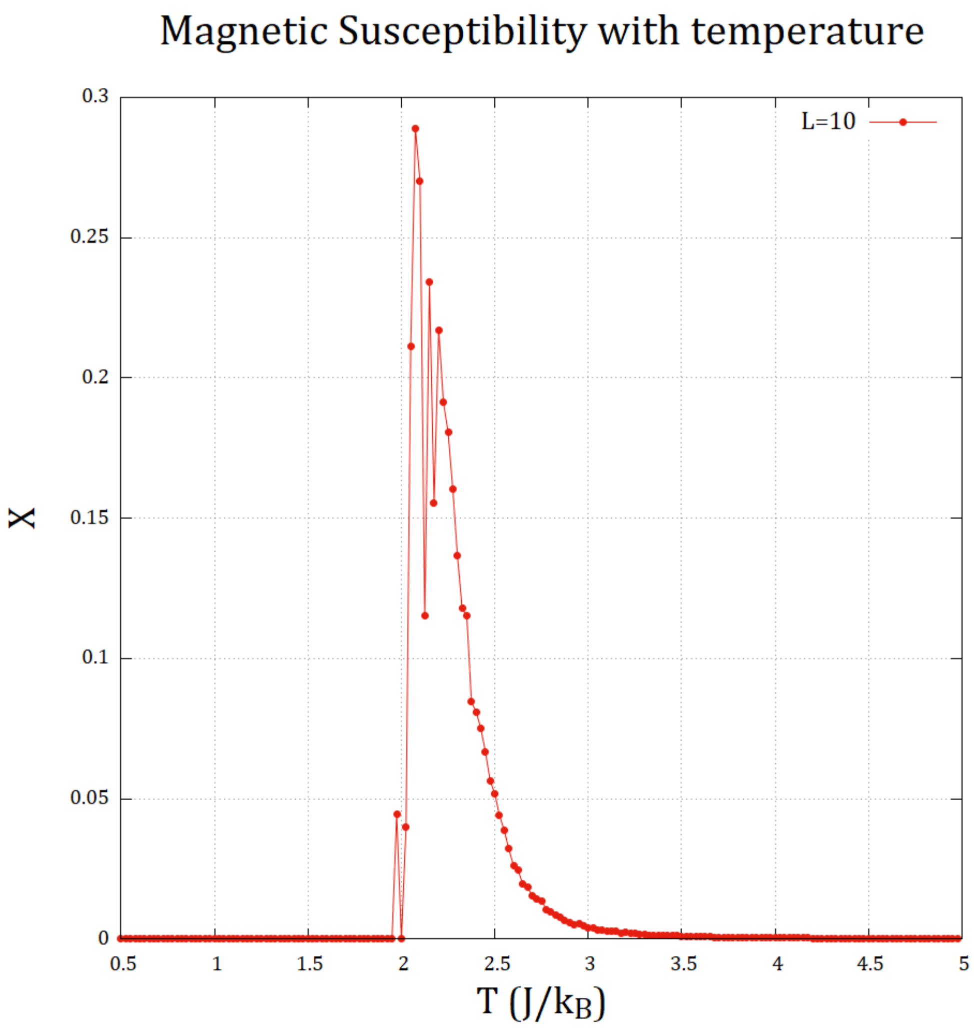


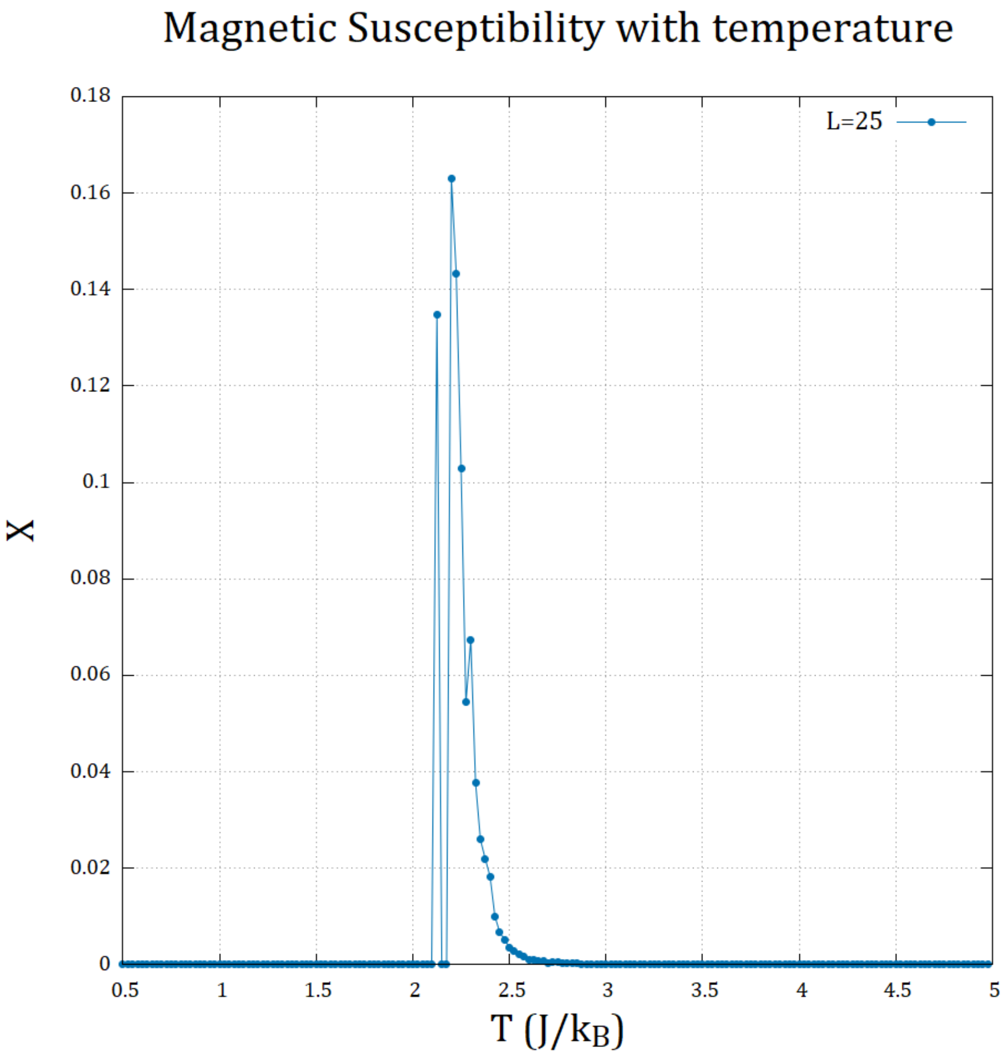
System Size and 2D Analysis

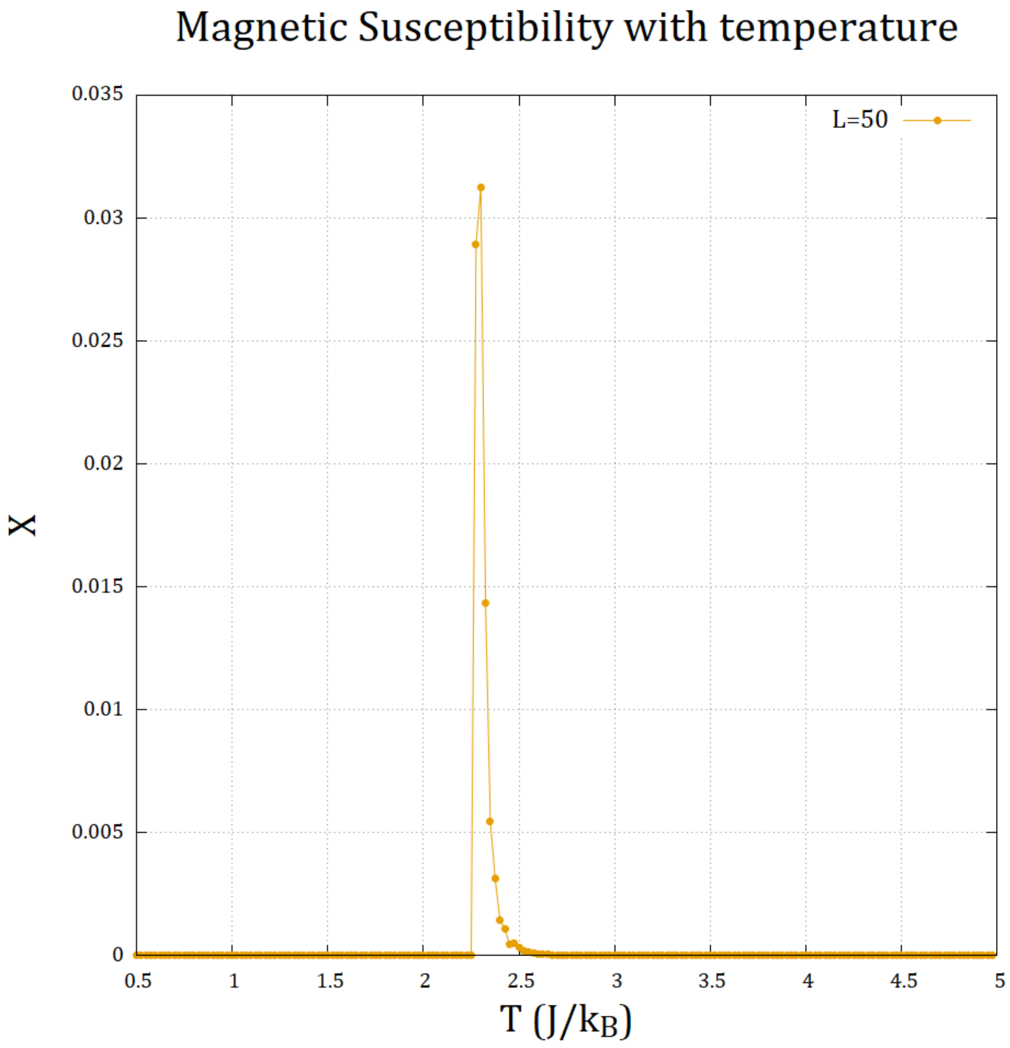
SUSCEPTIBILITY vs TEMPERATURE
X vs. T

In Ising model, magnetic susceptibility is given by:

$$\chi = \frac{(\Delta M)^2}{k_B T}$$




Magnetic Susceptibility with temperature
L=25
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
X
T (J/kB)

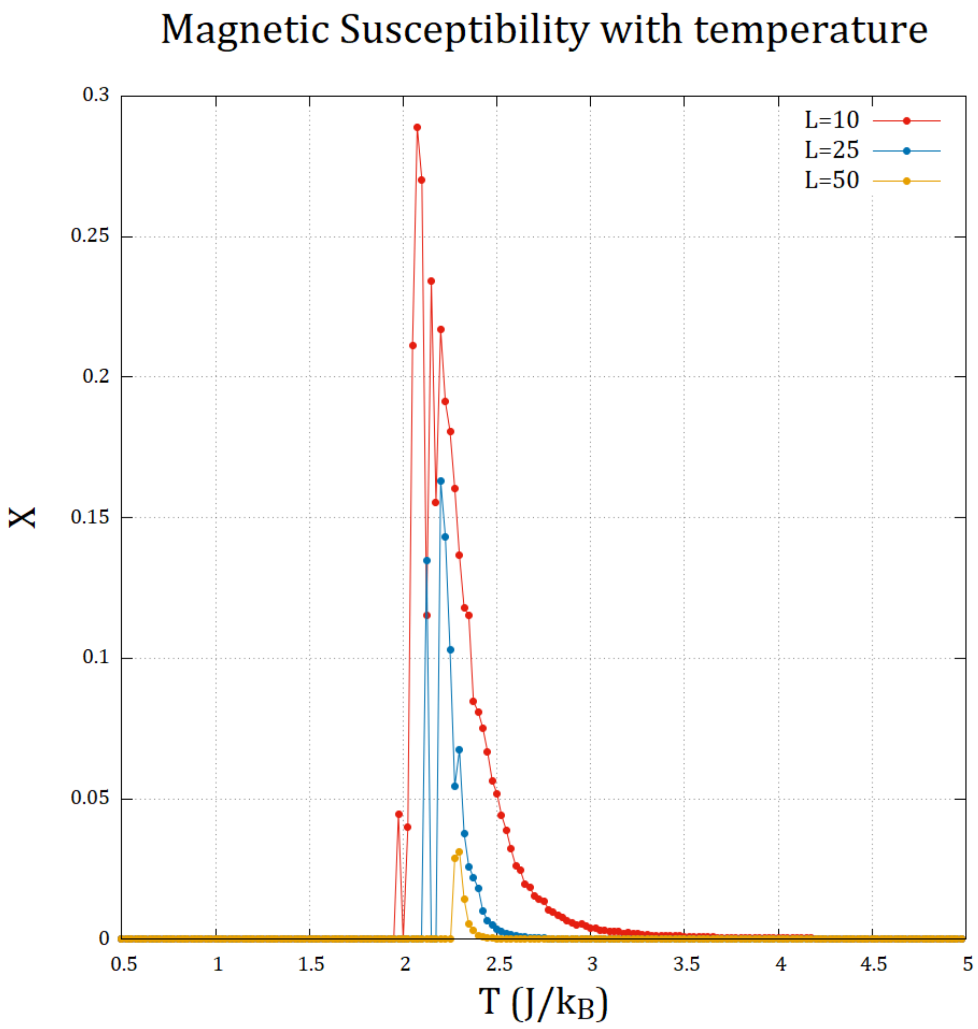

Magnetic Susceptibility with temperature
L=50
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
X
T (J/kB)

System Size and 2D Analysis

As we increase the system size (L) the magnet susceptibility diverges to infinity at the Curie temperature (Tc).

Magnet susceptibility decreases faster with increasing system size

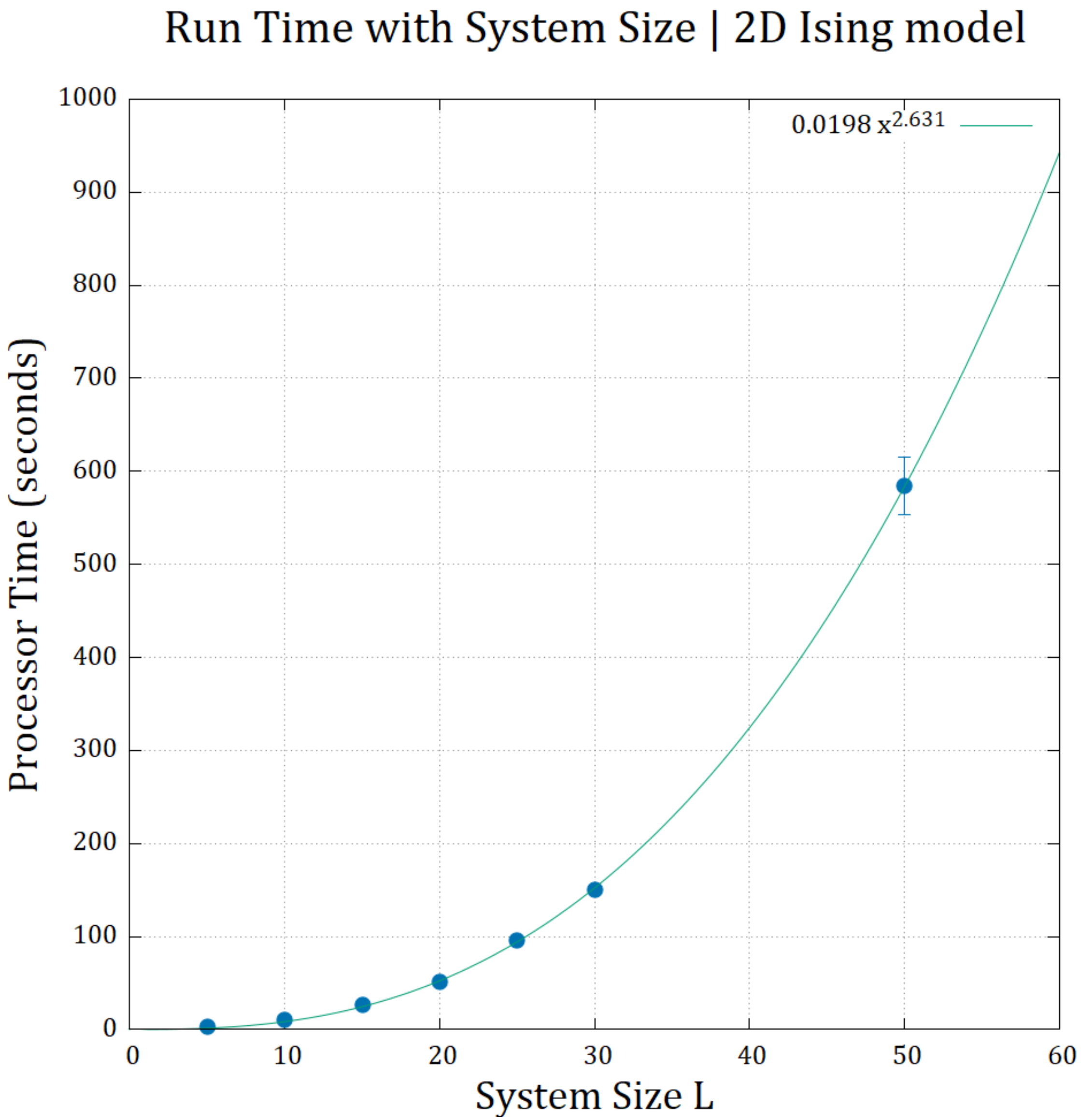
And the fluctuations decreases with increasing system size (L).



System Size and 2D Analysis

- Analyzing runtime with growing system sizes, we found that the 2D Ising model scales as a polynomial function of system size (L)

$$Runtime(L) = 0.0198x^{2.631}$$

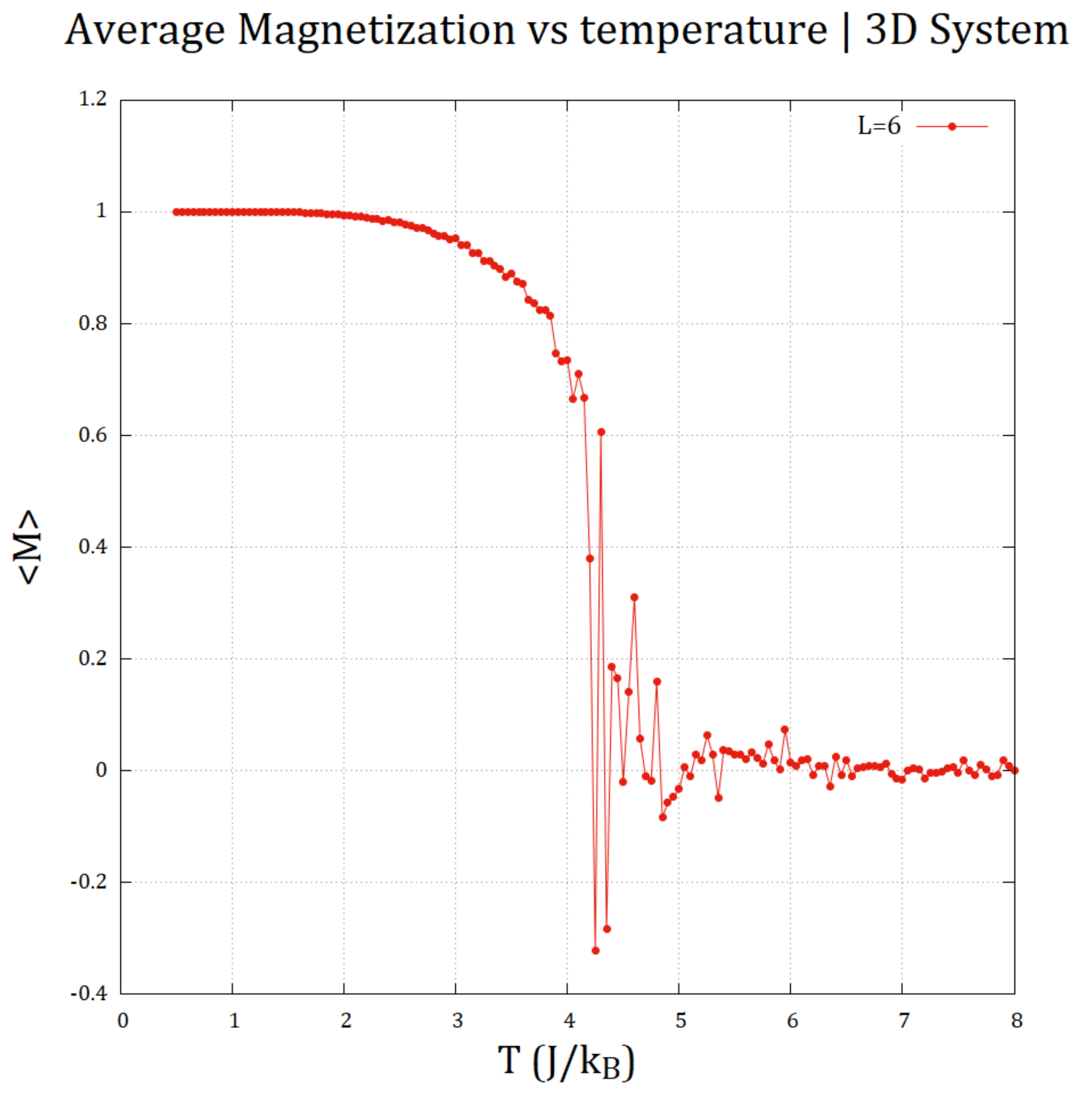


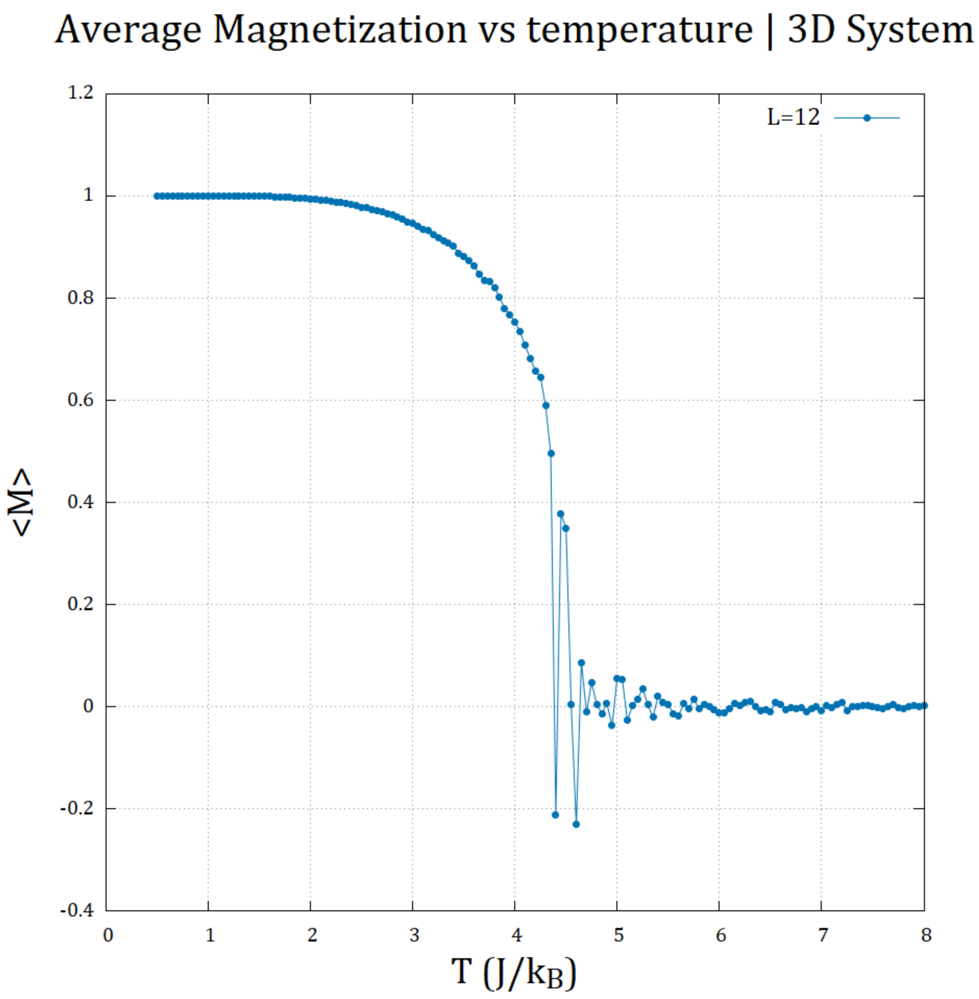
System Size and 3D Analysis

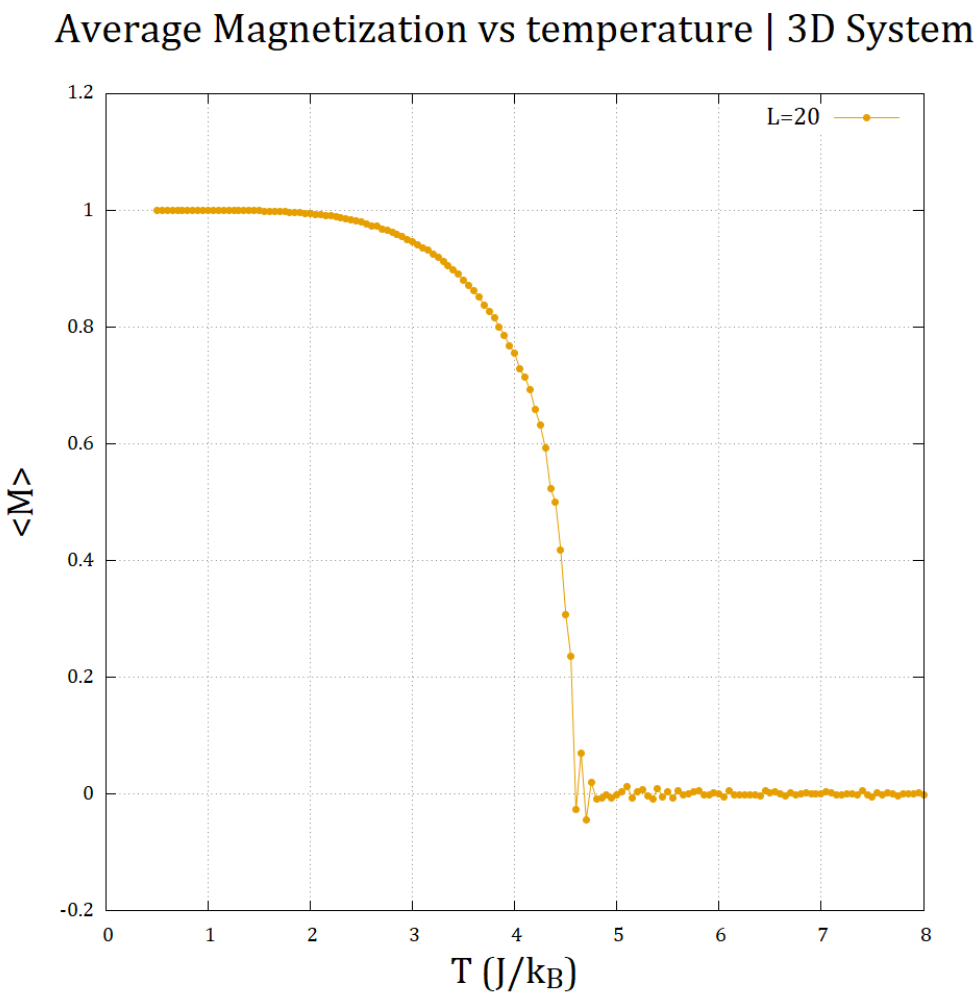
MAGNETIZATION vs TEMPERATURE
<M> vs. T

The behavior is identical to 2D.
The Curie temperature (Tc) is around 4.5 J/kB which is higher than in 2D.

Because in 3D the number of nearest neighbors is higher.



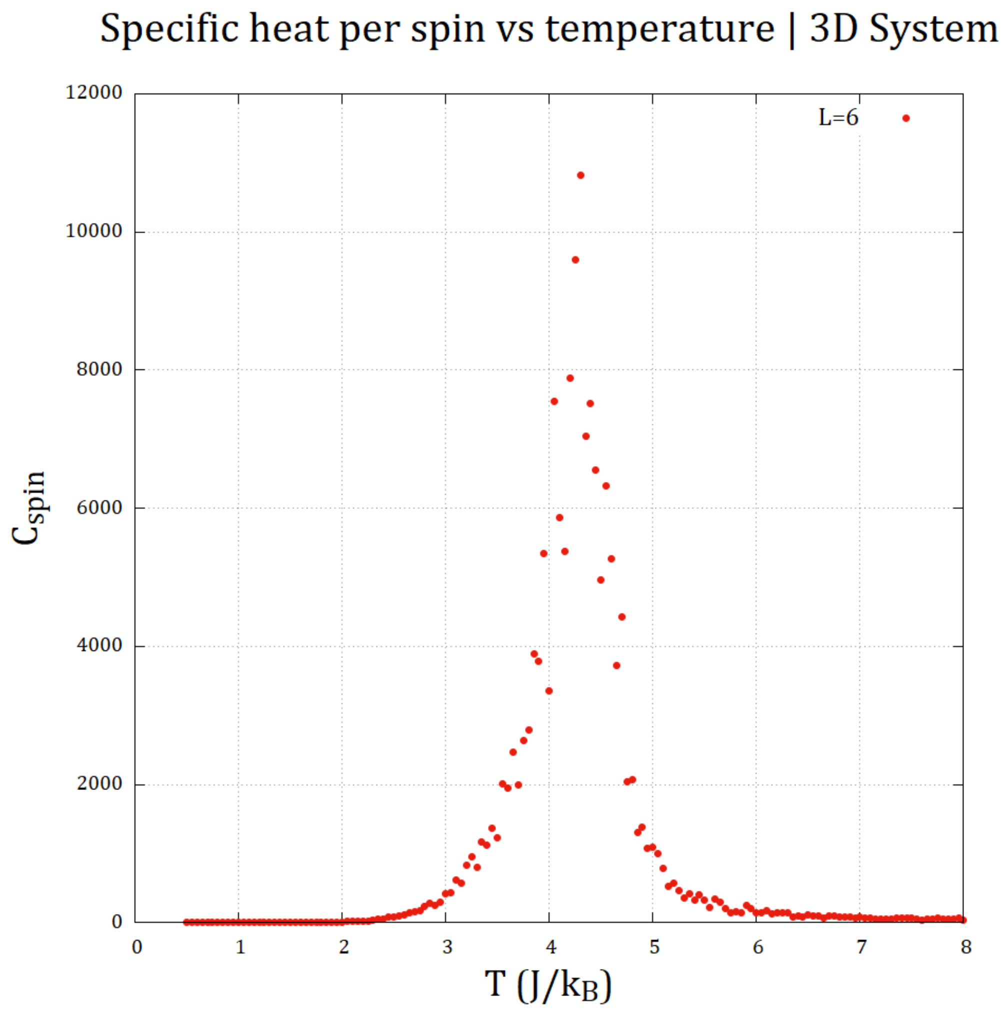

Average Magnetization vs temperature | 3D System
L=12
<M>
T (J/kB)
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
0
1
2
3
4
5
6
7
8

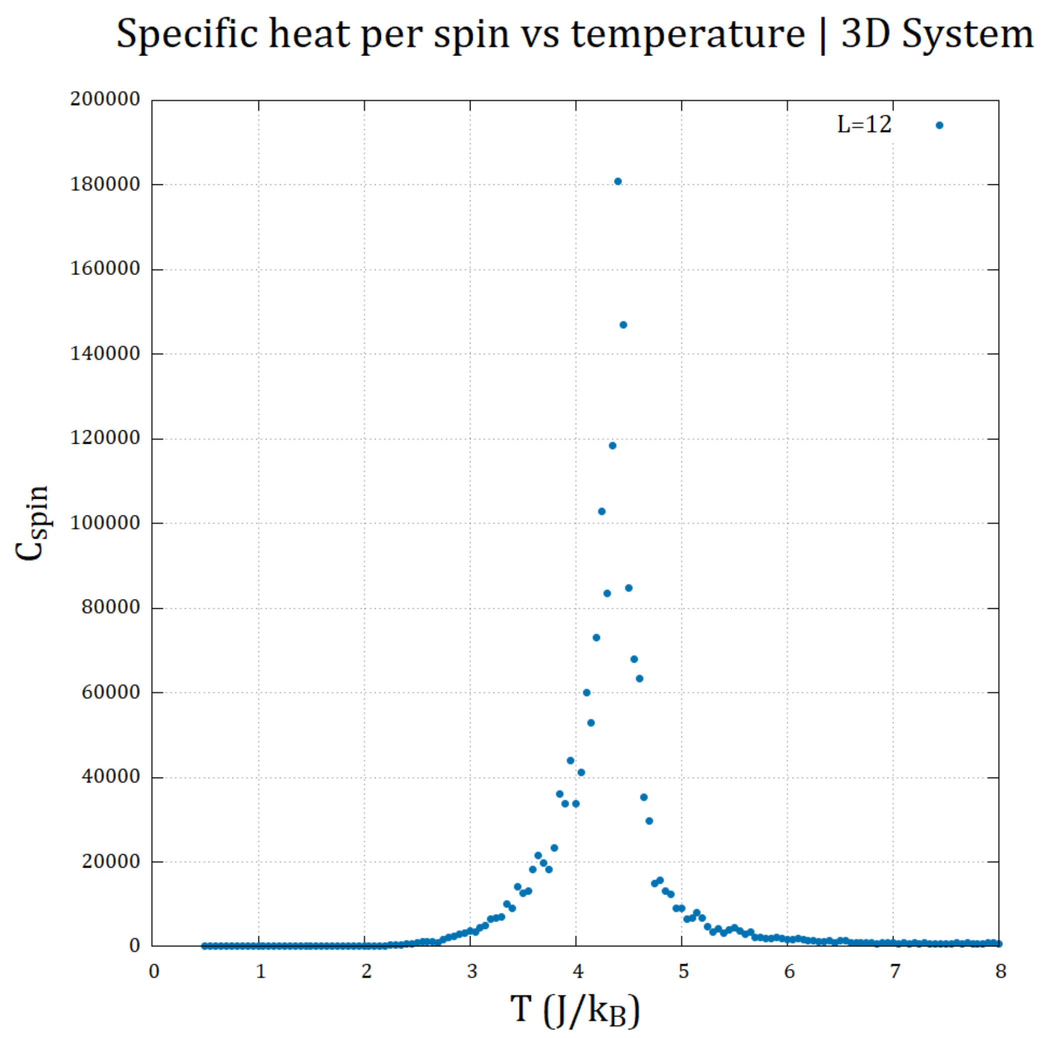

Average Magnetization vs temperature | 3D System
L=20
<M>
T (J/kB)
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
1
2
3
4
5
6
7
8

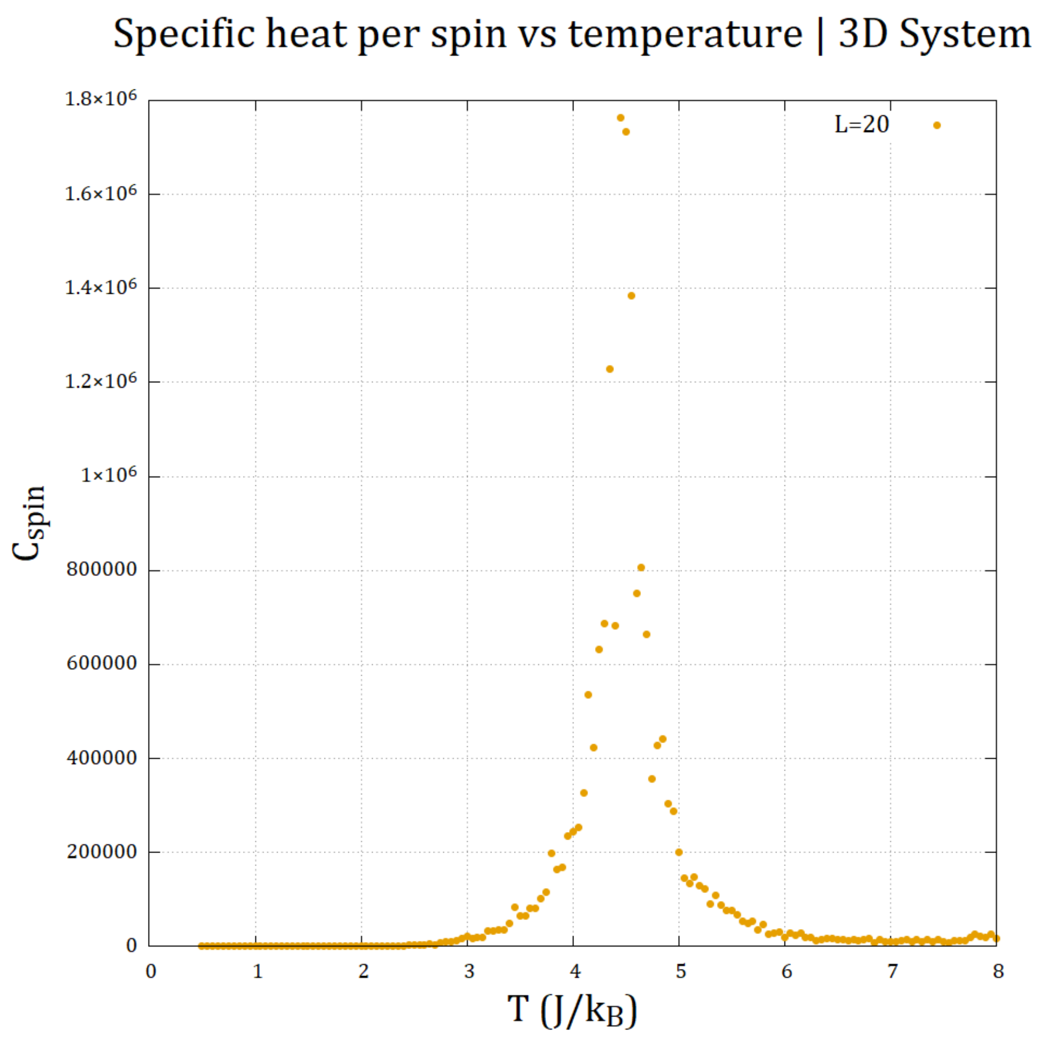
System Size and 3D Analysis

HEAT CAPACITY vs TEMPERATURE
C vs. T

The behavior is identical to 2D.
The Curie temperature (Tc) is around 4.5 J/kB which is higher than in 2D.

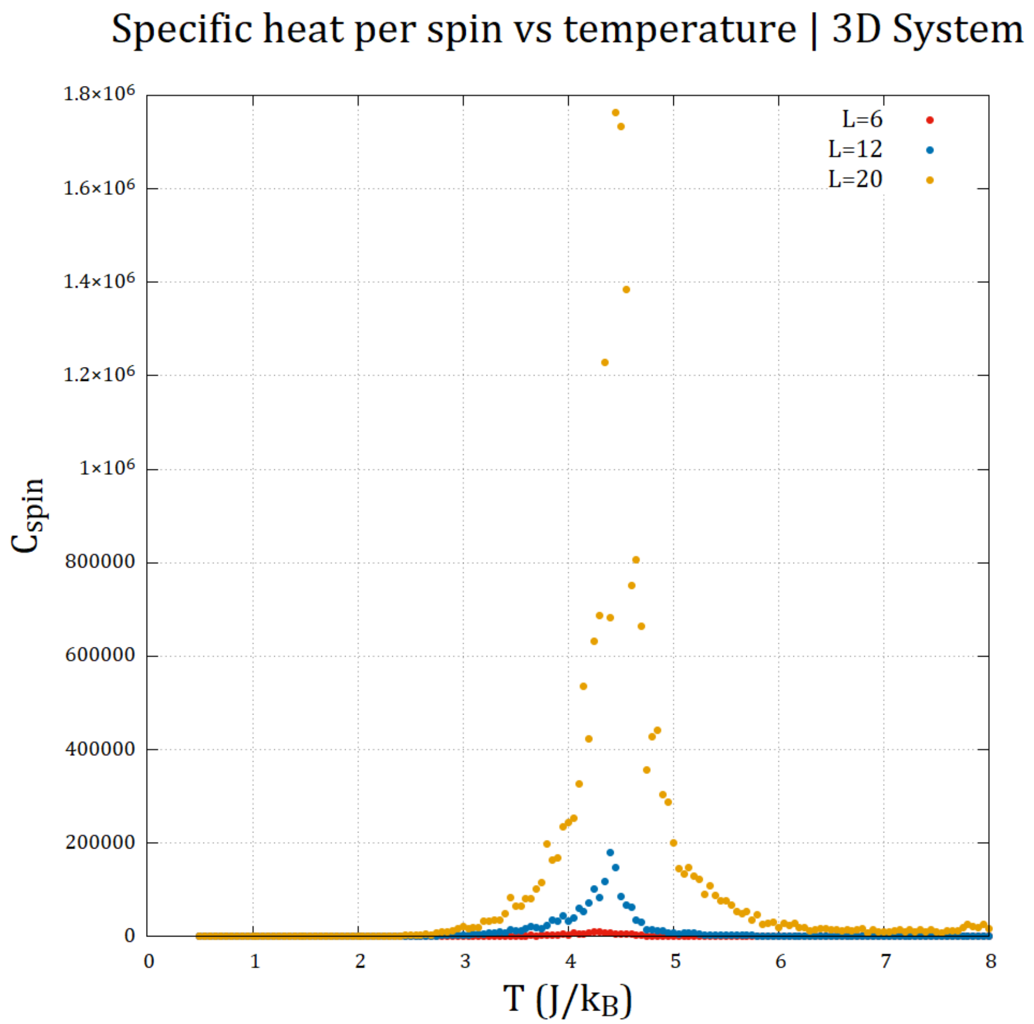



Specific heat per spin vs temperature | 3D System
L=12
Cspin
T (J/kB)
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
0
1
2
3
4
5
6
7
8


Specific heat per spin vs temperature | 3D System
L=20
Cspin
T (J/kB)
1.8×10⁶
1.6×10⁶
1.4×10⁶
1.2×10⁶
1×10⁶
800000
600000
400000
200000
0
0
1
2
3
4
5
6
7
8

System Size and 3D Analysis

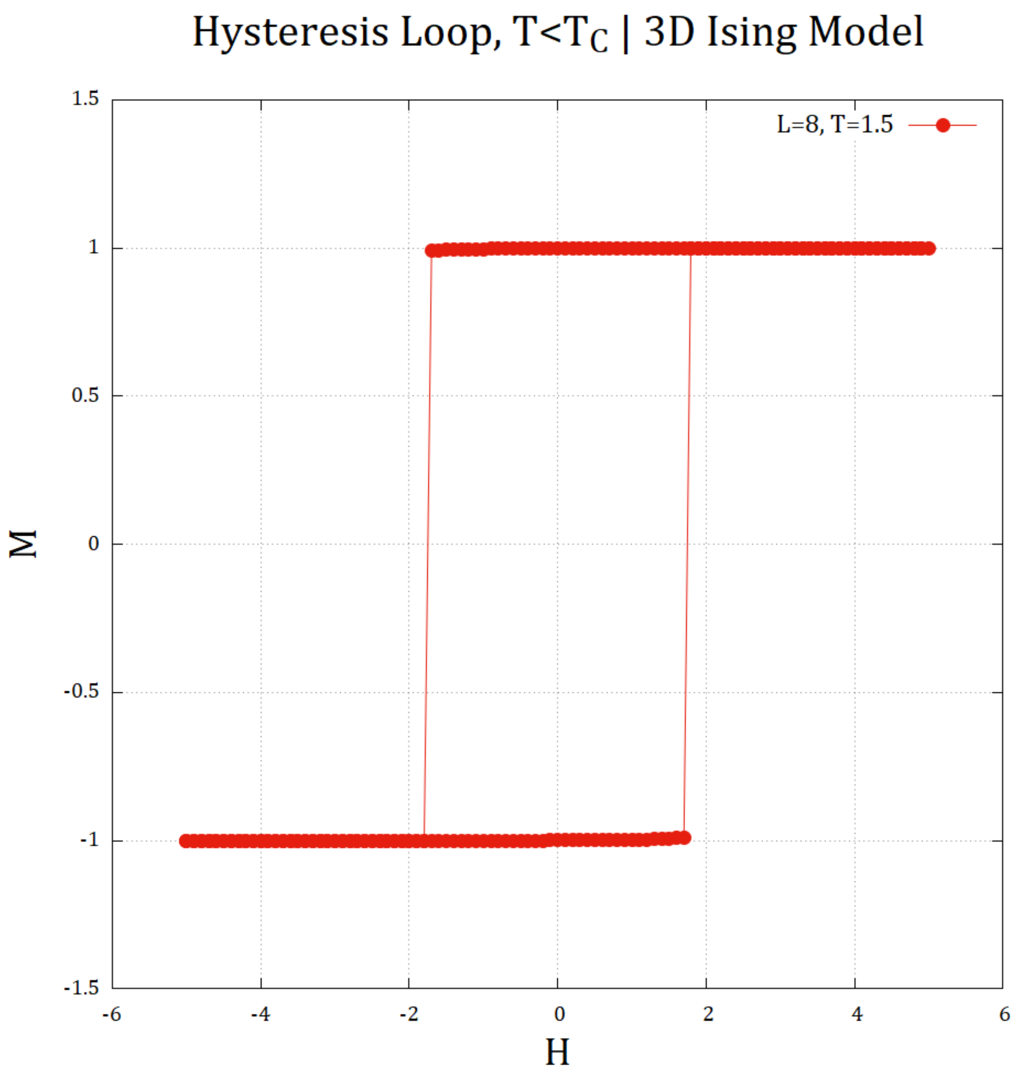
The noise is less than 2D.



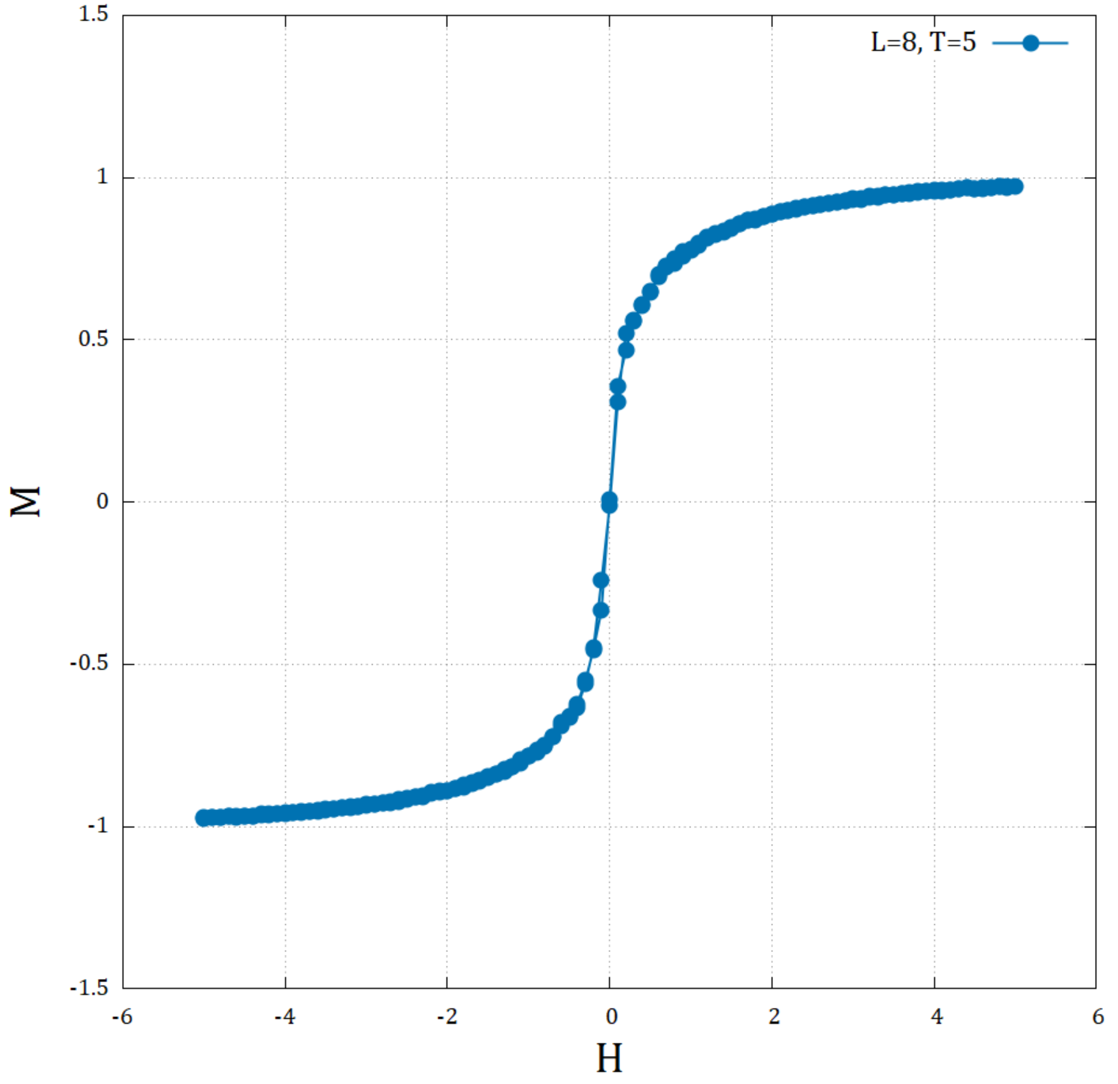
System Size and 3D Analysis

HYSTERESIS LOOP
<M> vs. B

There is hysteresis loop in 3D. The same as 2D.



Hysteresis Loop, $T>T_C$ | 3D Ising Model

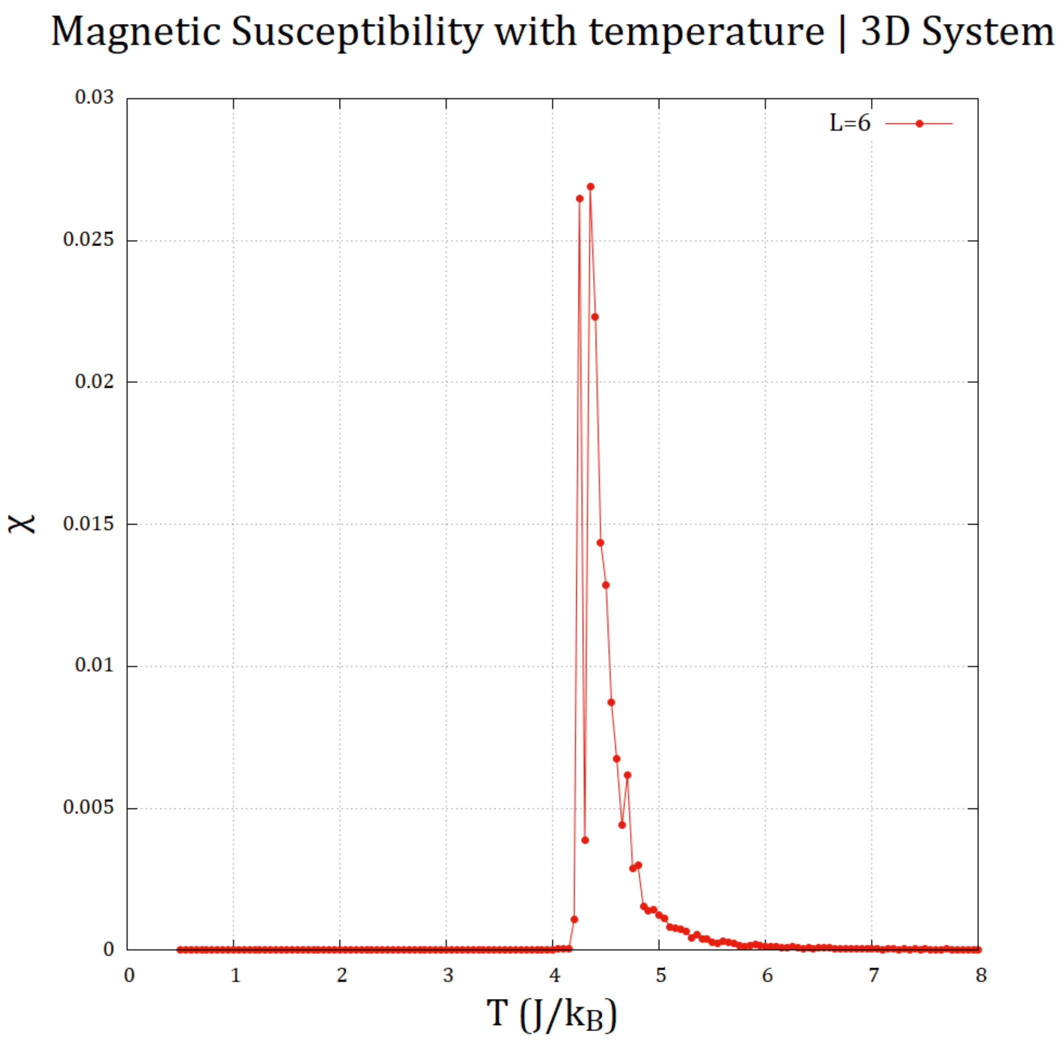


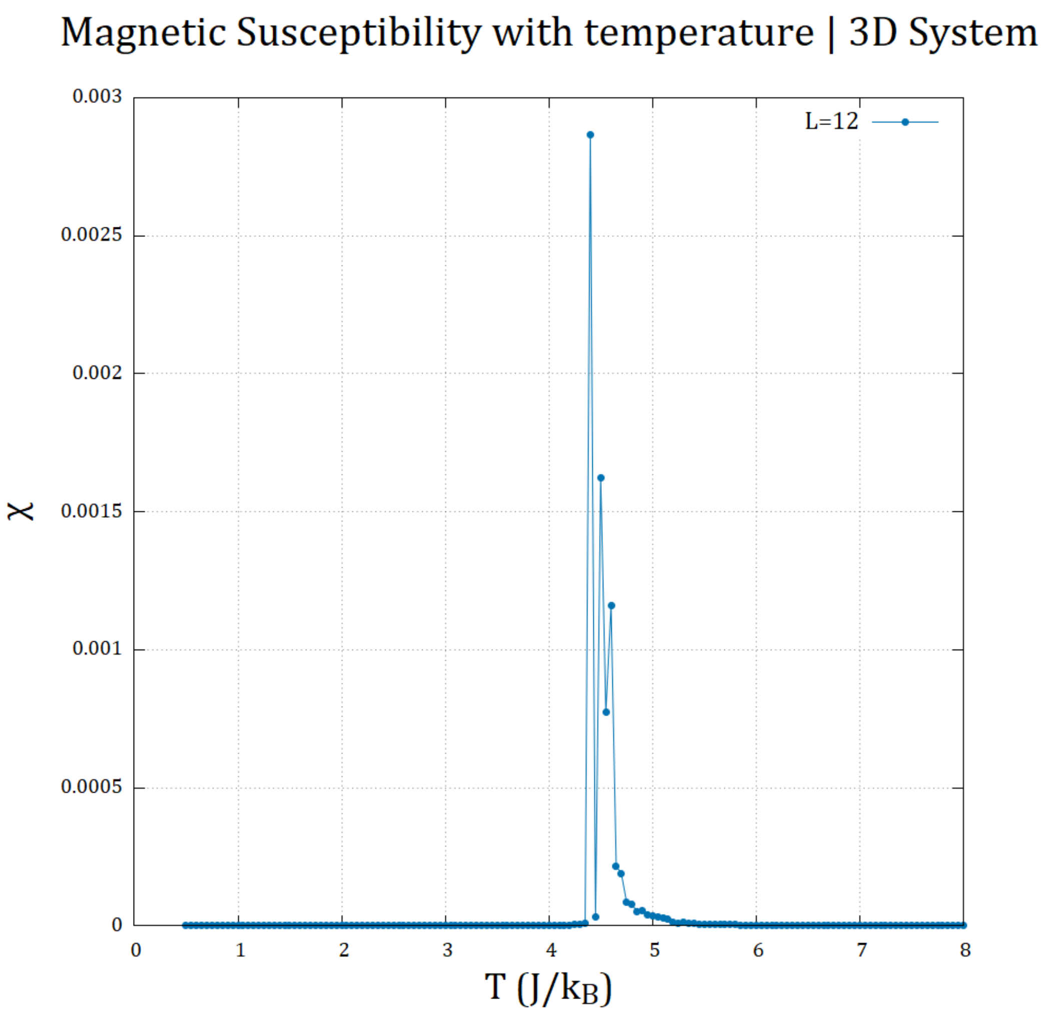
System Size and 3D Analysis

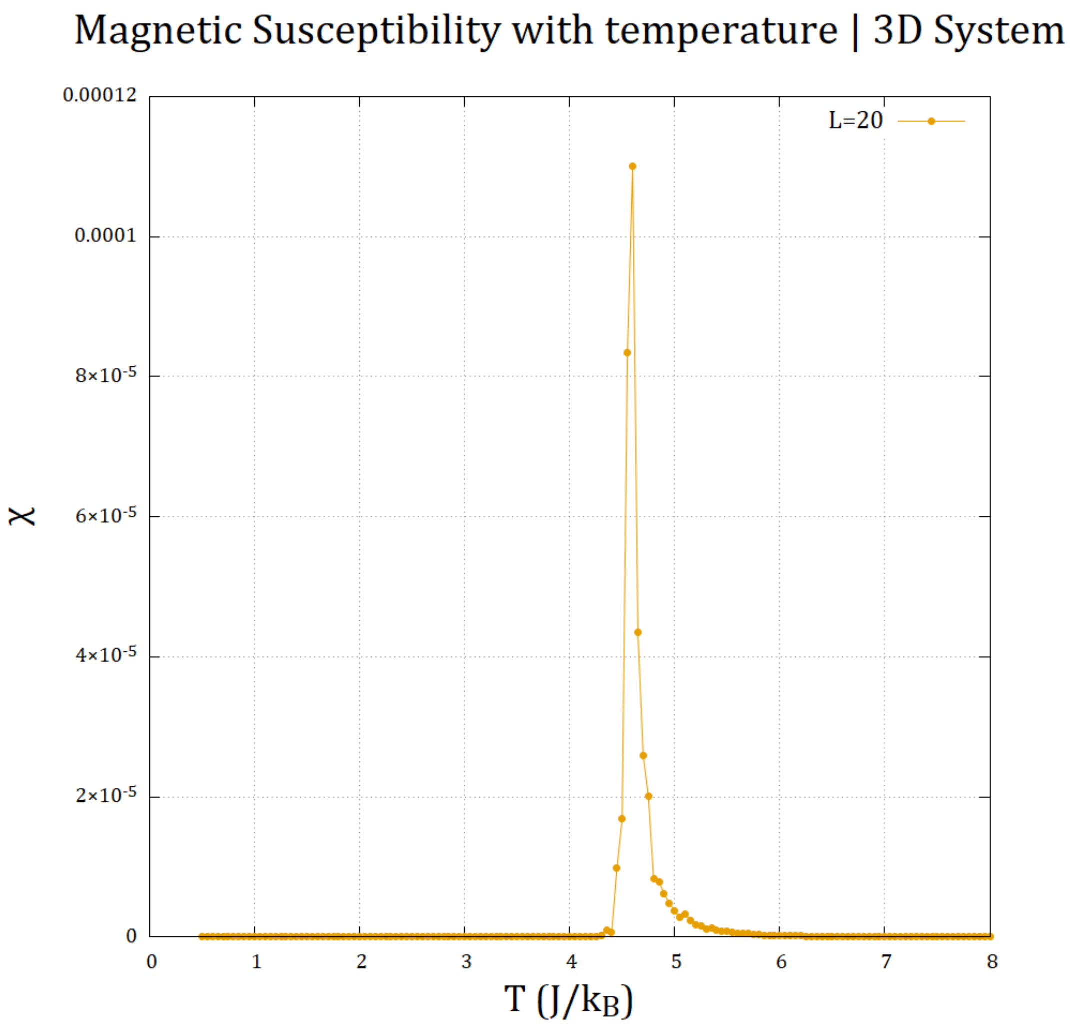
SUSCEPTIBILITY vs TEMPERATURE
X vs. T

The behavior is similar to the 2D results

The susceptibility reduces with system size, while Tc increases.

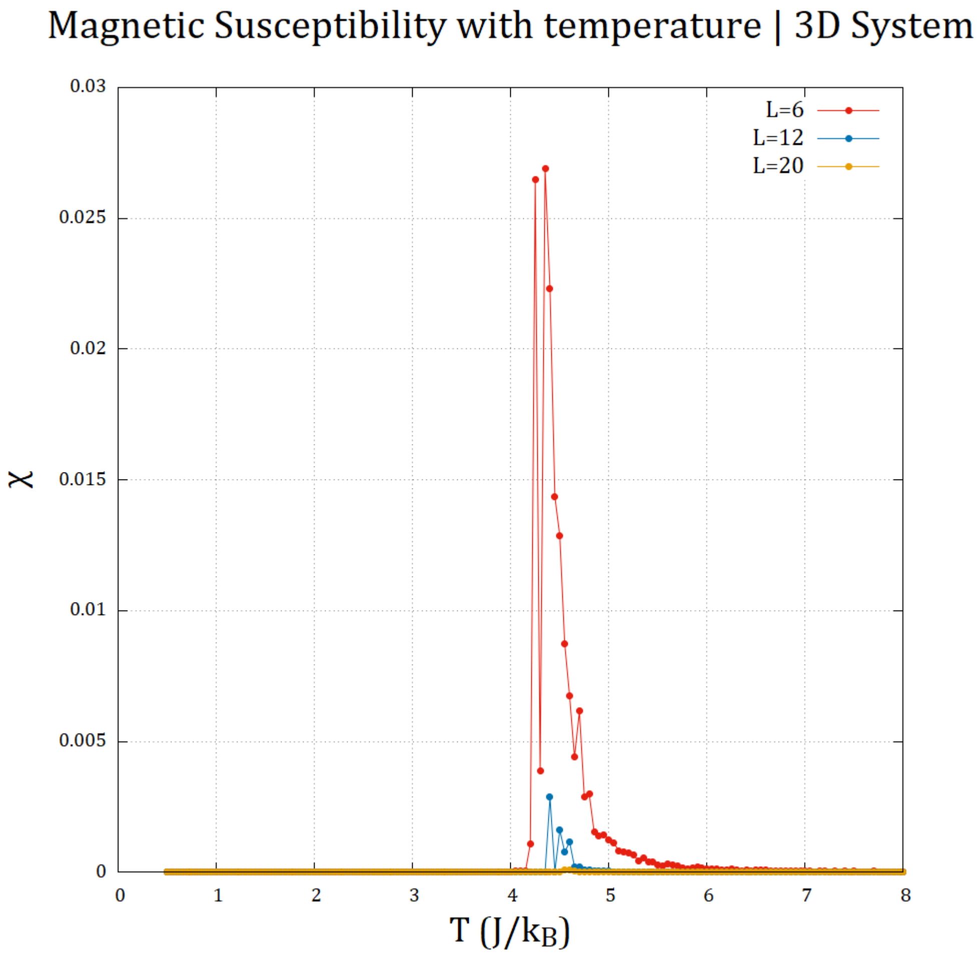



Magnetic Susceptibility with temperature | 3D System
L=12
0.003
0.0025
0.002
0.0015
0.001
0.0005
0
χ
0 1 2 3 4 5 6 7 8
T (J/kB)


Magnetic Susceptibility with temperature | 3D System
L=20
0.00012
0.0001
8×10-5
6×10-5
4×10-5
2×10-5
0
χ
0 1 2 3 4 5 6 7 8
T (J/kB)

System Size and 3D Analysis

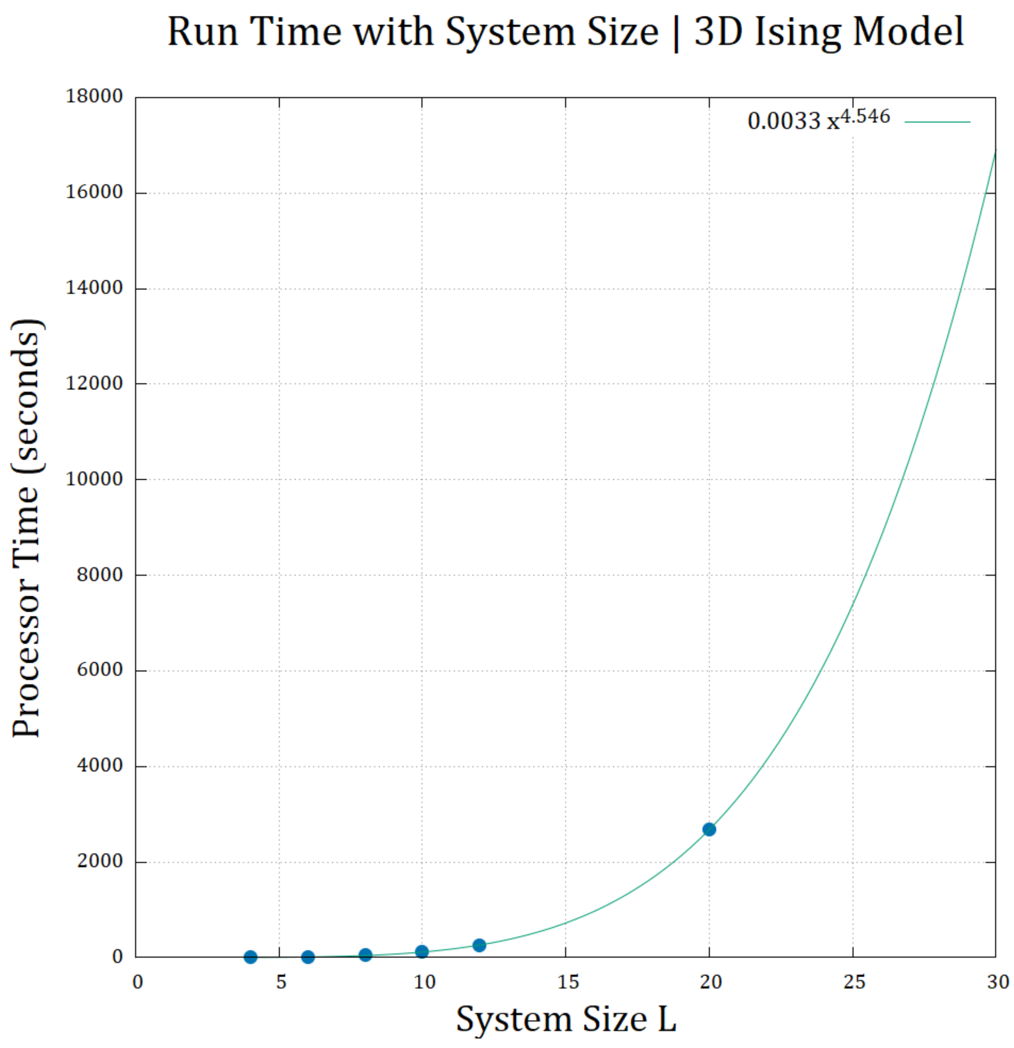
The Susceptibility decreases, while the Curie temperature increases marginally.



System Size and 3D Analysis

- Analyzing runtime with growing system sizes, we found that the 3D Ising model scales as a polynomial function of system size (L)

$$Runtime(L) = 0.0033x^{4.546}$$

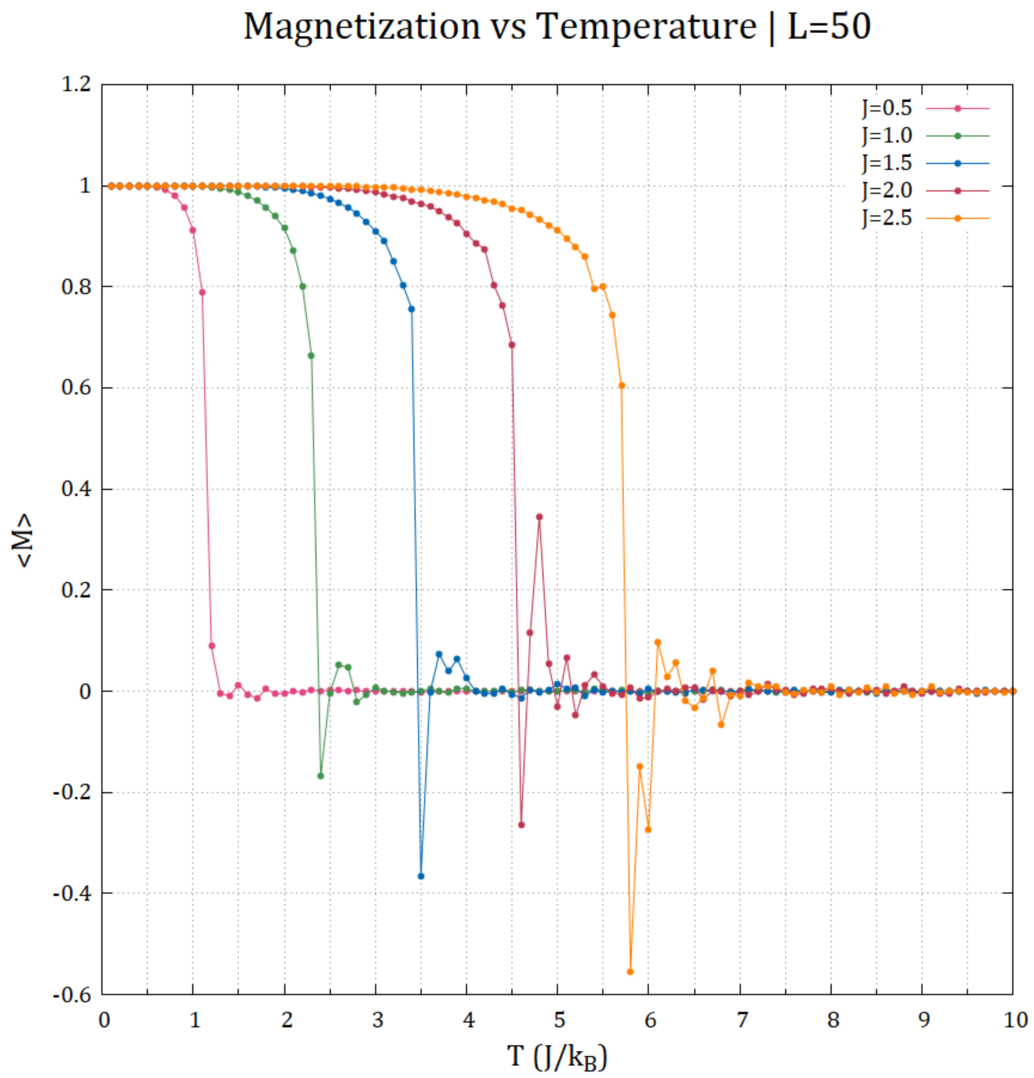



ME WHEN THE
WHEN THE 3D ISING MODEL FINALLY STOPS RUNNING

Coupling Constant Analysis

MAGNETIZATION vs TEMPERATURE
<M> vs. T

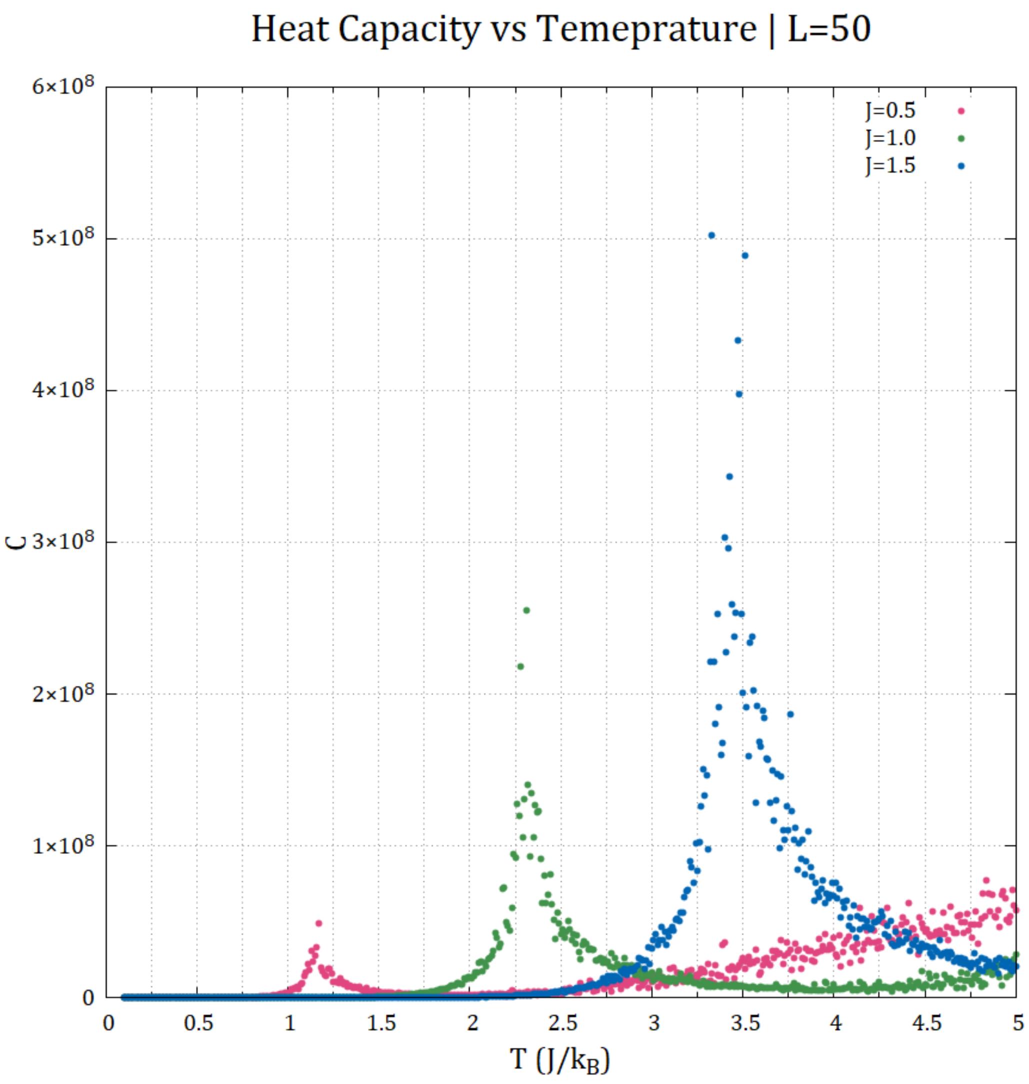
As we increases the coupling strength as the Curie temperature increases.



Coupling Constant Analysis

HEAT CAPACITY vs TEMPERATURE
C vs. T

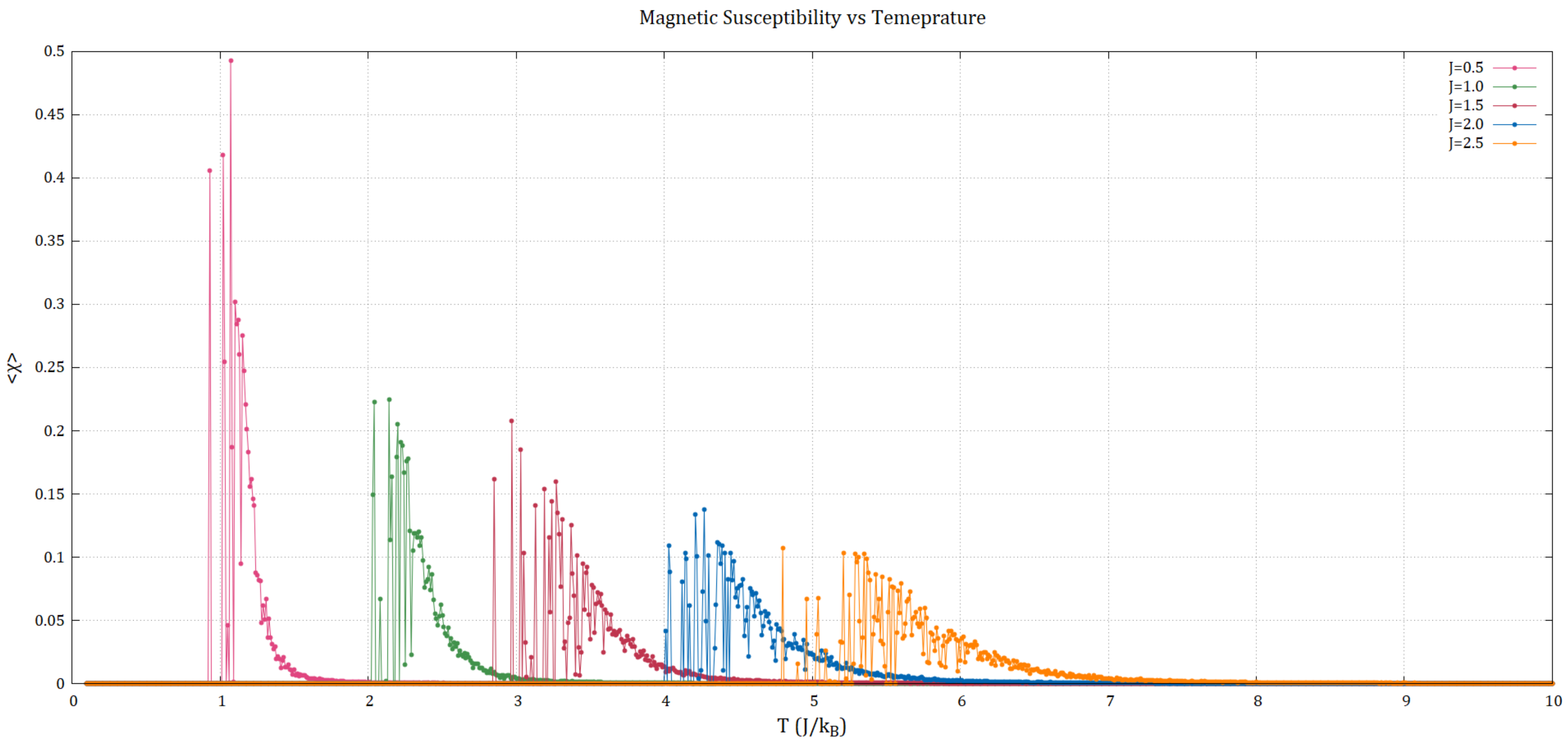
The results agree with the results of magnetization vs temperature. Which the Curie temperature increases by increasing the coupling strength.



Coupling Constant Analysis

SUSCEPTIBILITY vs TEMPERATURE
X vs. T

Again, the results agreed with the previous two.
You can notice that the singularity of the susceptibility shifts to the right.



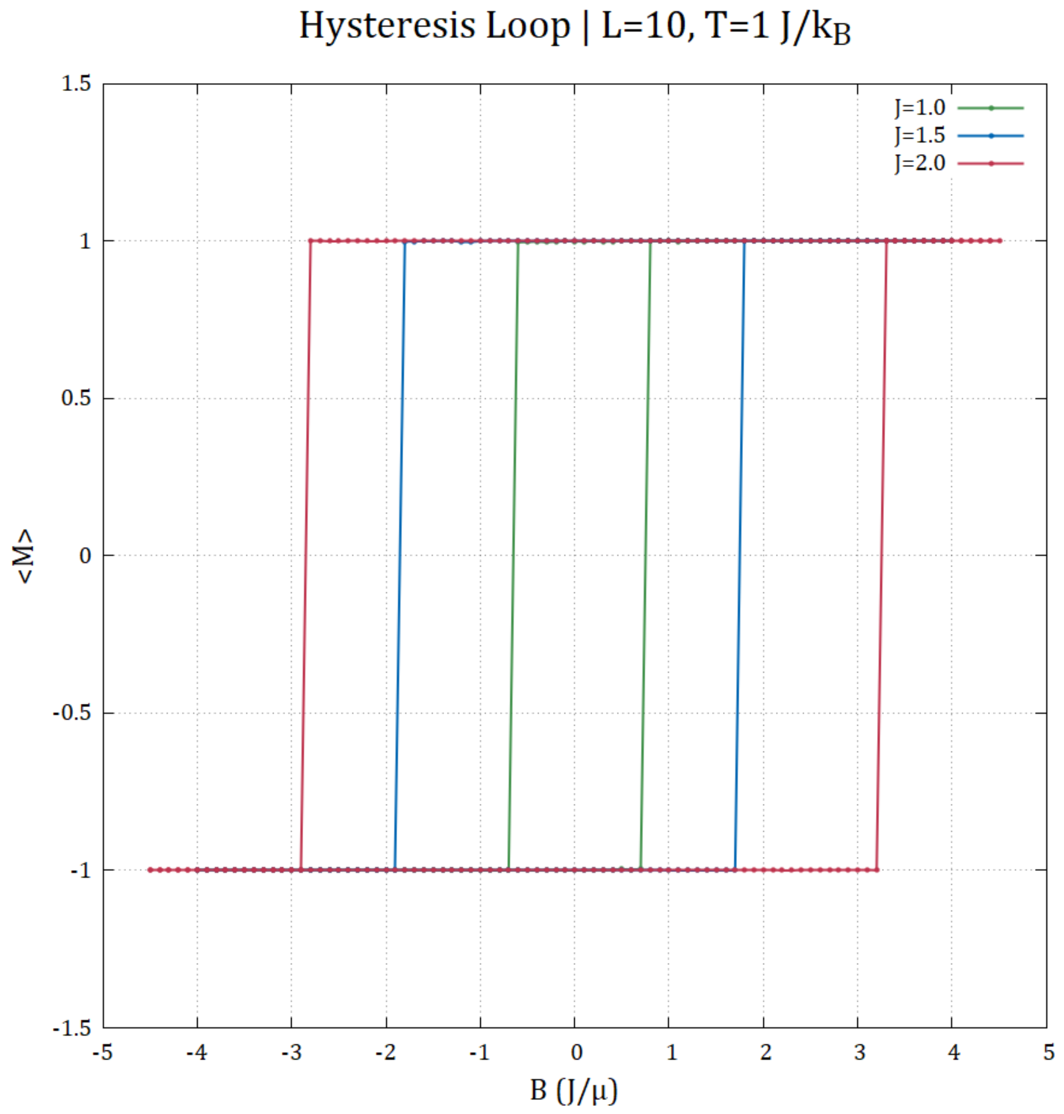
Magnetic Susceptibility vs Temeprature
<χ>
T (J/k_B)
J=0.5
J=1.0
J=1.5
J=2.0
J=2.5
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0
1
2
3
4
5
6
7
8
9
10

30

Coupling Constant Analysis

HYSTERESIS LOOP
<M> vs. B

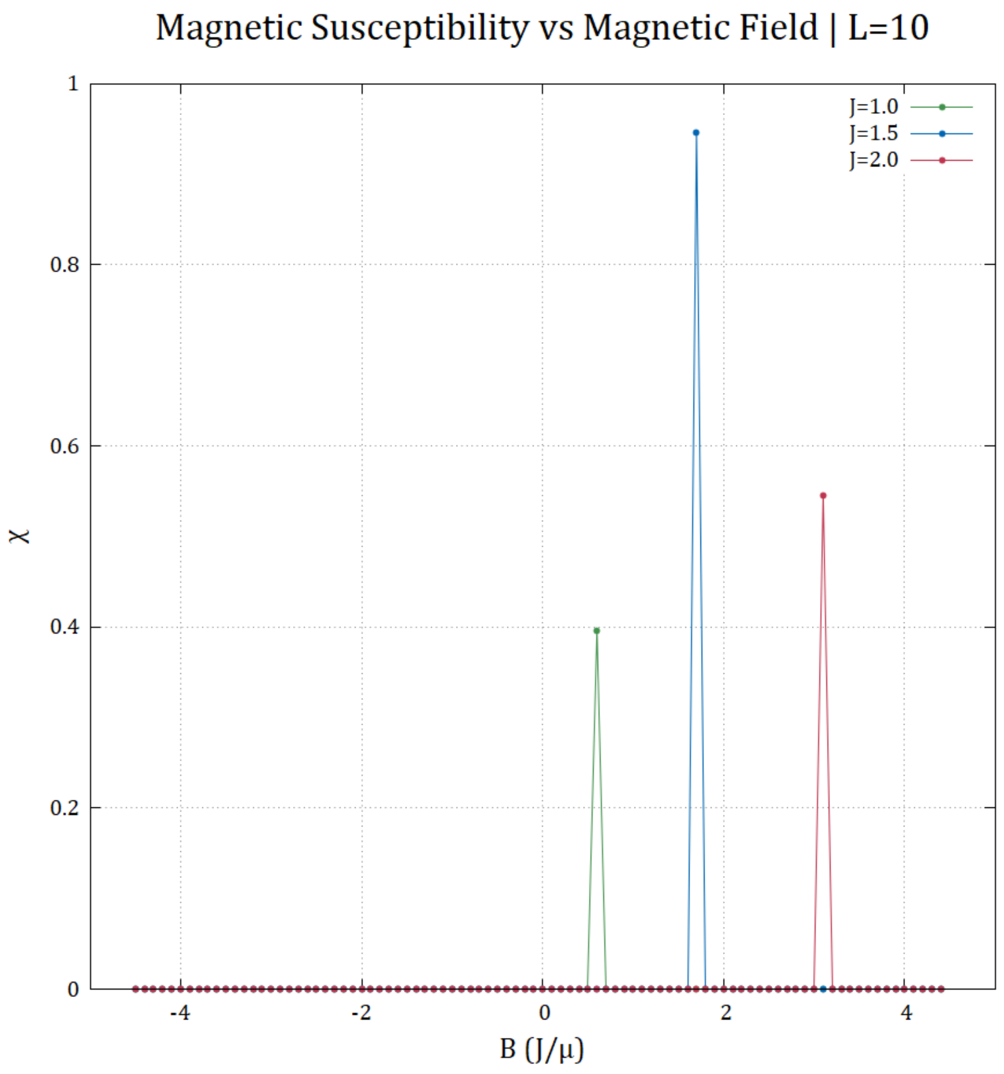
As the coupling constant increases, as the material becomes more ferromagnetic, that means it's highly magnetized. So, the coercive field is higher for higher coupling constant.



Coupling Constant Analysis

SUSCEPTIBILITY vs MAGNETIC FIELD
X vs. B

These results agrees with the previous, because the maxima of susceptibility represents the coercive field. Which is increasing with coupling strength.

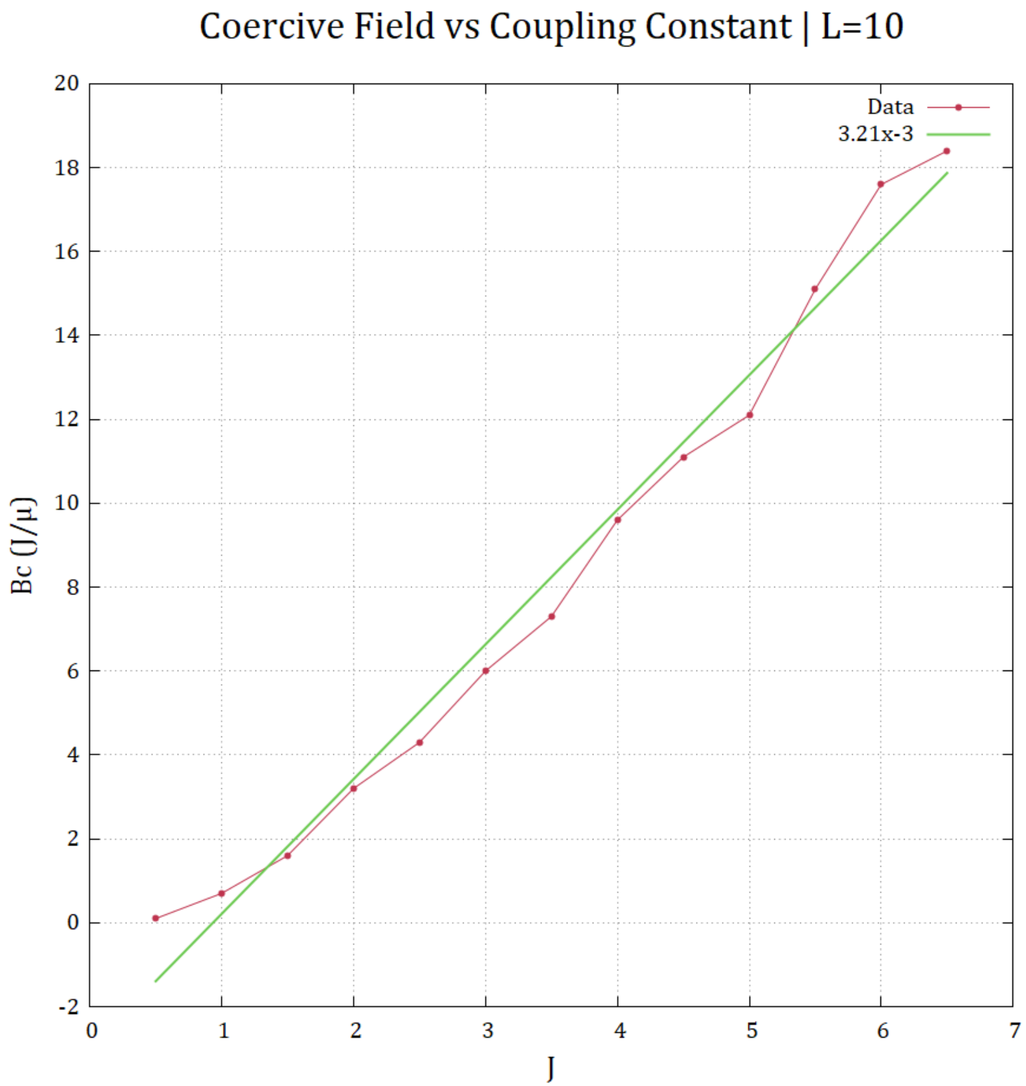


Coupling Constant Analysis

COERCIVE FIELD vs COUPLING CON.
Bc vs. J

Fitting the behavior of coercive field with the coupling strength. Which is found to be linear by this equation:

$$B_c = 3.21x - 3$$

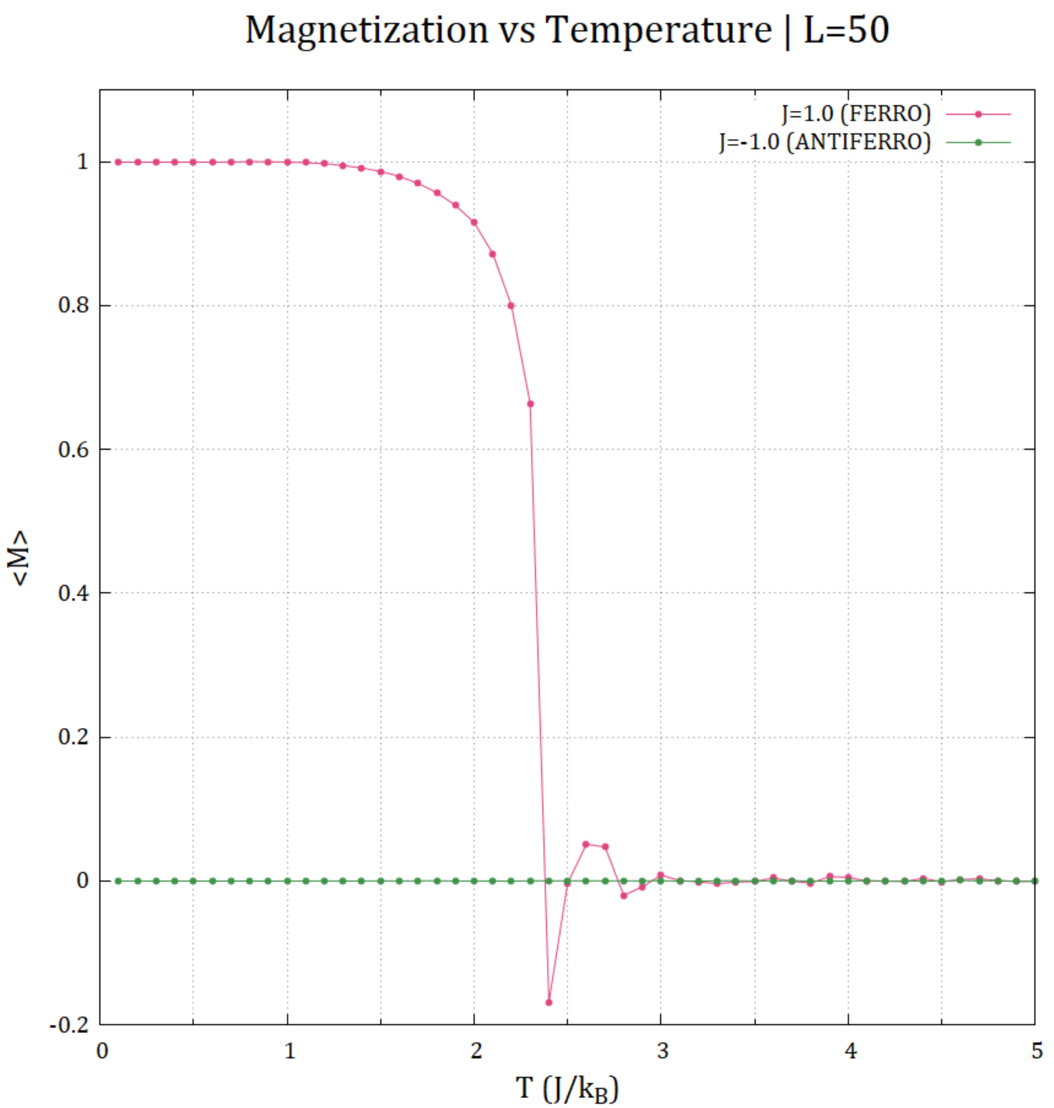


Anti-ferromagnetism

MAGNETIZATION vs TEMPERATURE
<M> vs. T

Trying to find the Neel temperature or phase transition of antiferromagnetic material by studying M vs. T.

Which is NOT useful, because the average of magnetization is zero in both antiferro- and para- regions.

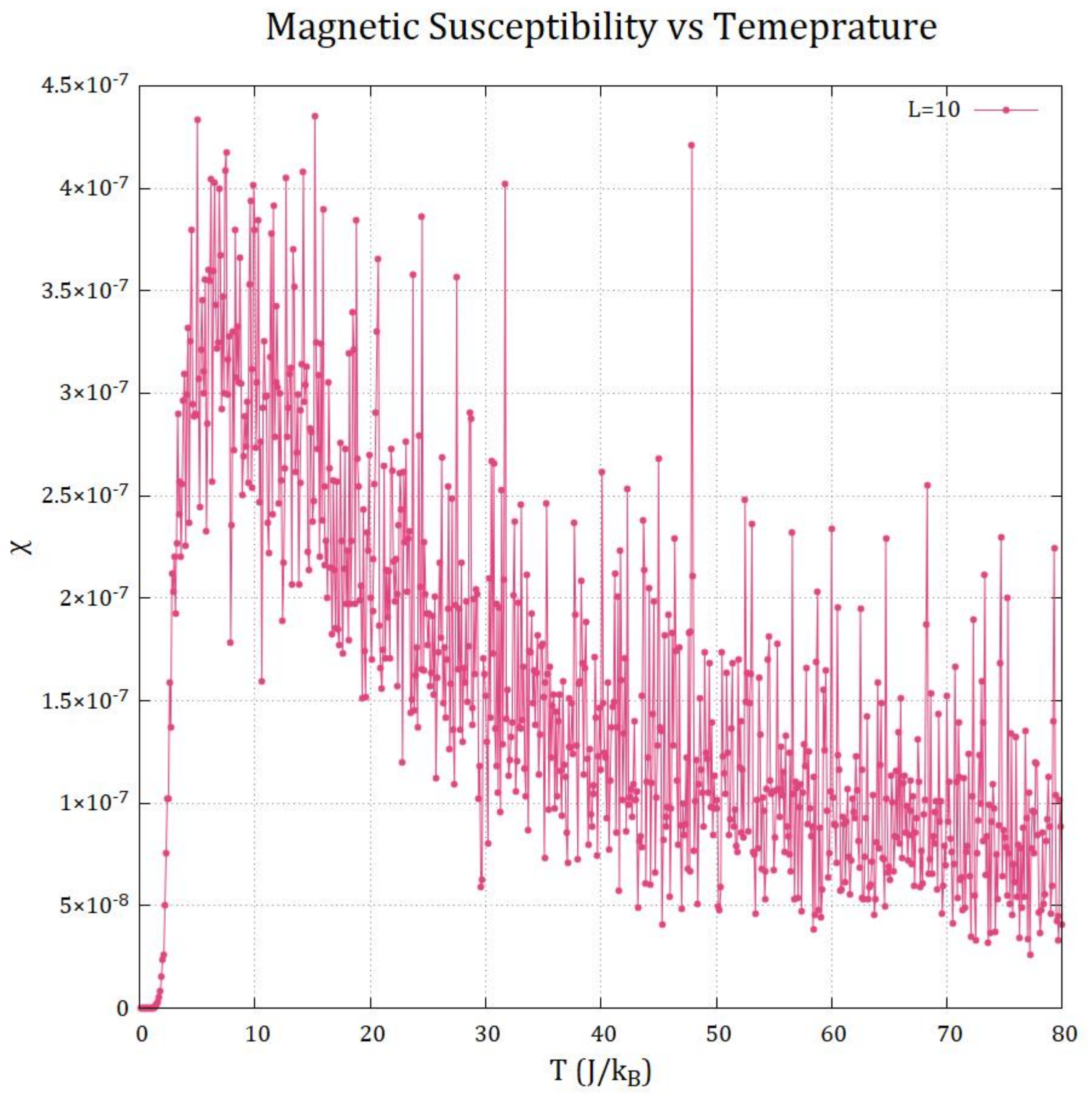


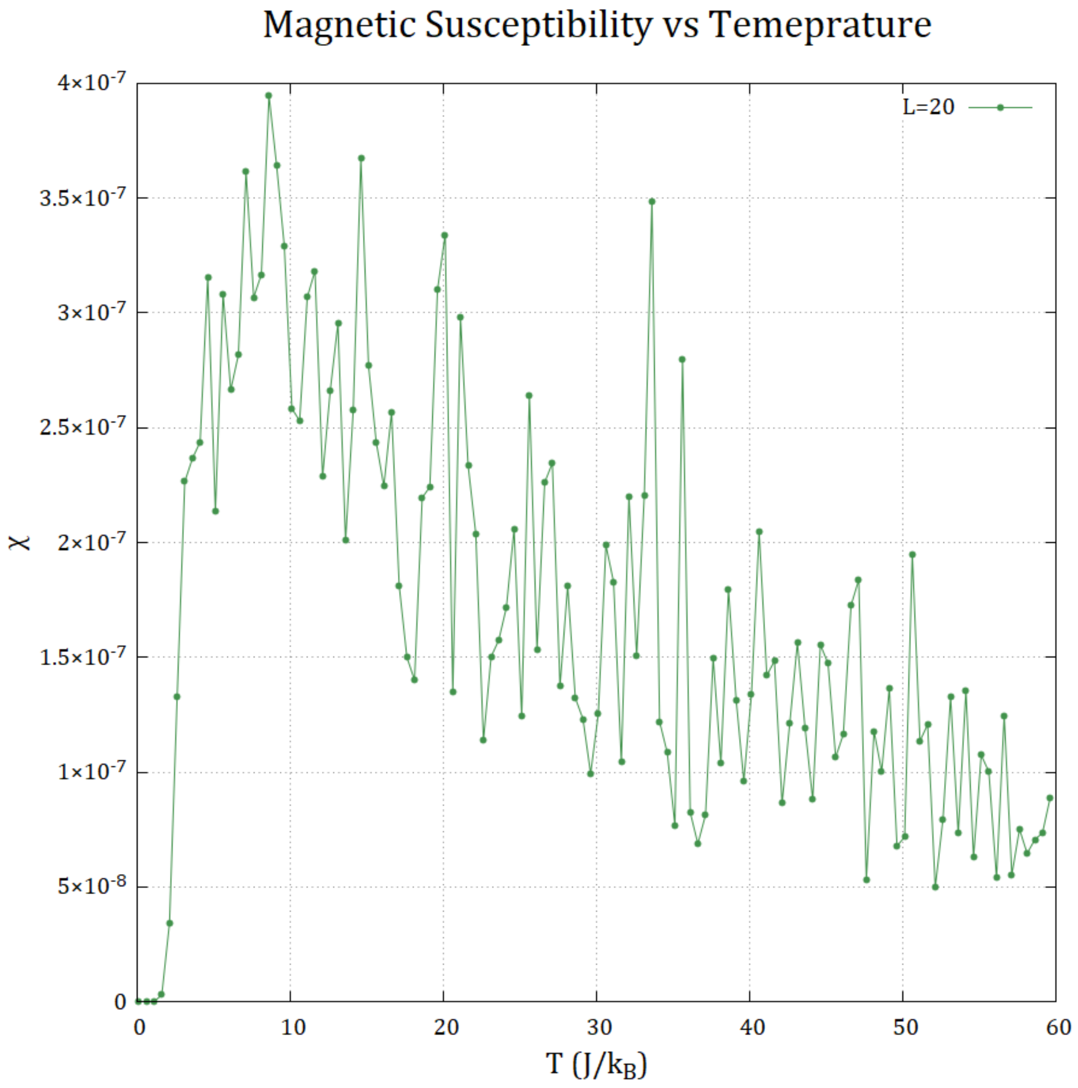
Anti-ferromagnetism

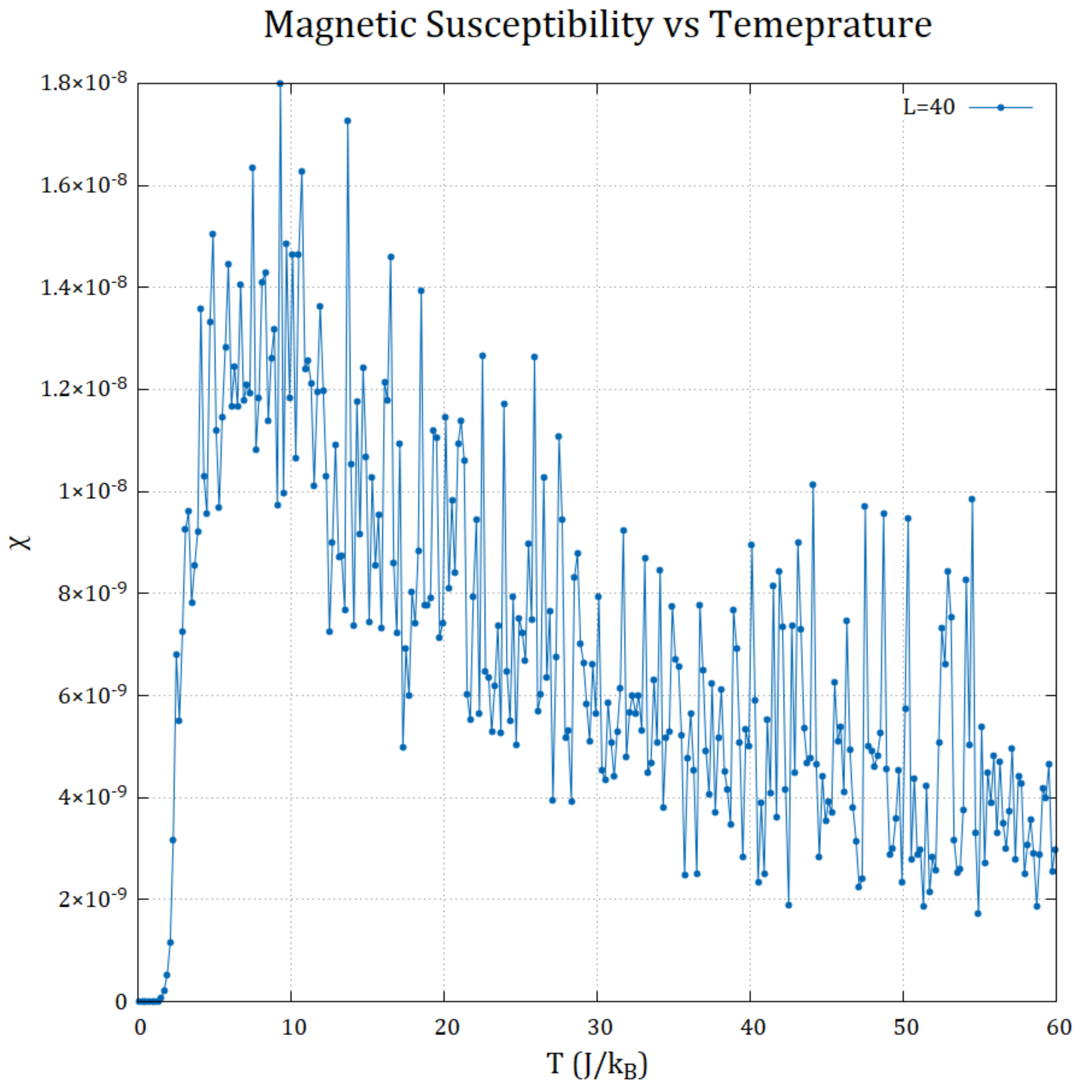
SUSCEPTIBILITY vs TEMPERATURE
χ vs. T

Finding Néel temperature by studying susceptibility with temperature.

Here, the Néel temperature at the maxima of susceptibility.




Magnetic Susceptibility vs Temeprature
L=20
χ
T (J/k_B)
0
10
20
30
40
50
60
0
5×10^-8
1×10^-7
1.5×10^-7
2×10^-7
2.5×10^-7
3×10^-7
3.5×10^-7
4×10^-7

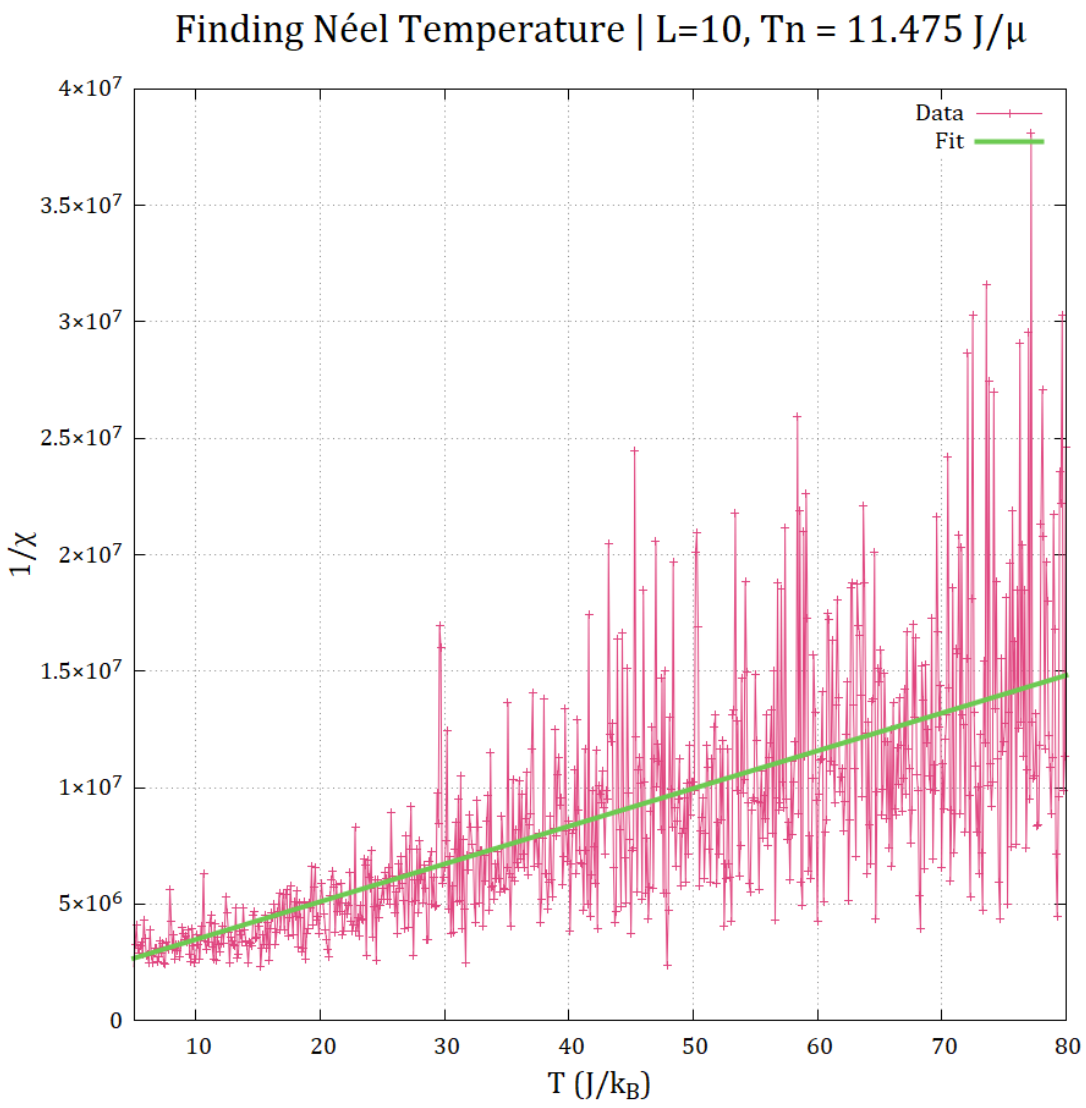

Magnetic Susceptibility vs Temeprature
L=40
χ
T (J/k_B)
0
10
20
30
40
50
60
0
2×10^-9
4×10^-9
6×10^-9
8×10^-9
1×10^-8
1.2×10^-8
1.4×10^-8
1.6×10^-8
1.8×10^-8

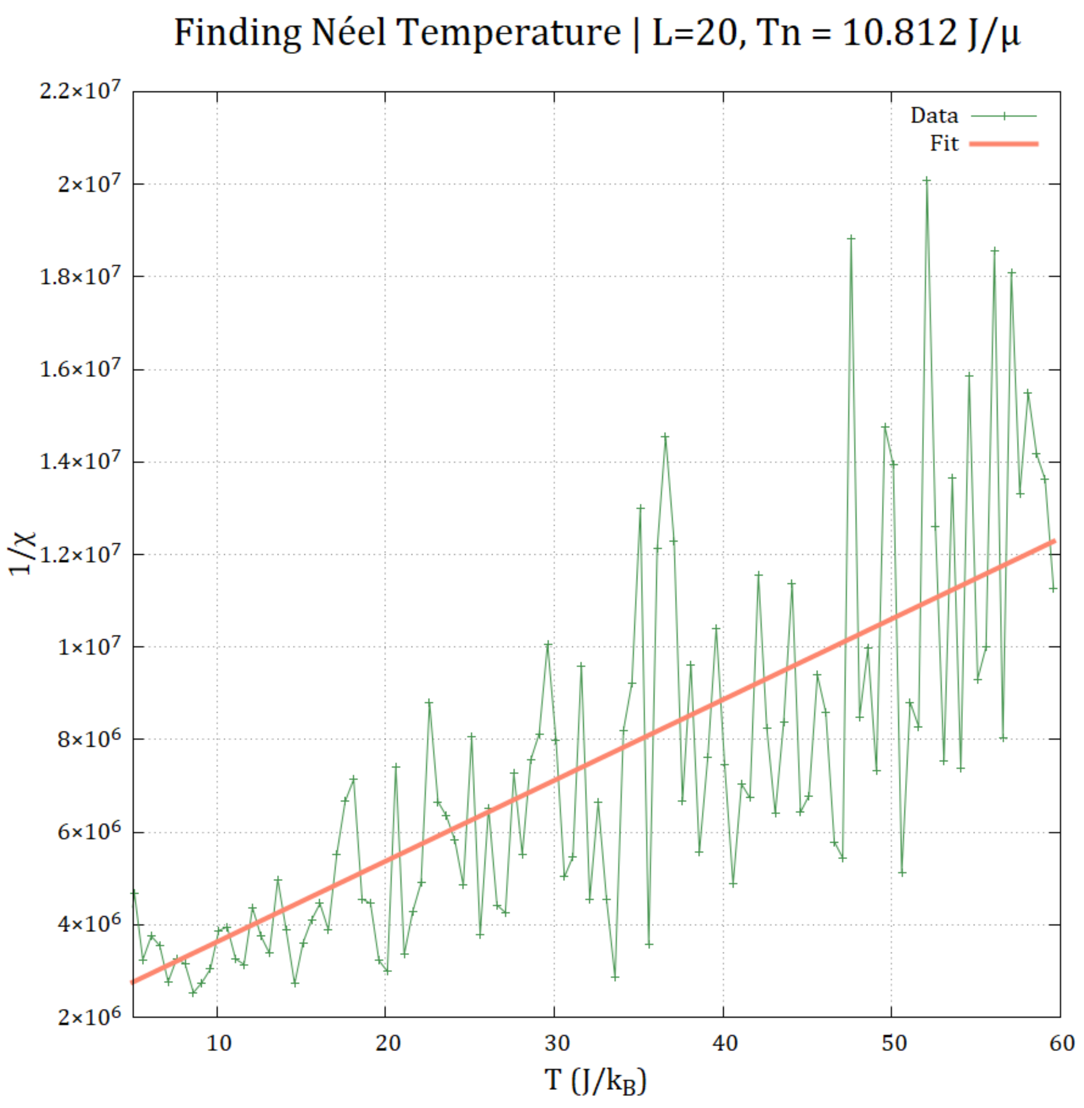
Anti-ferromagnetism

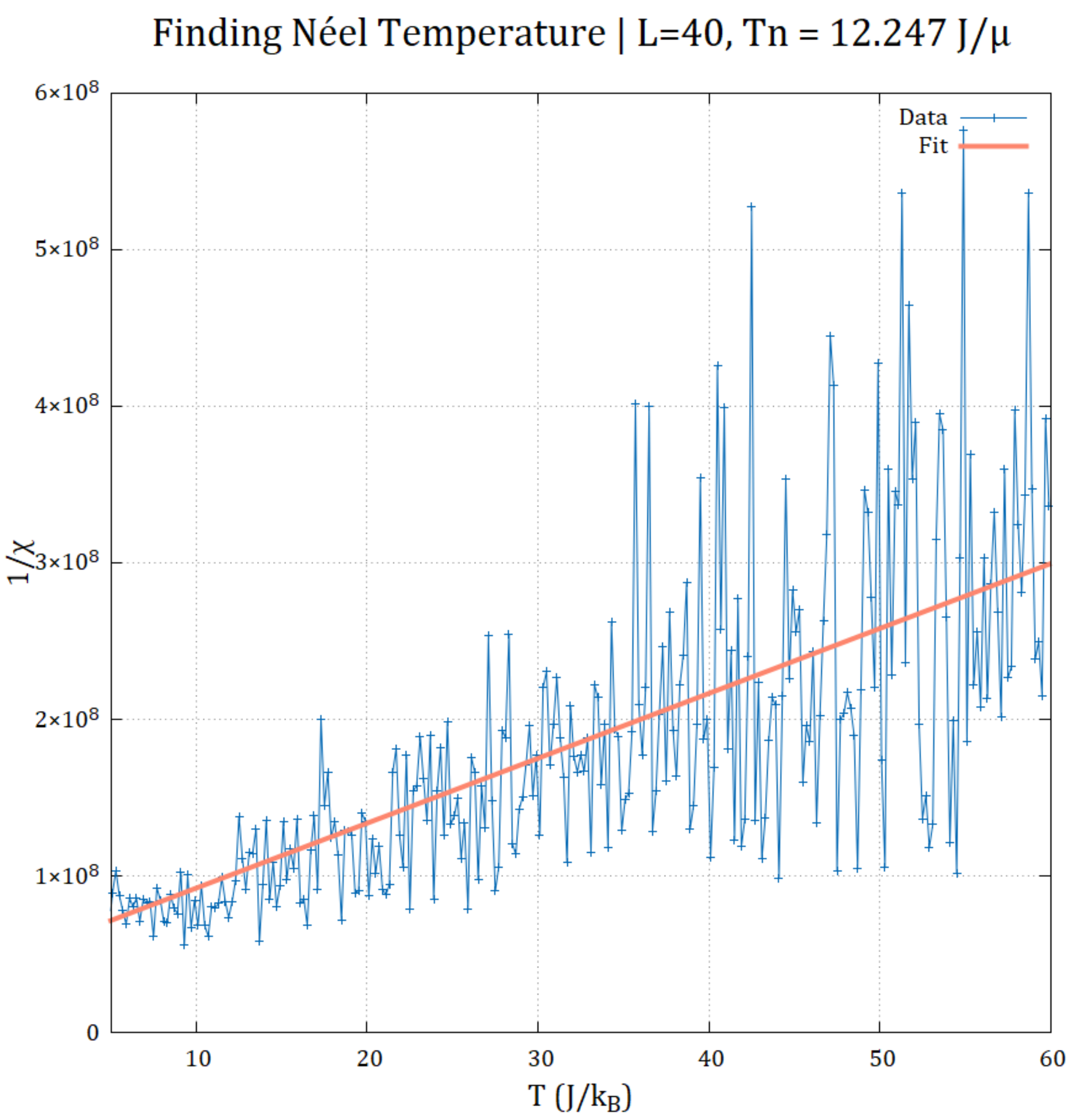
FINDING NÉEL TEMPERATURE

By fitting 1/X vs. T with a linear equation, during to Curie-Weiss law.

Note that Curie-Weiss law is derived from mean field, so this is just an estimate.




Finding Néel Temperature | L=20, Tn = 10.812 J/μ
Data
Fit
1/χ
2.2×10^7
2×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1×10^7
8×10^6
6×10^6
4×10^6
2×10^6
10
20
30
40
50
60
T (J/k_B)

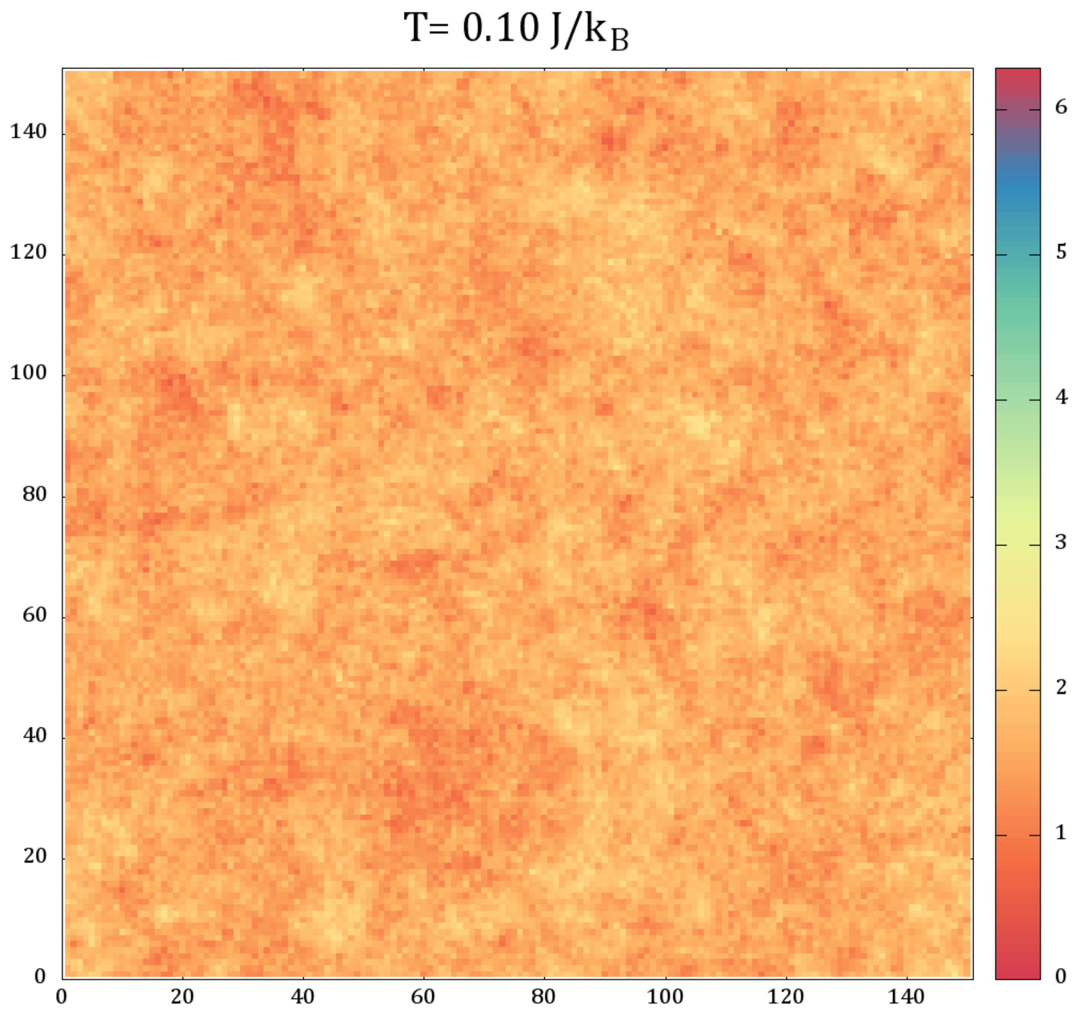

Finding Néel Temperature | L=40, Tn = 12.247 J/μ
Data
Fit
1/χ
6×10^8
5×10^8
4×10^8
3×10^8
2×10^8
1×10^8
0
10
20
30
40
50
60
T (J/k_B)

Arbitrary Spin Direction in 2D

PHASE TRANSITION

Ferro to Para by Increasing Temp.

This animation shows the spins of the system in the transition from ferro- to para- magnetism by increasing temperature.

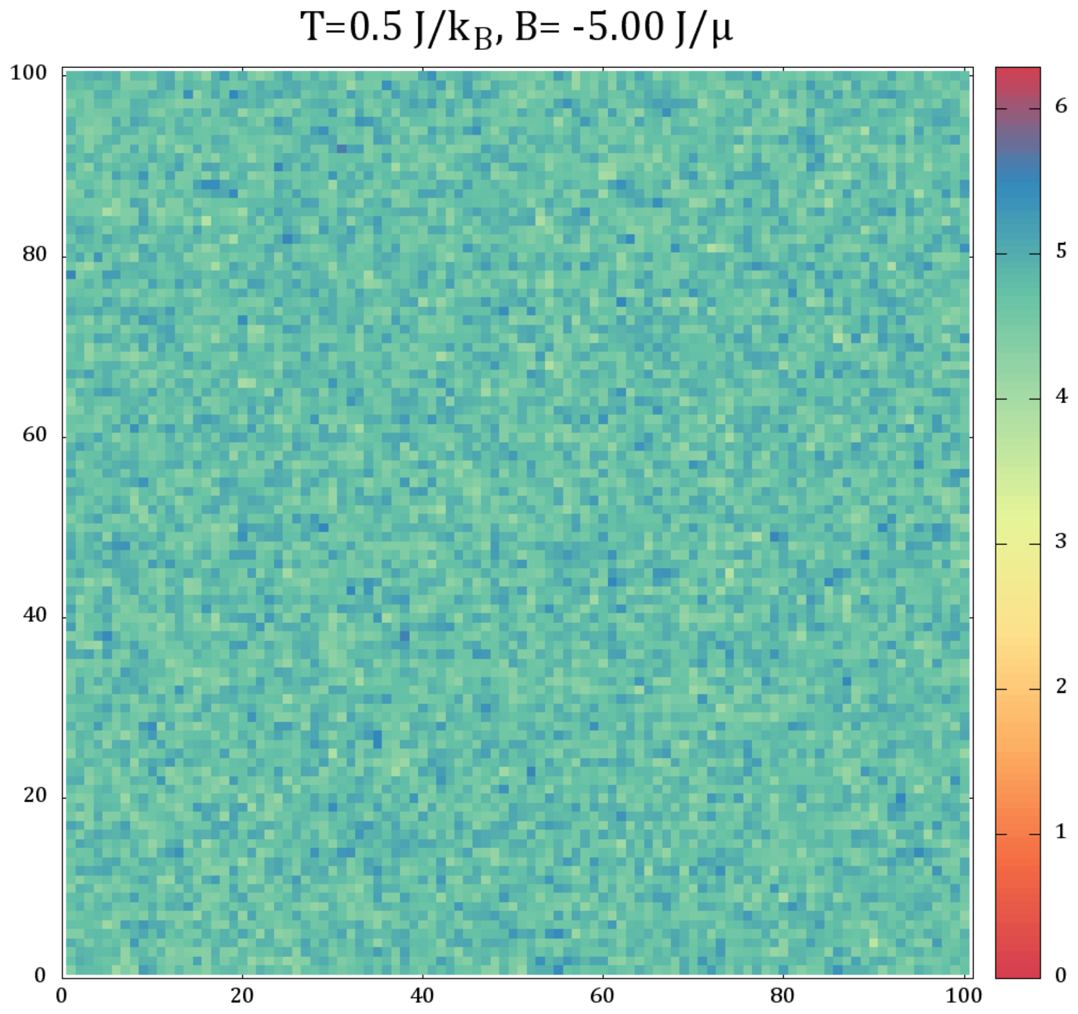


Arbitrary Spin Direction in 2D

HYSTERESIS LOOP
<M> vs. B

Visualizing the hysteresis loop by showing the spins as the magnetic field changes.

Try to find the coercive field!



FUTURE WORK

- Apply parallelization to run systems larger
- Try other algorithms than Monte Carlo Metropolis, like Wolff algorithm
- Consider other term on Hamiltonian
- Calculate the critical exponents of Ising model
- Study universality, scale invariance of Ising model

SUMMARY

- 2D and 3D Ising models were simulated
- Effects of system size were studied
- General spin direction was implemented
- The effect of coupling strength is studied
- Anti-ferromagnetism was studied using Ising model

WORK DISTRIBUTION

Kumail

Asif


THANK YOU