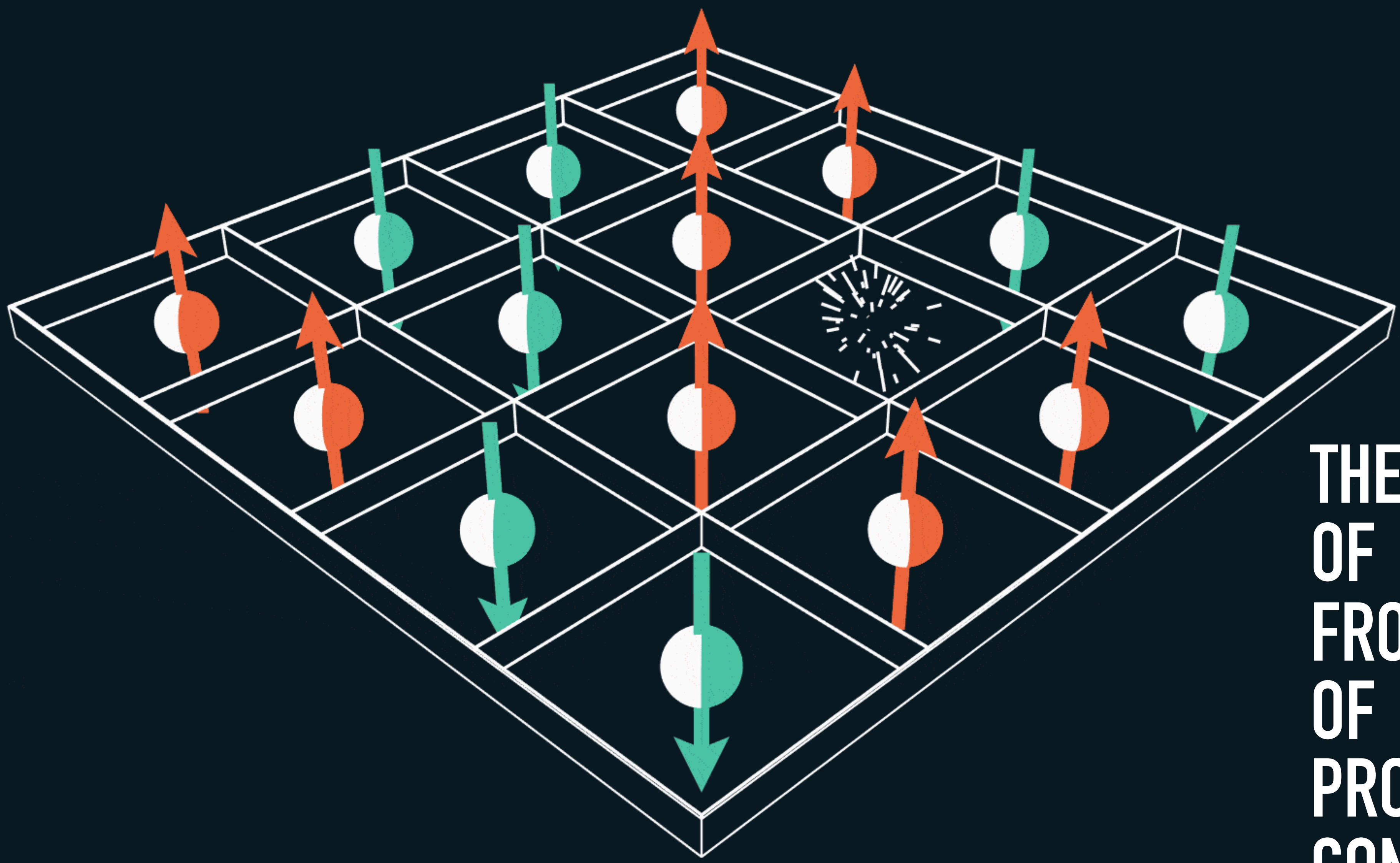
NICOLÁS VERGARA - NANOMAGNETISM LABORATORY

MONTECARLO SIMULATION OF MAGNETIC NANOSTRUCTURES .

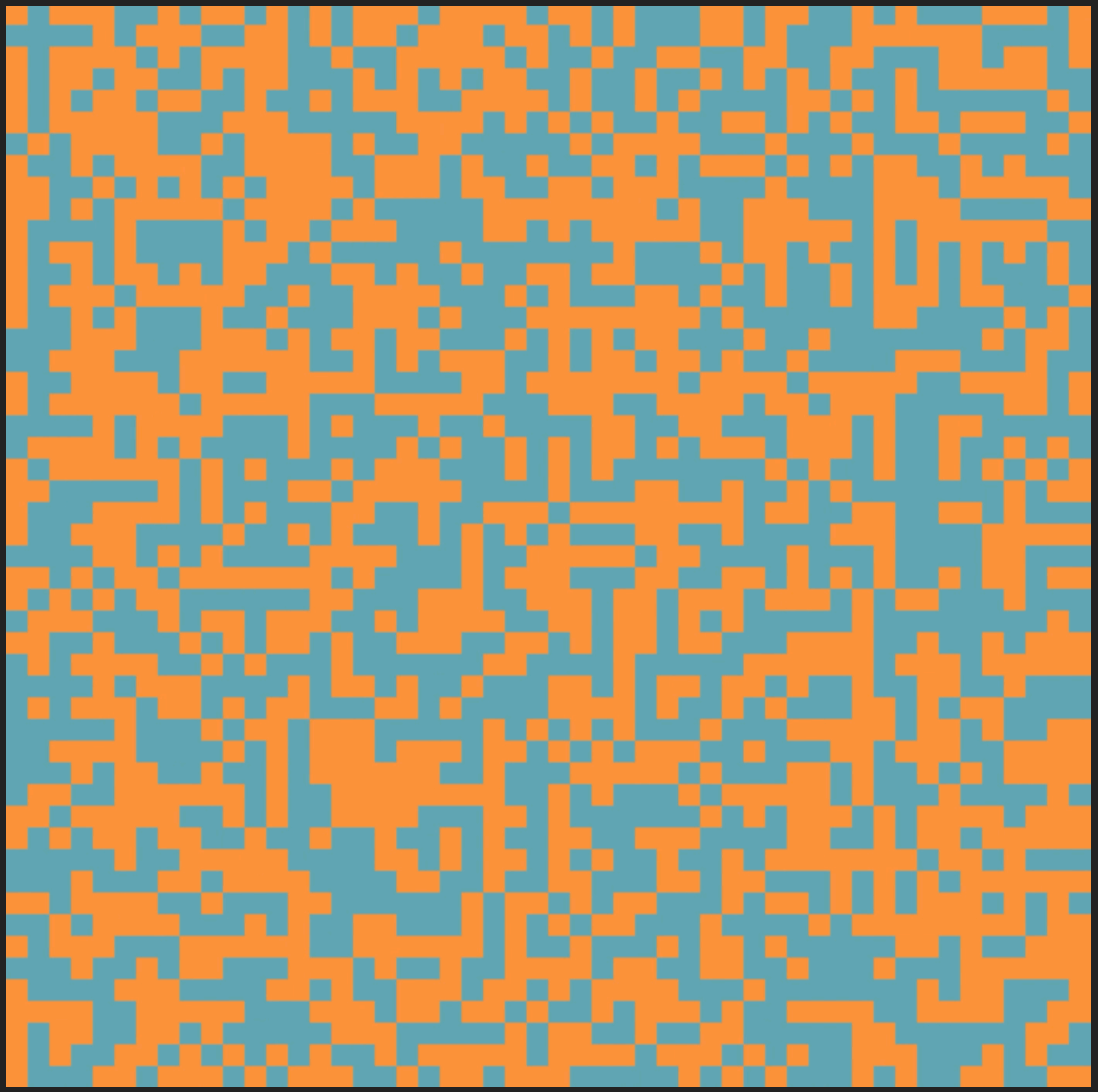
MAGNETS



THE MAGNETIC PROPERTIES OF THE MATERIALS ARISES FROM ELECTRONS. THE SUM OF THE ELECTRONS PROPERTIES DESCRIBES COMPLETELY THE MAGNET

QuantaMagazine: https://www.quantamagazine.org/a-childs-puzzle-has-helped-unlock-the-secrets-of-magnetism-20190124/

WE SIMULATE A MAGNET AS AN ARRAY OF SPINS. EVERY TIME WE INITIALIZE IT WE MUST ASSURE A RANDOM STATE



ORANGE IS SPIN UP AND BLUE IS SPIN DOWN

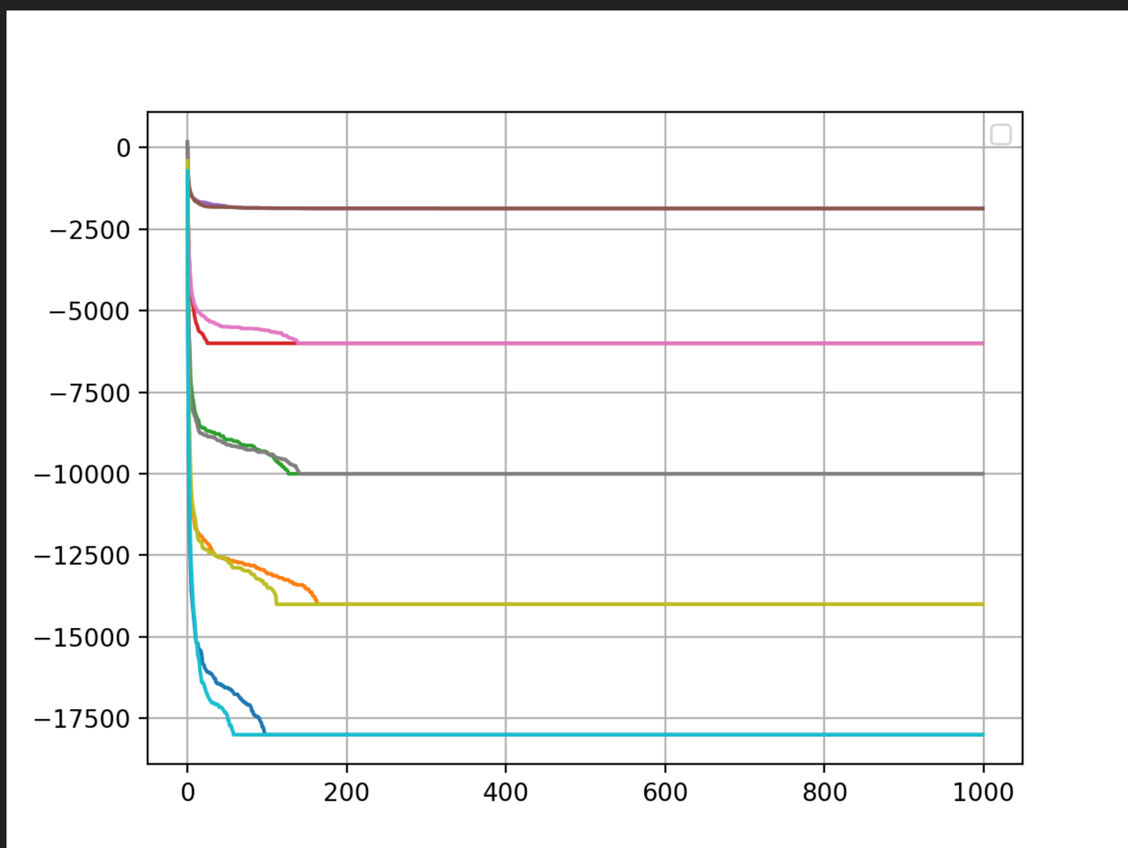
2D MODEL

```
SYSTEM = HBAR*2 * (0.5 - NP.RANDOM.RANDINT(0, 2,SIZE=[L, L, L]))
```

BUT WHAT ABOUT THE DYNAMICS ?

MINIMIZATION OF ENERGY

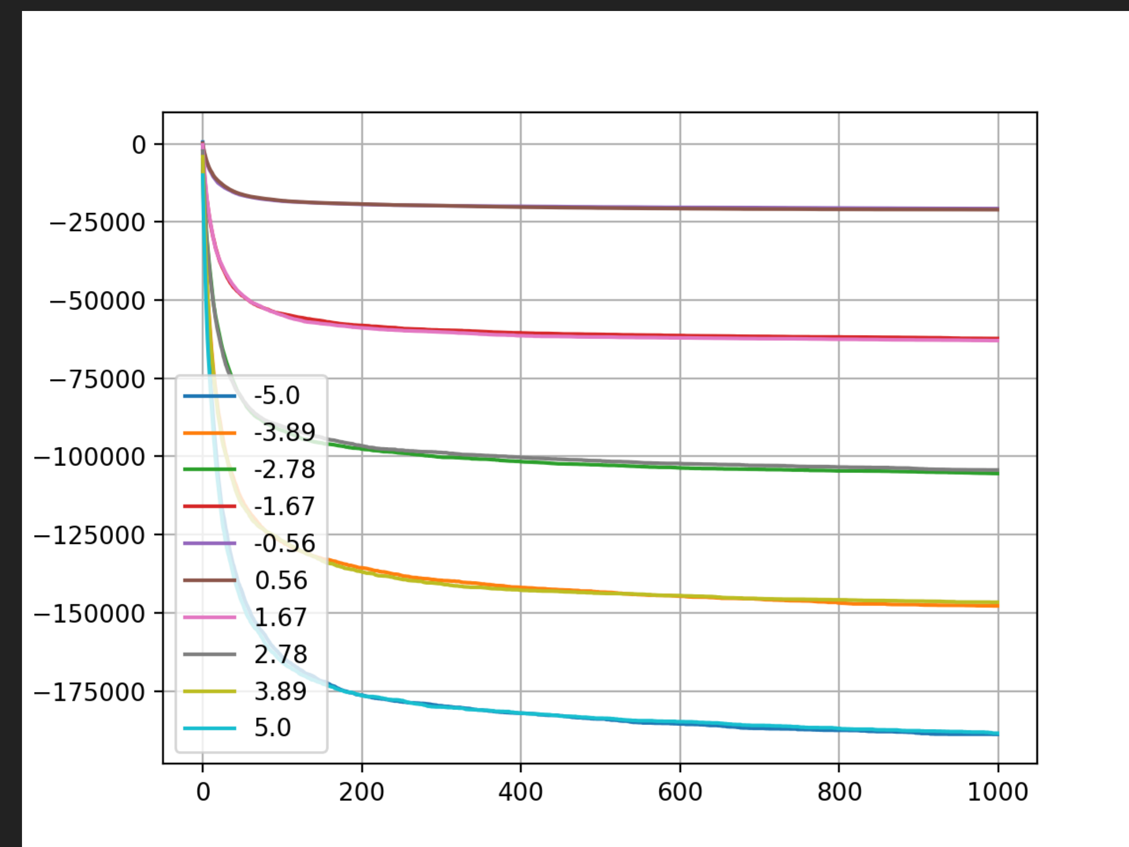
Energy



Iterations

M=30x30

Energy



Iterations

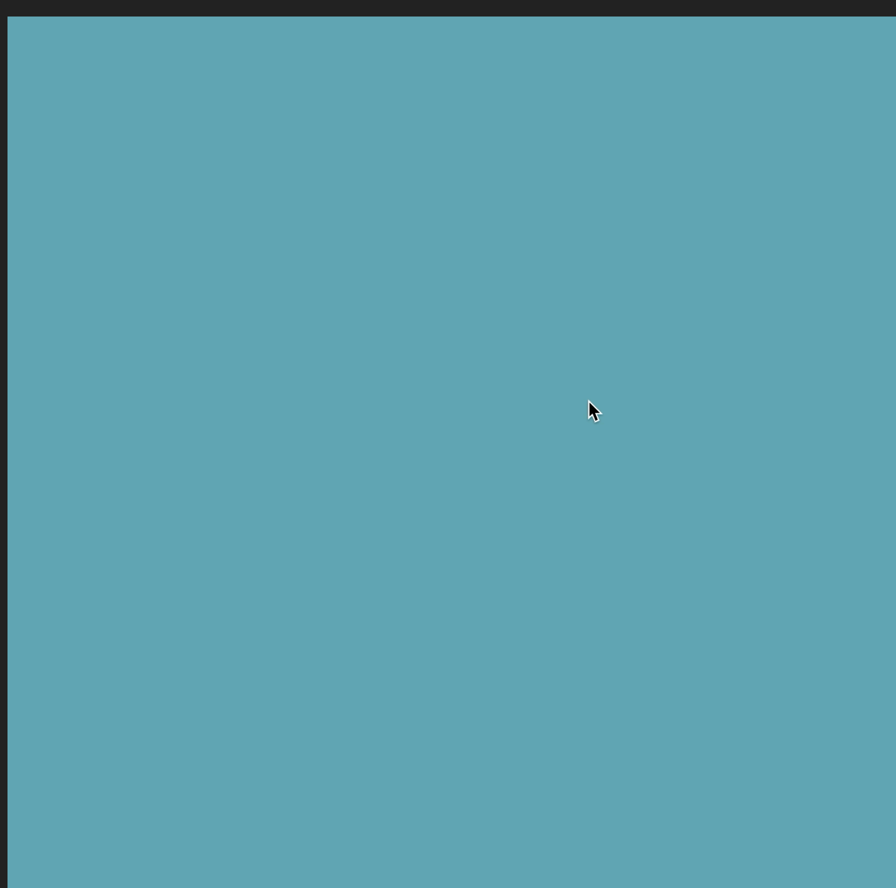
M=100x100

$$p_i = \frac{1}{Z} e^{-E_i/(K_B T)}$$

SO IF WE FIX THE ENERGY, ASSUMING IT'S ALREDY MINIMUM , WE CAN EXPECT THAT THE TEMPERATURE GIVE INFORMATION ABOUT THE MOST PROBABLE STATE OF THE SYSTEM

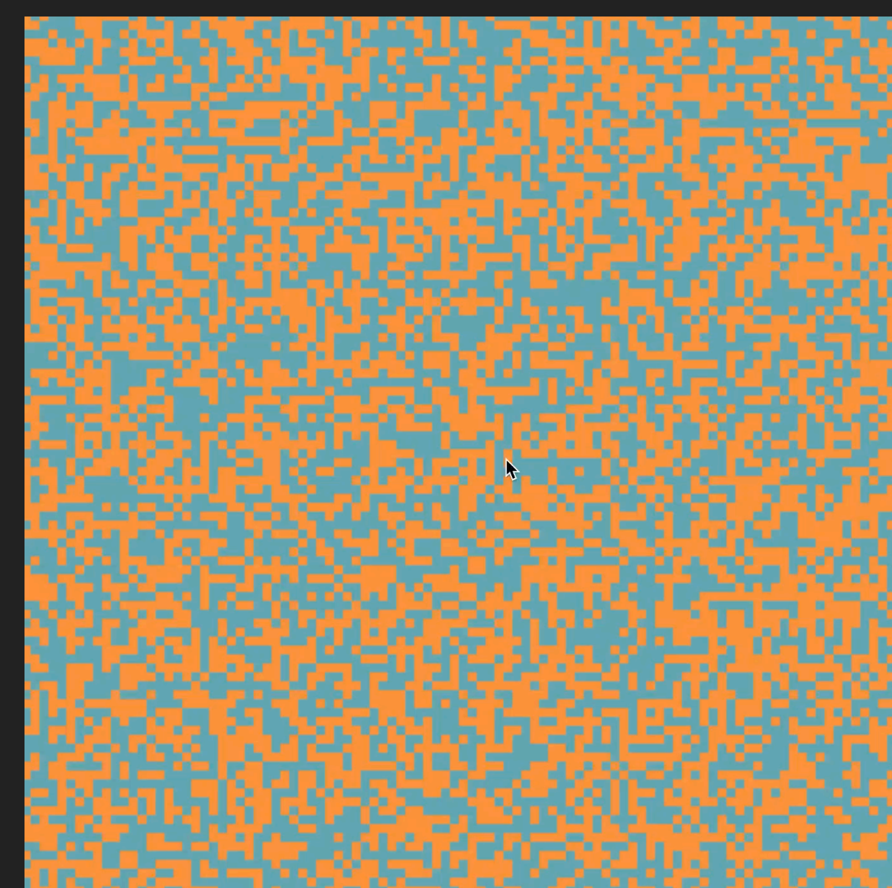
$$T \to 0 \Rightarrow p_i \approx 1$$

THERE IS ONE REALLY PROBABLE STATE

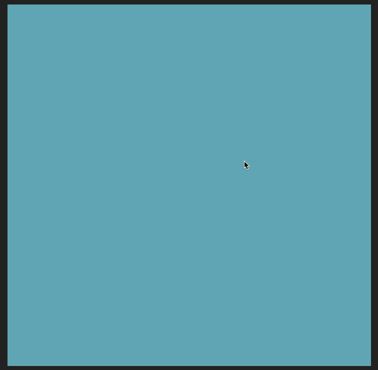


$$T \to \infty \Rightarrow p_i \approx 0$$

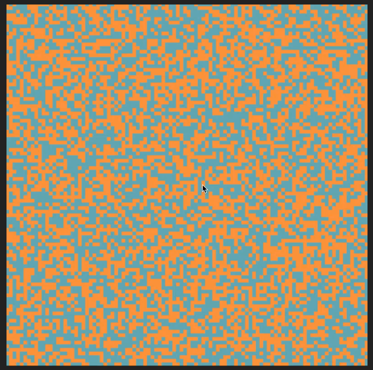
THERE ARE MANY PROBABLE MICRO-STATES

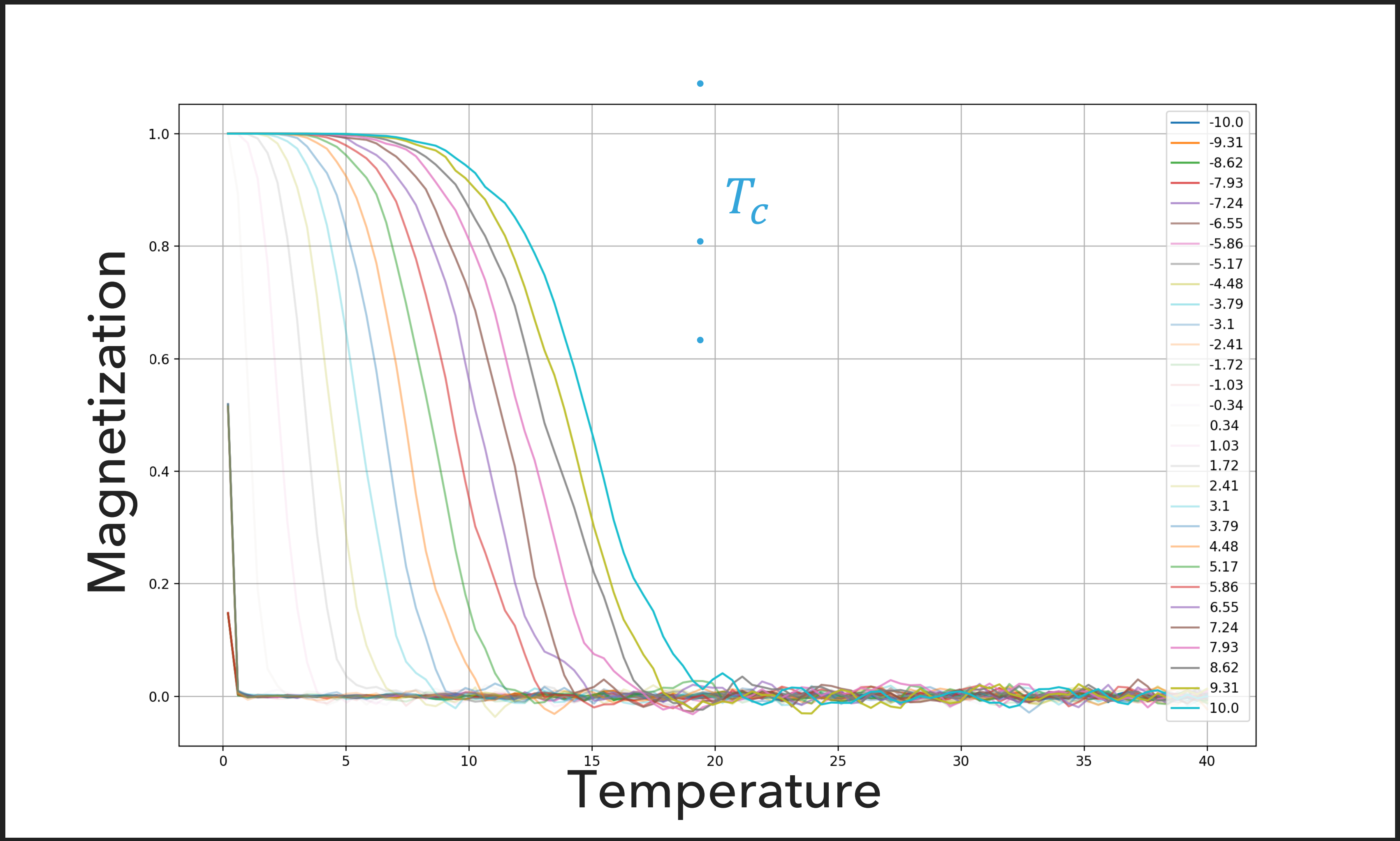


THE TEMPERATURE OF TRANSITION BETWEEN THIS TWO STATES, IT'S CALLED THE CURIE TEMPERATURE : T_c

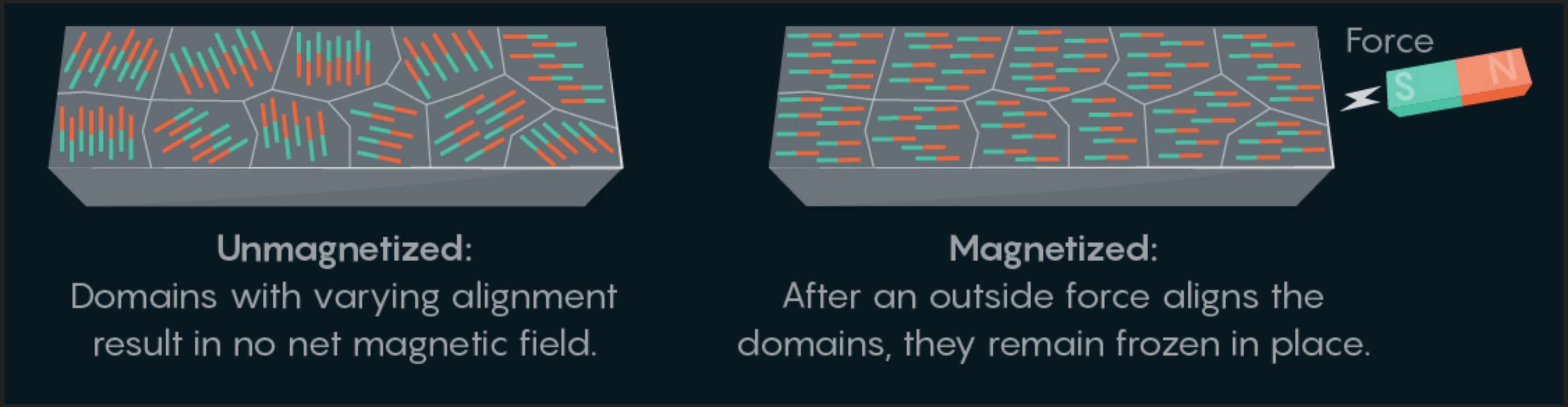


$\rightarrow$

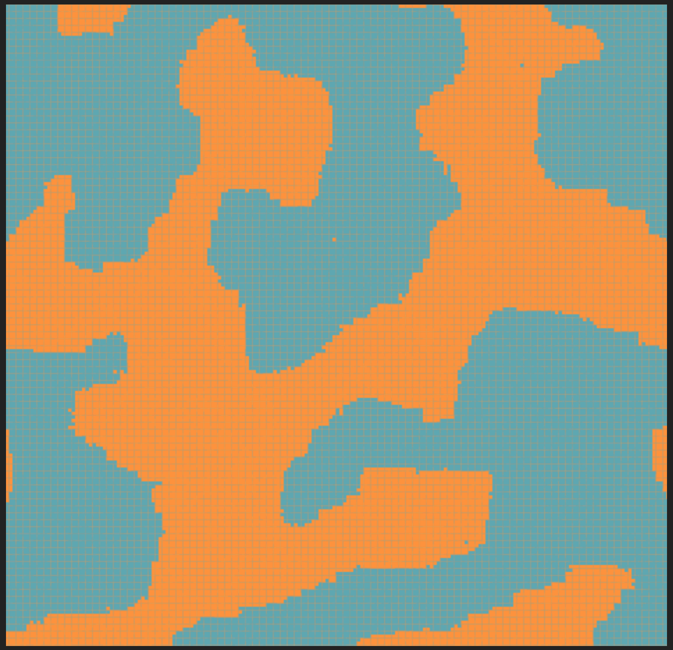




Transition of state, for different simulated systems



THANKS TO THE SIMULATION WE PREDICT THE FORMATION OF DOMAINS FOR TEMPERATURES IN THE RANGE OF THE TRANSITION OF STATE $0 < T < T_C$



Ernst Ising, Contribution to the Theory of Ferromagnetism. http://www.hs-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html

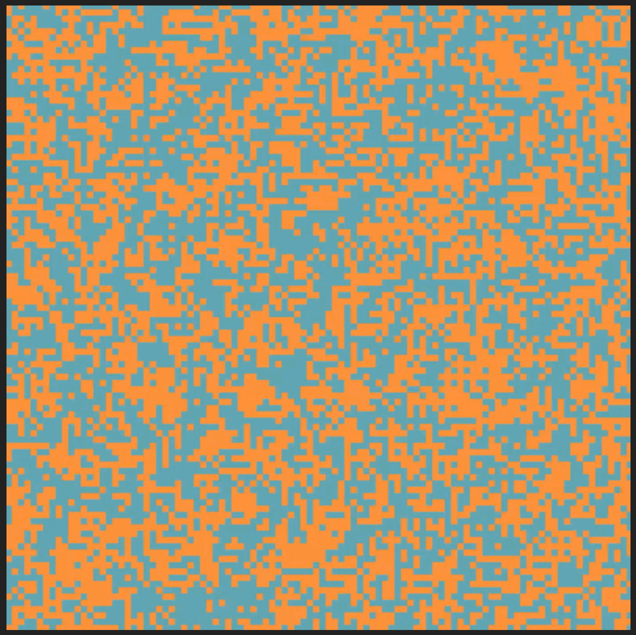
WHAT IF THERE IS AN EXTERNAL MAGNETIC FIELD?

$$E_i \equiv \mathcal{H}_i = s_{iz}\sum_j J_{ij} s_{j_z} \rightarrow \mathcal{H}_i = s_{iz}\sum_j J_{ij} s_{j_z} + B s_{iz}$$

SPINS TENDS TO ALING TO THE FIELD

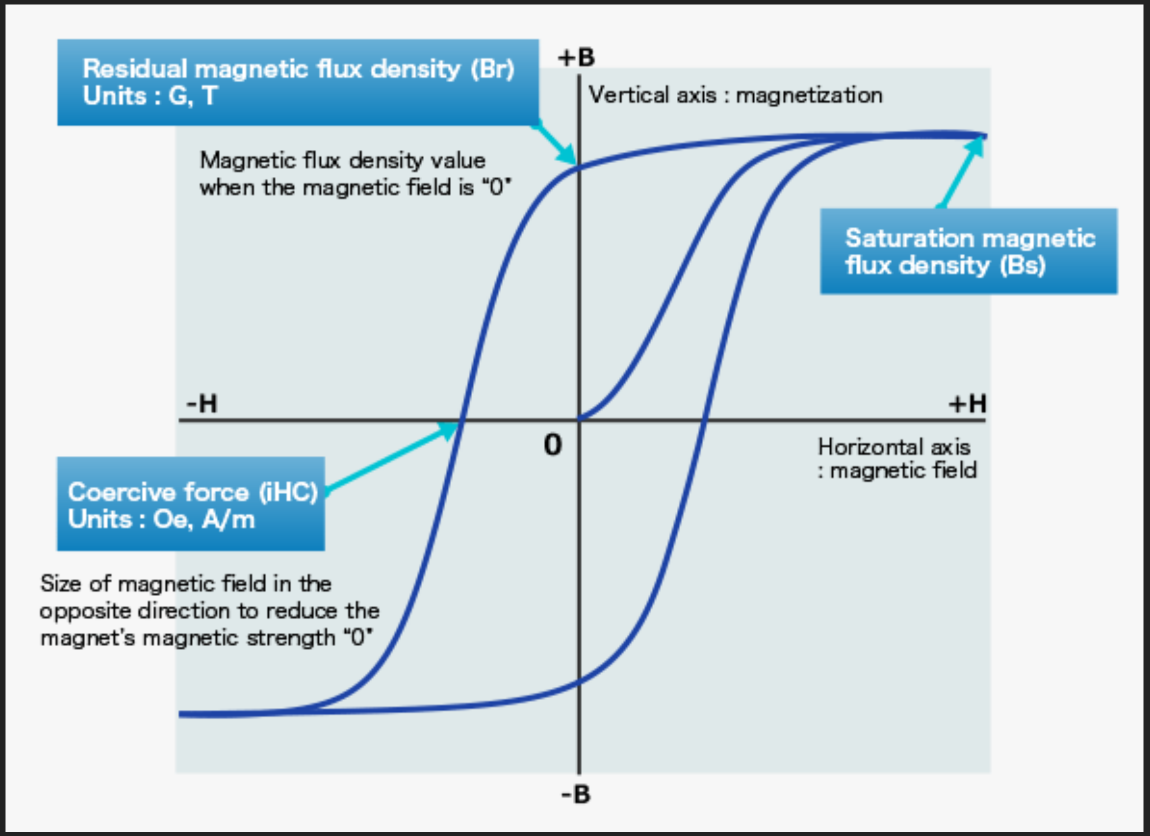
$T < T_c$

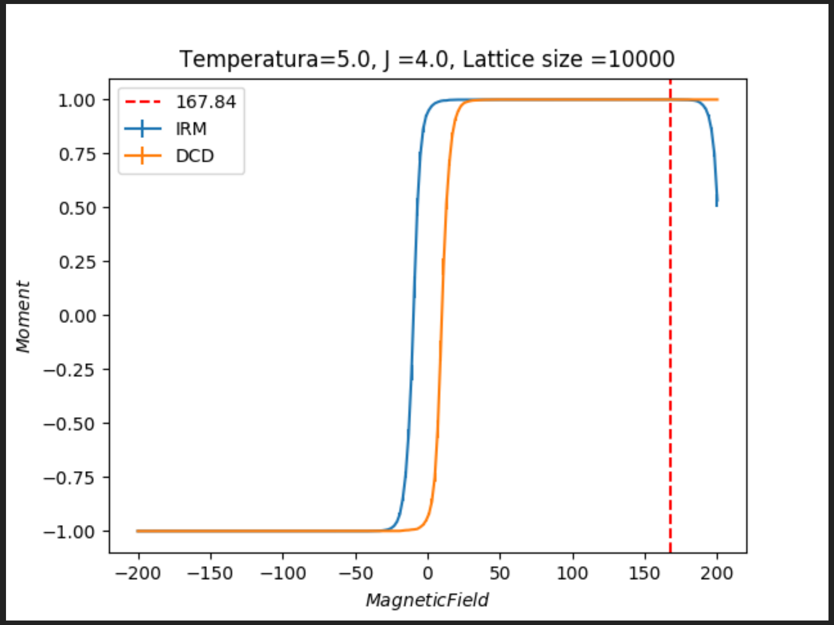
$T > T_c$

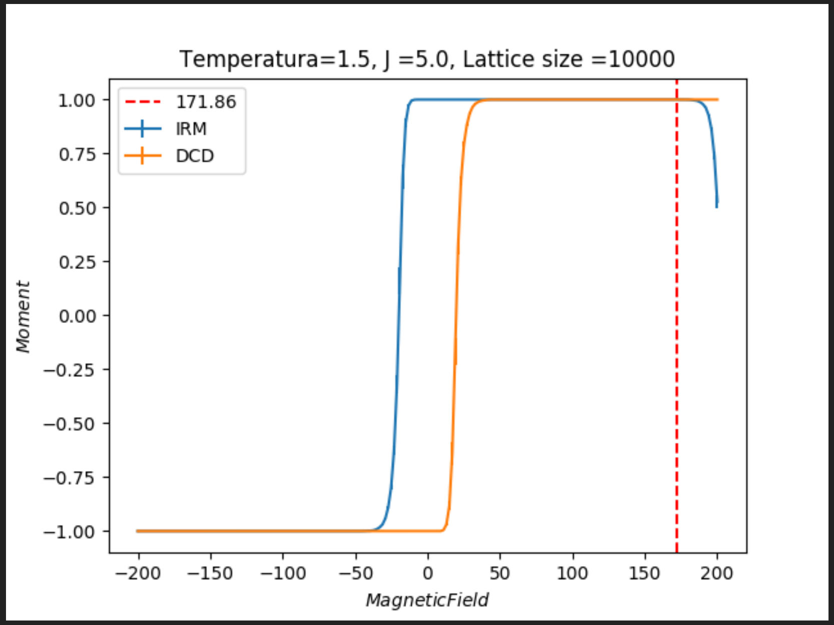


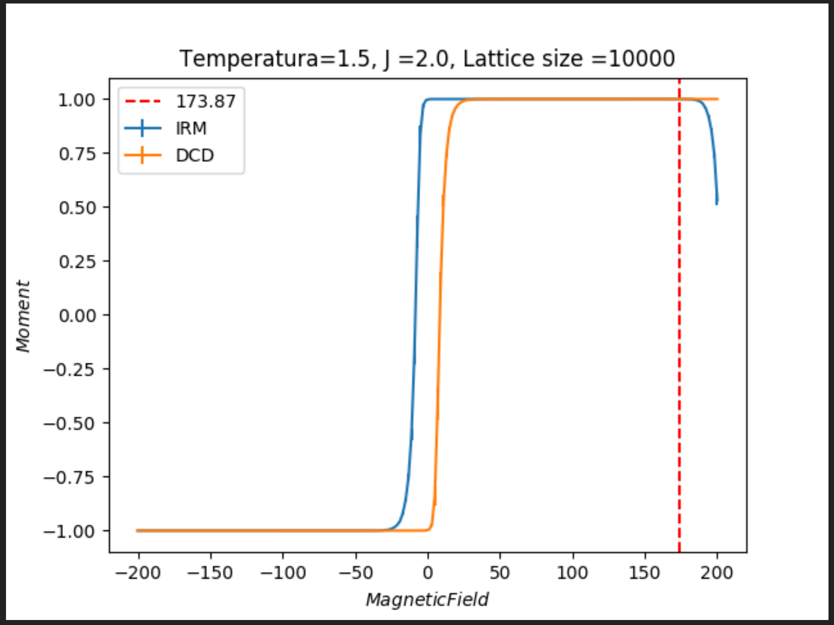
WHAT HAPPEN IF WE VARY THE FIELD, FROM REALLY STRONG IN ONE DIRECTION,TO THE OTHER, AND MEASURE THE MAGNETIZATION?

IT BEHAVES AS THE MAGNET HAS MEMORY. BECAUSE ,WE OBTAIN AN HYSTERESIS LOOP, IN OTHER WORDS IT DOES NOT RETURN BACK AT THE SAME PATH.



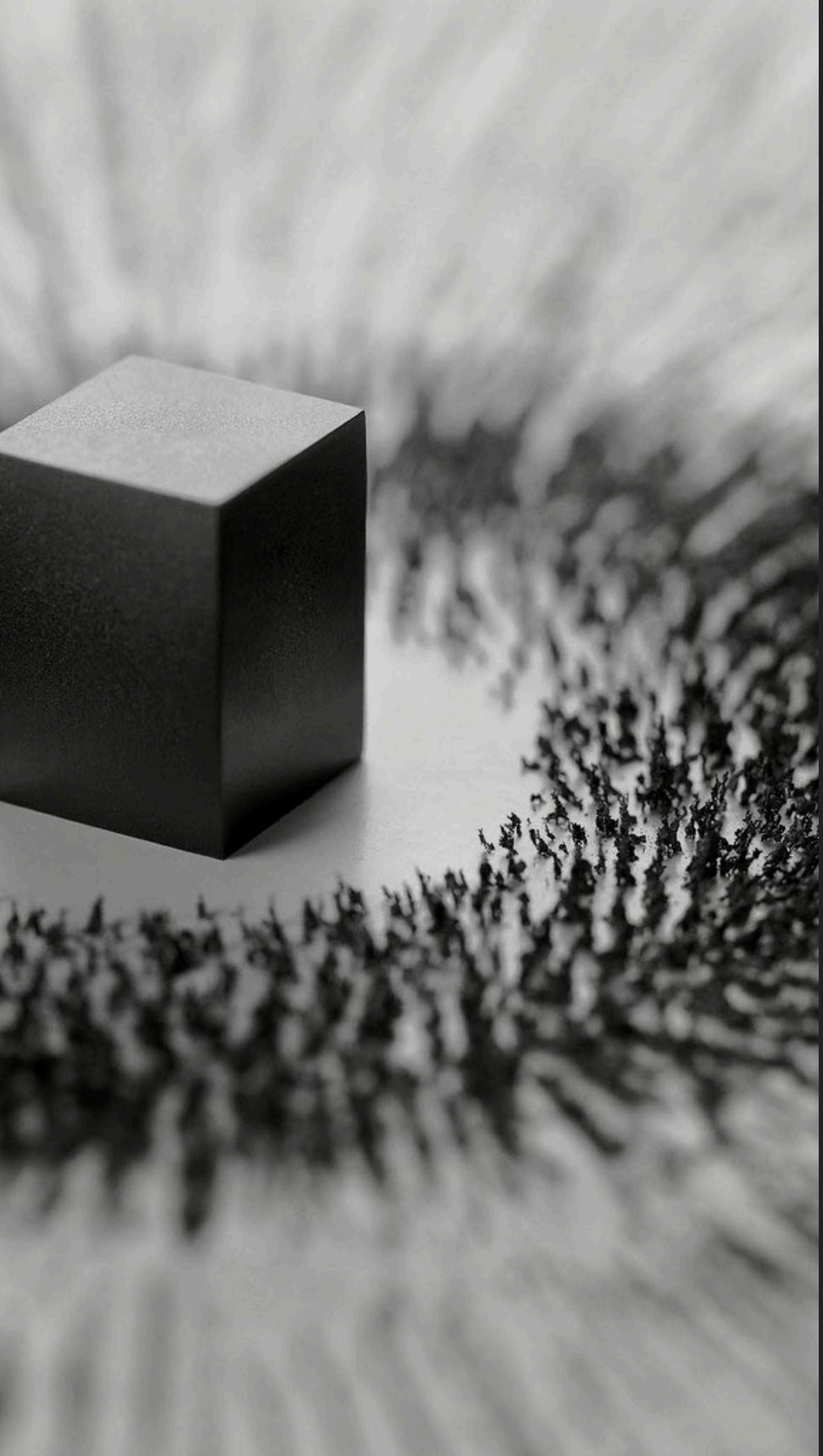






CAN WE REPRODUCE THIS BEHAVIOR WITH OUR SIMULATION?

YES, THE 2D ISING MODEL HAS MEMORY.



BUT WHAT OTHER MEASURES CAN WE REPRODUCE WITH THIS MODEL AND THE METROPOLIS ALGORITHM?

ISOTHERMAL REMANENT MAGNETIZATION

DIRECT CURRENT DEMAGNETIZATION

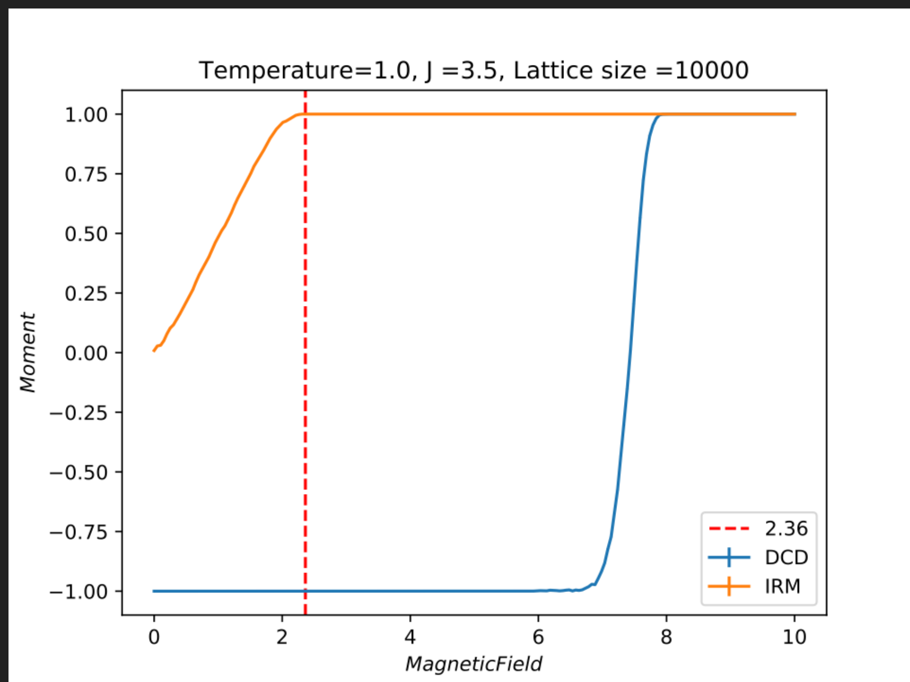
HEAT CAPACITY

SUSCEPTIBILITY

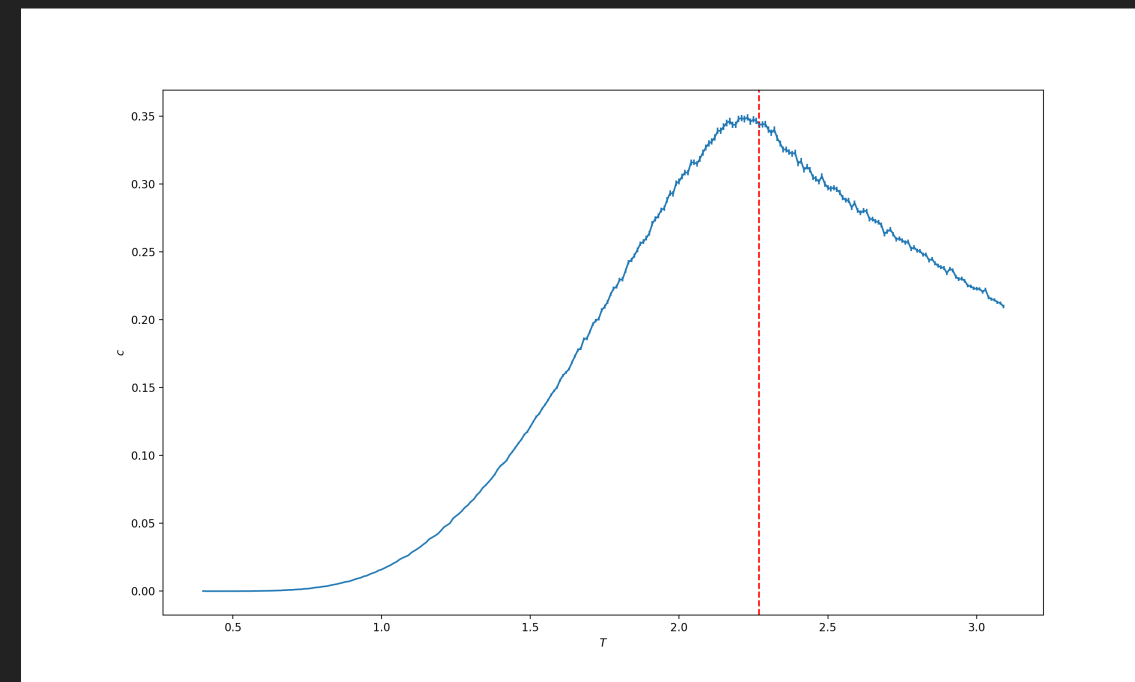
ENERGY

STANDARD BEHAVIOR

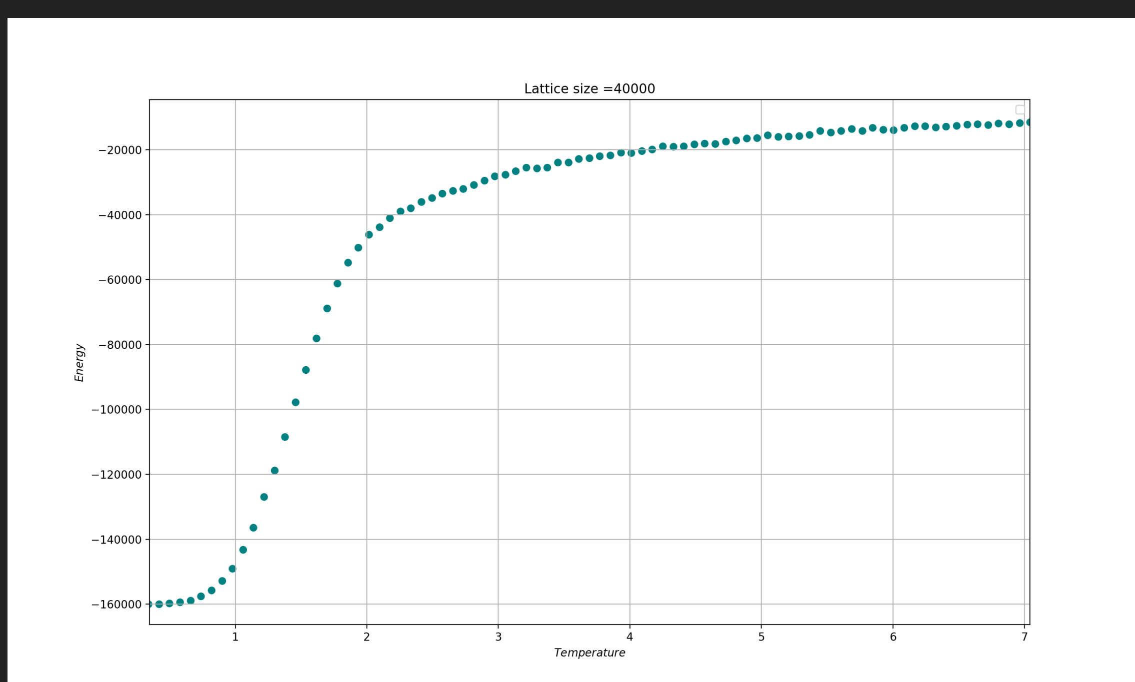
IRM AND DCD



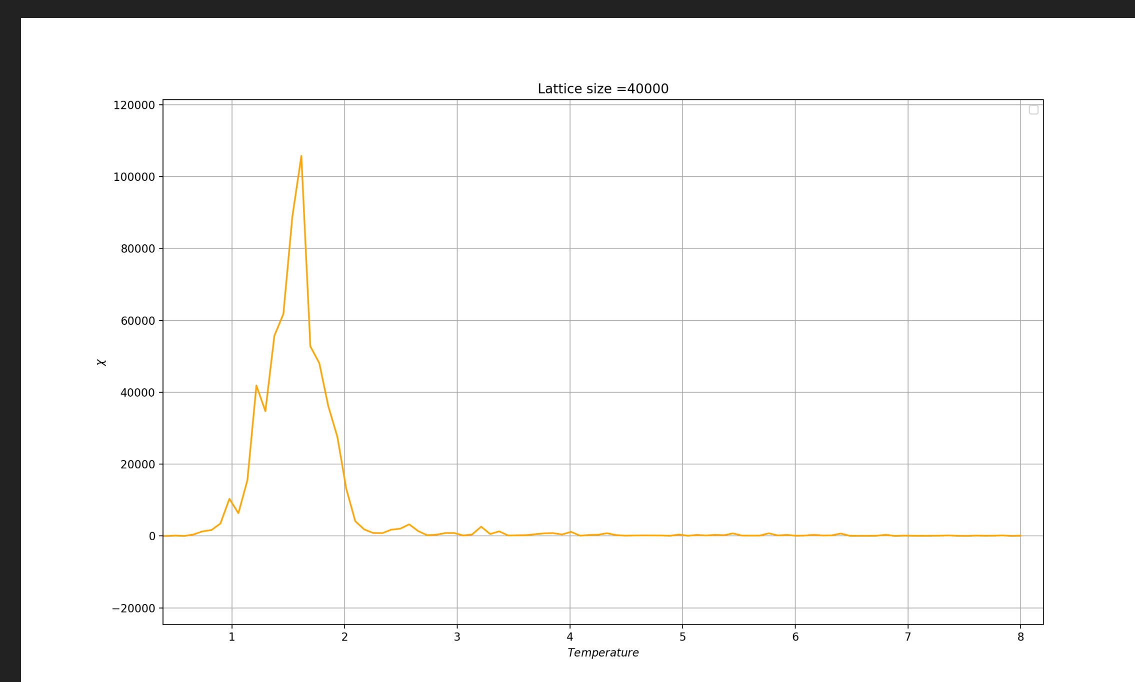
HEAT CAPACITY AS FUNCTION OF T



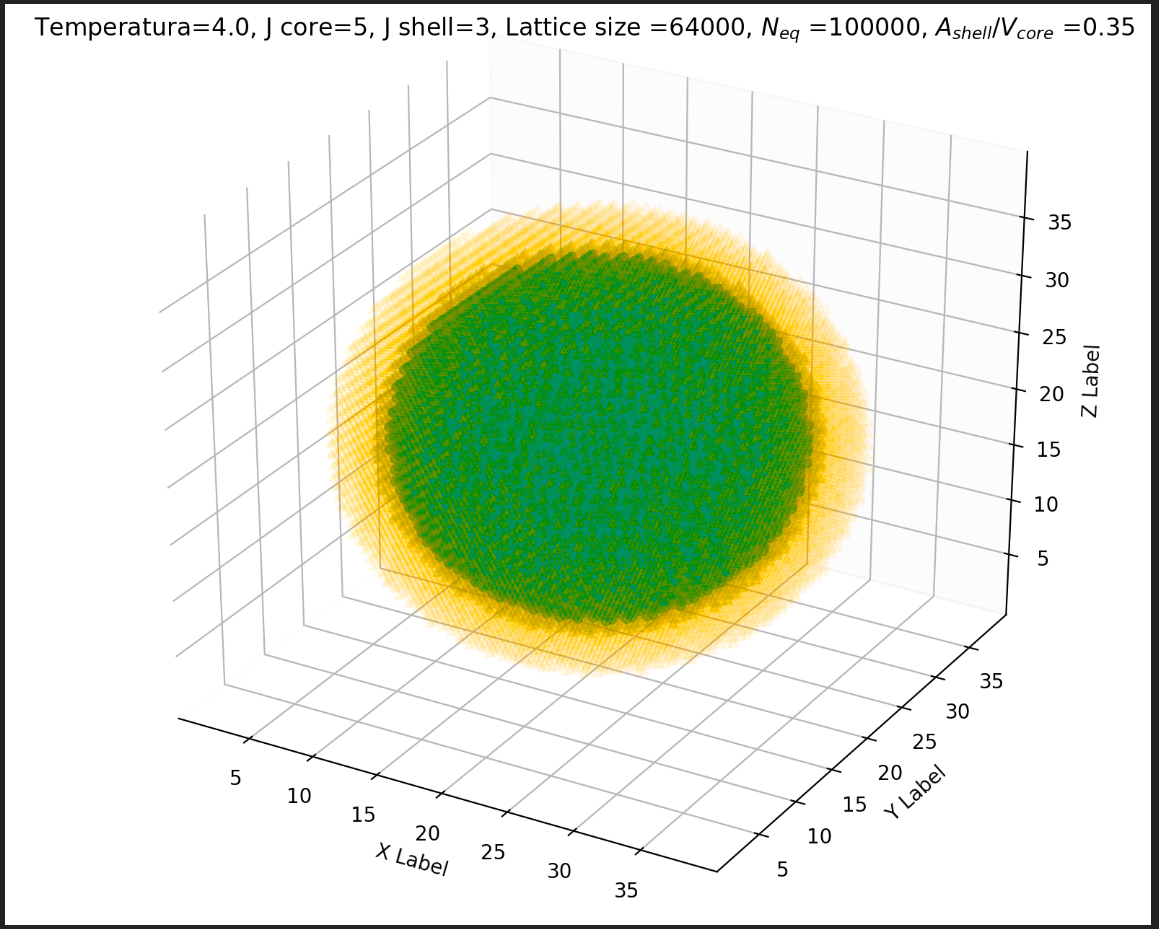
ENERGY AS FUNCTION OF T



SUSCEPTIBILITY AS FUNCTION OF T



WE SIMULATE A NANO-PARTICLE AS AN SPHERICAL ARRAY OF SPINS. WE ALSO COVER A CONFIGURATION CALLED CORE-SHELL

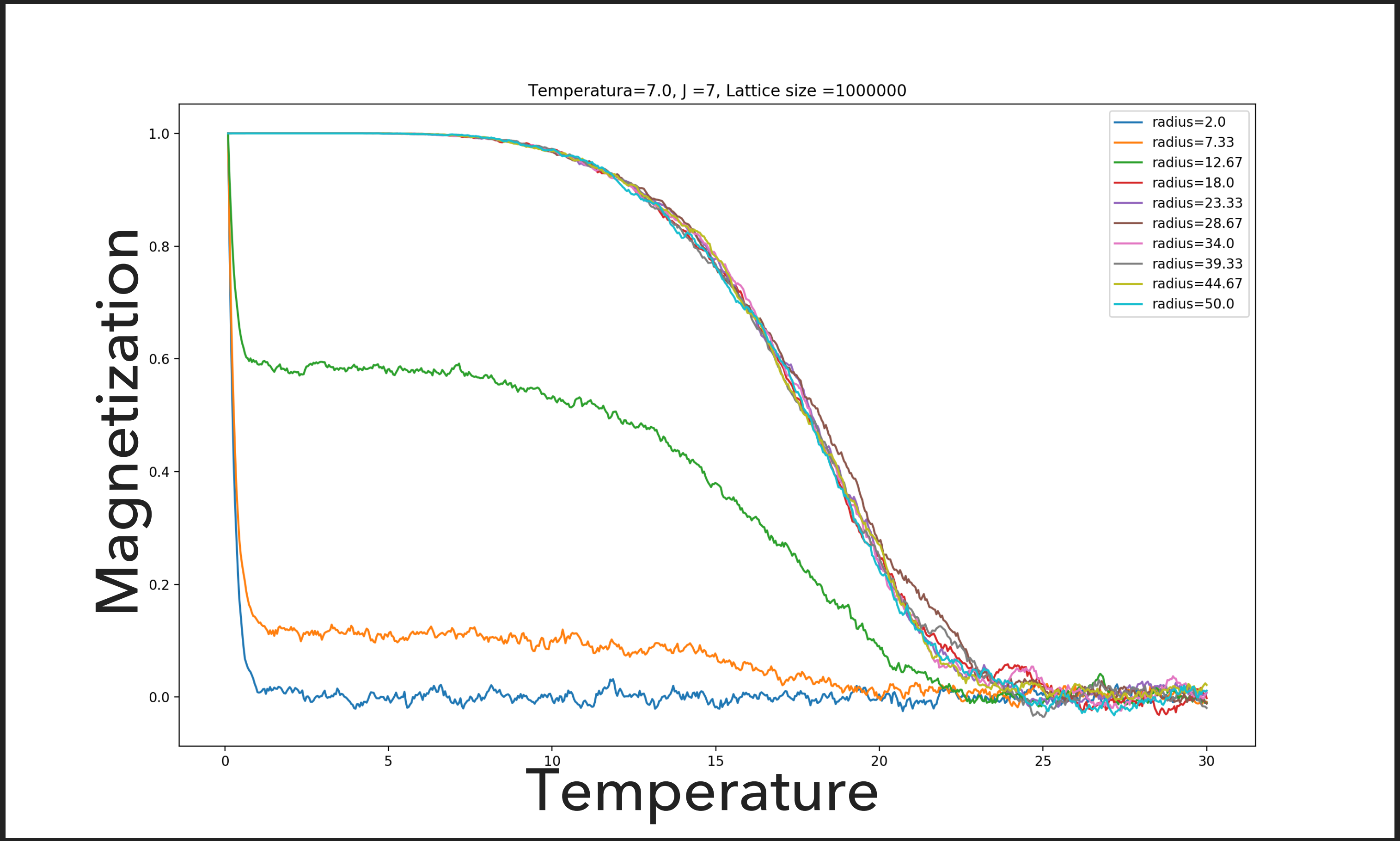


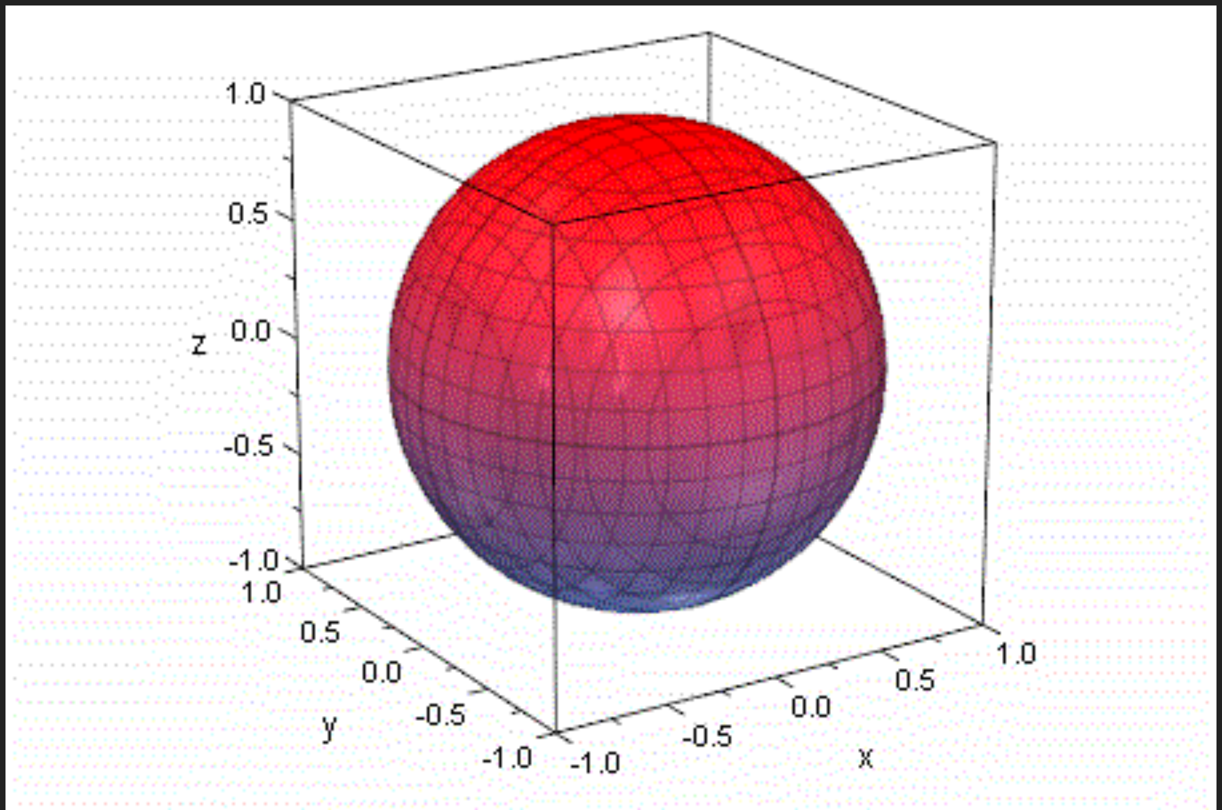
GRENN IS THE CORE, ORANGE THE INTERFACE, EVERY DOMAIN HAS A DIFFERENT COUPLING CONSTANT

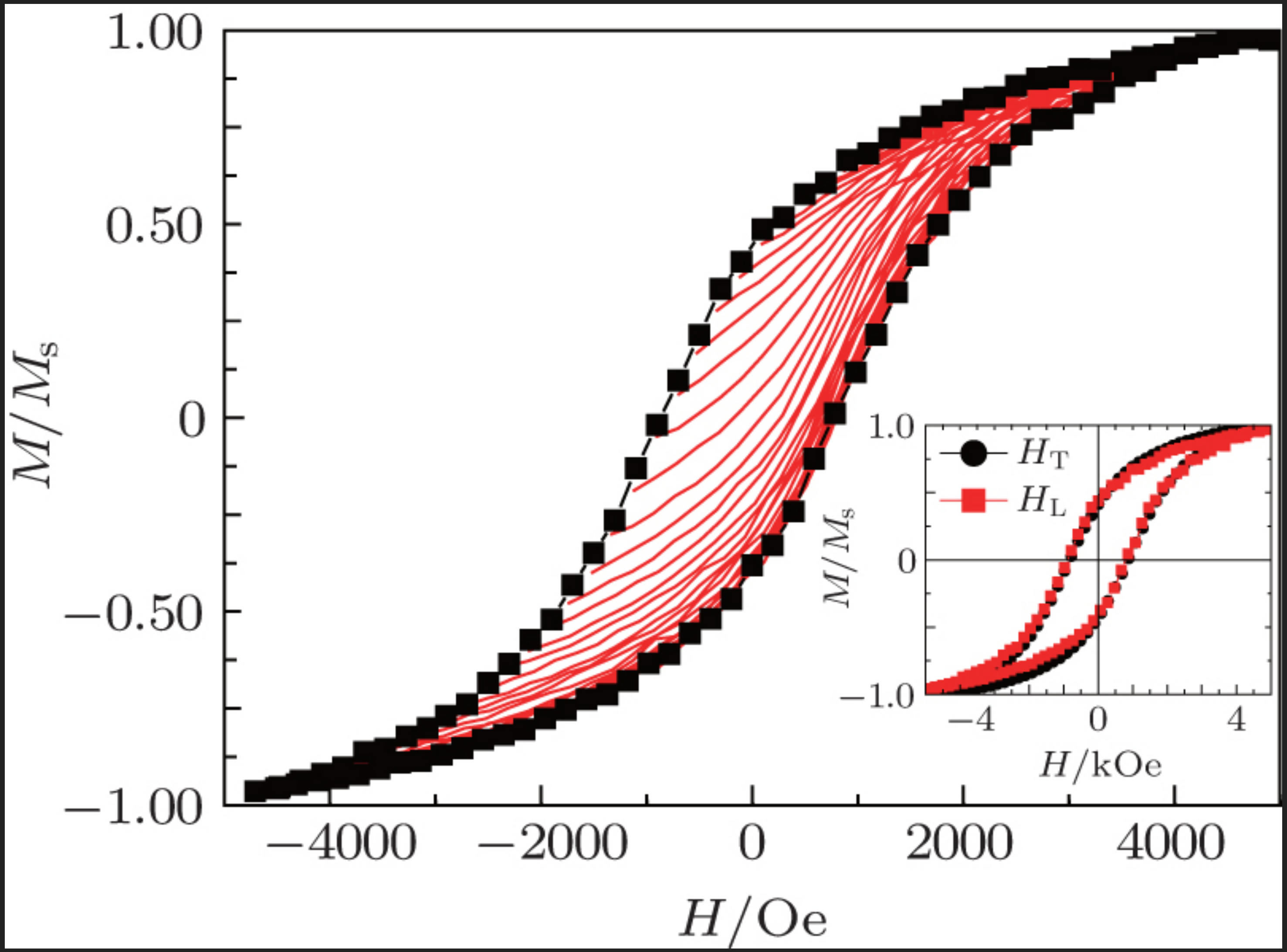
3D MODEL

WHIT THIS NEW MODEL WE DISCOVER THAT:

NANO LIMIT


Temperatura=7.0, J =7, Lattice size =1000000
Magnetization
Temperature
radius=2.0
radius=7.33
radius=12.67
radius=18.0
radius=23.33
radius=28.67
radius=34.0
radius=39.33
radius=44.67
radius=50.0
1.0
0.8
0.6
0.4
0.2
0.0
0
5
10
15
20
25
30

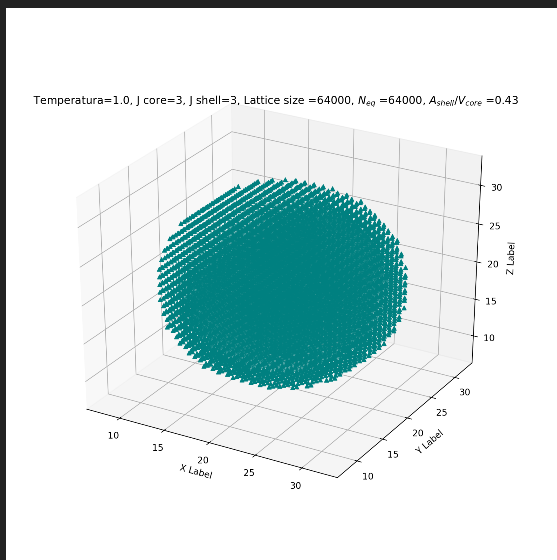

z
y
x
1.0
0.5
0.0
-0.5
-1.0



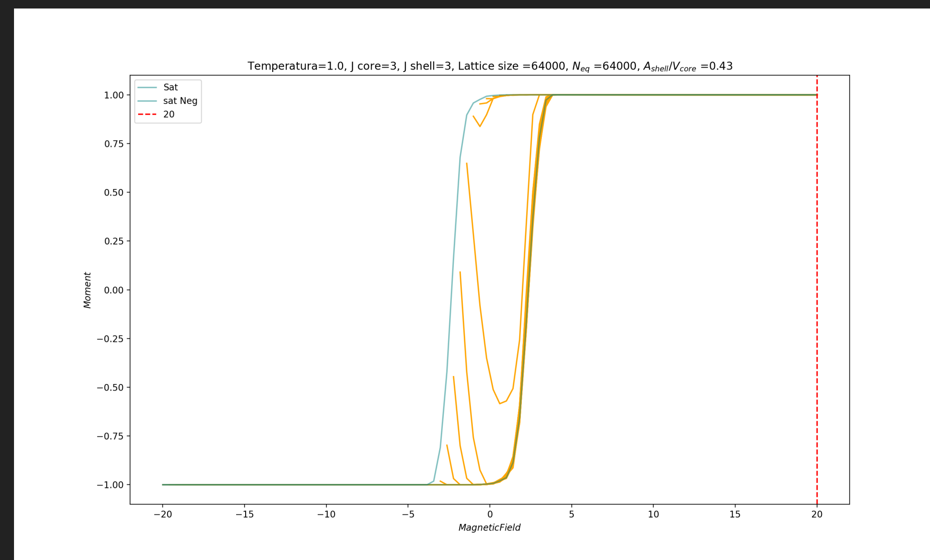
FORC

CITE: Fabrication of CoFe2O4 ferrite nanowire arrays in porous silicon template and their local magnetic properties

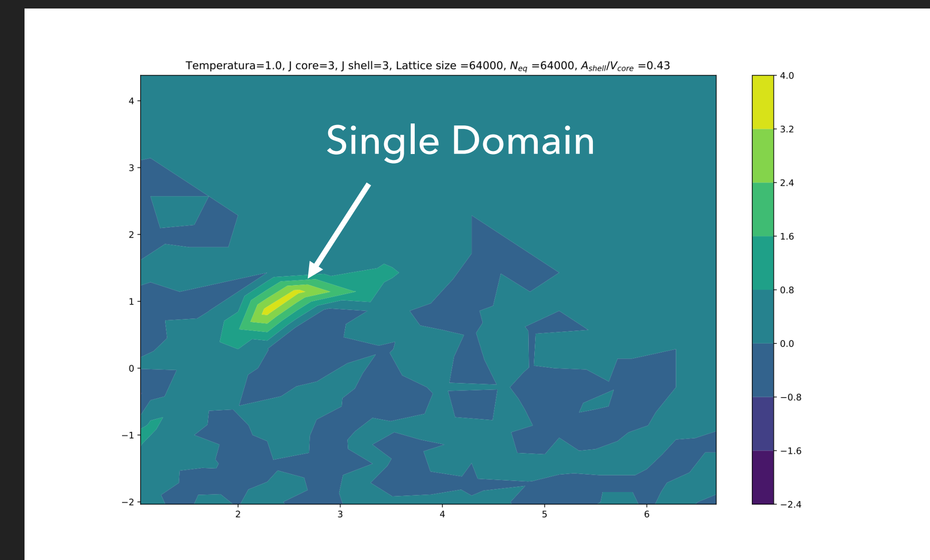
DOMAINS



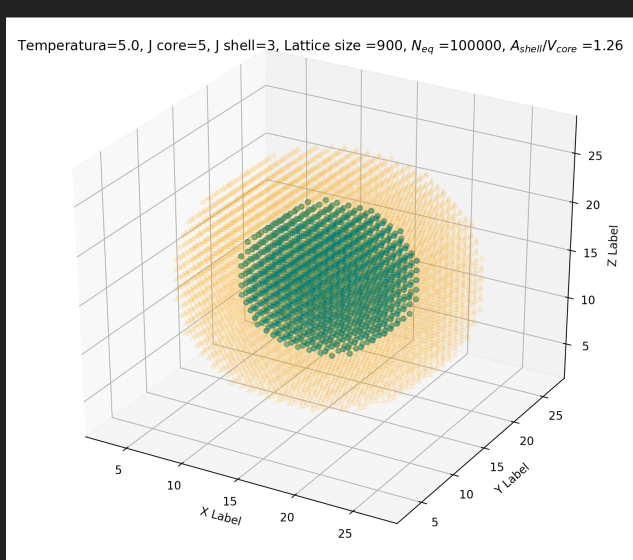
Temperatura=1.0, J core=3, J shell=3, Lattice size =64000, N_{eq} =64000, A_{shell}/V_{core} =0.43
X Label
Y Label
Z Label



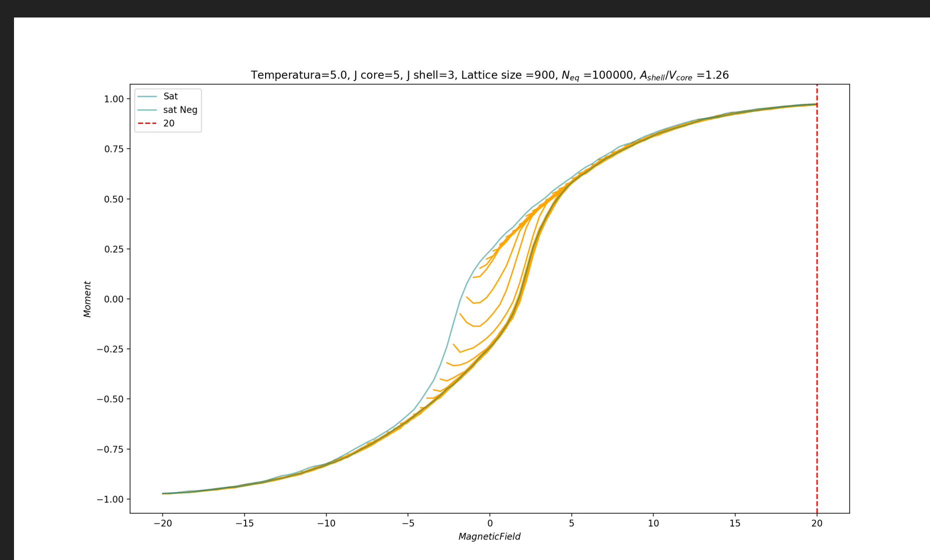
Temperatura=1.0, J core=3, J shell=3, Lattice size =64000, N_{eq} =64000, A_{shell}/V_{core} =0.43
Sat
sat Neg
20
Moment
MagneticField



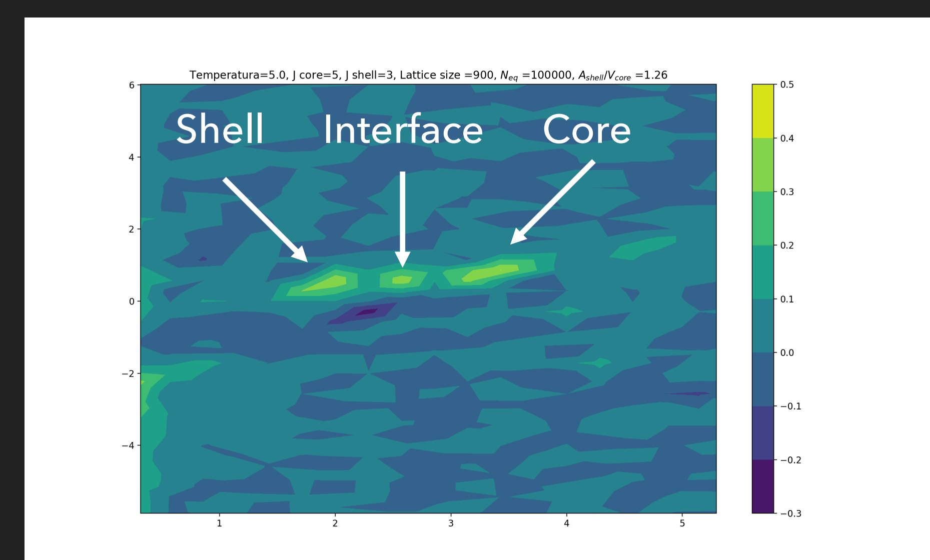
Temperatura=1.0, J core=3, J shell=3, Lattice size =64000, N_{eq} =64000, A_{shell}/V_{core} =0.43
Single Domain



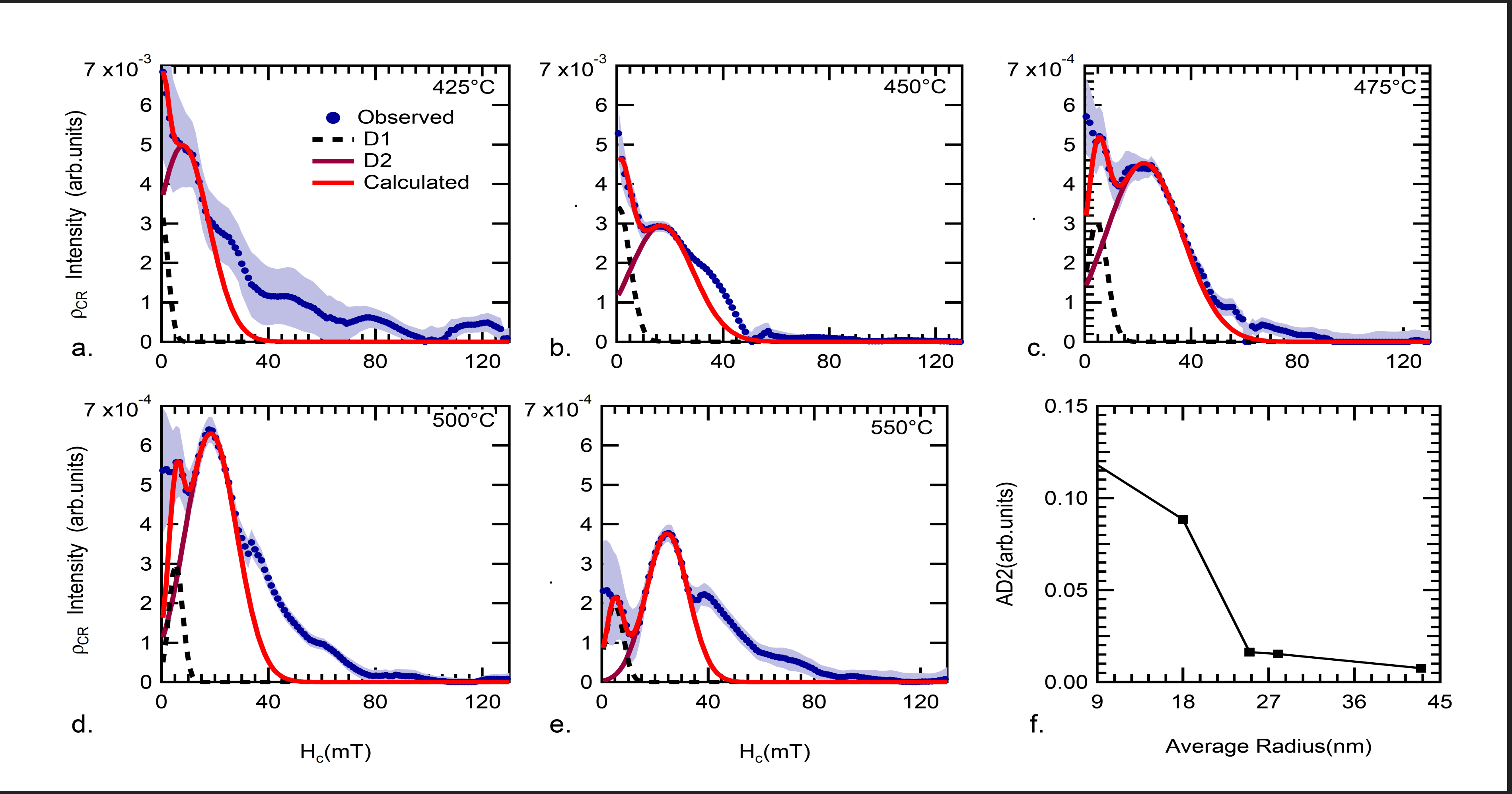
Temperatura=5.0, J core=5, J shell=3, Lattice size =900, N_{eq} =100000, A_{shell}/V_{core} =1.26
X Label
Y Label
Z Label



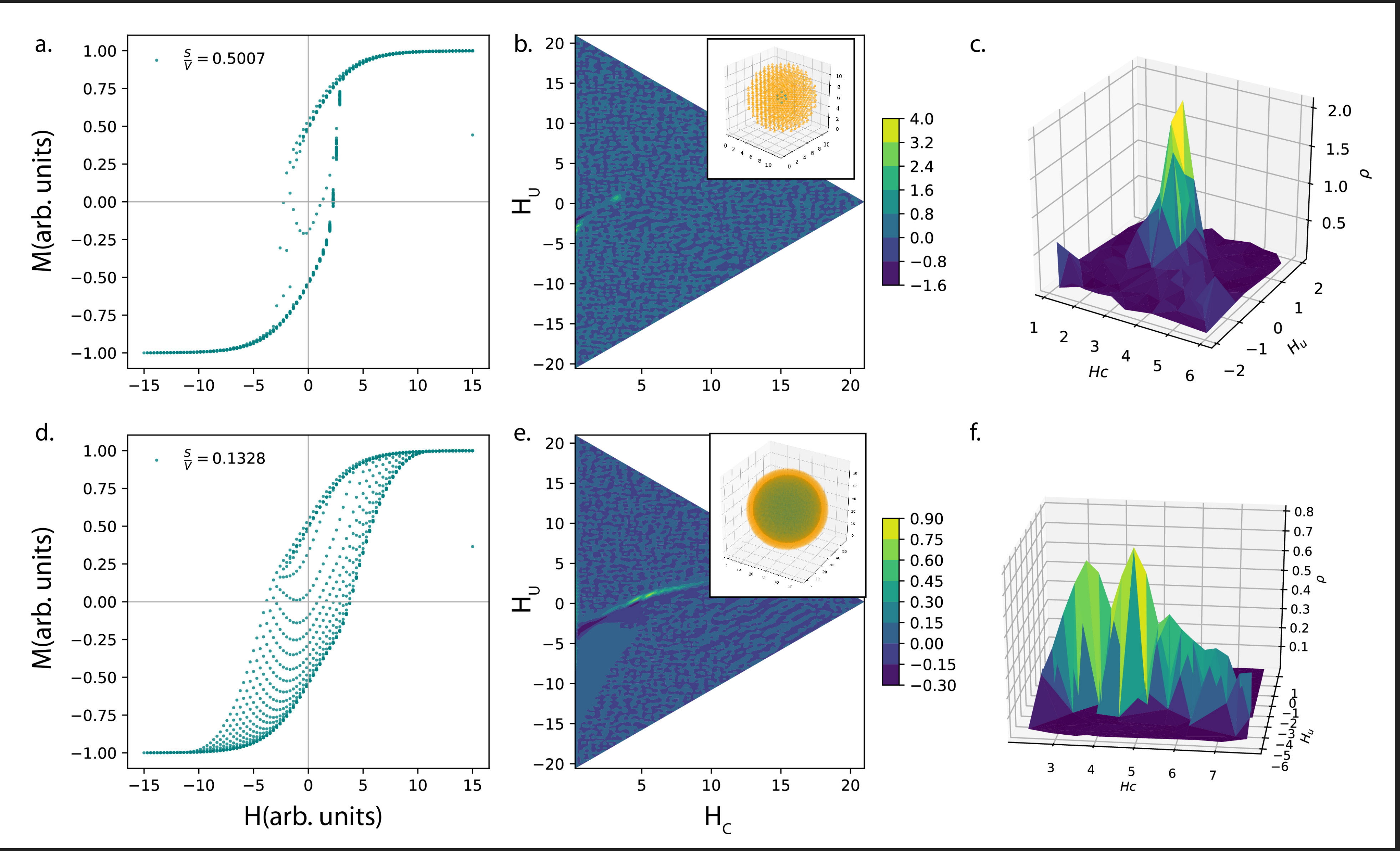
Temperatura=5.0, J core=5, J shell=3, Lattice size =900, N_{eq} =100000, A_{shell}/V_{core} =1.26
Sat
sat Neg
20
Moment
MagneticField



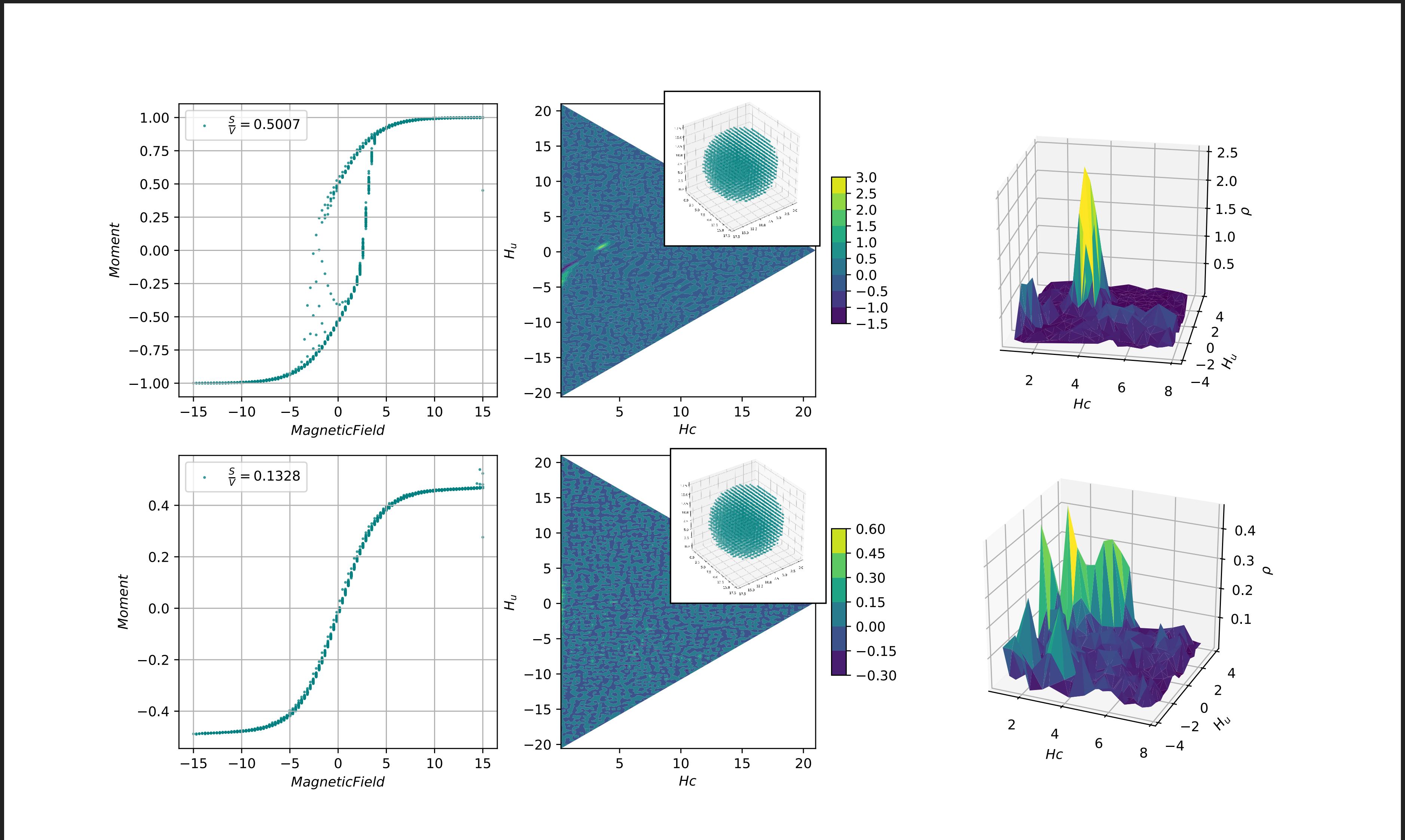
Temperatura=5.0, J core=5, J shell=3, Lattice size =900, N_{eq} =100000, A_{shell}/V_{core} =1.26
Shell
Interface
Core



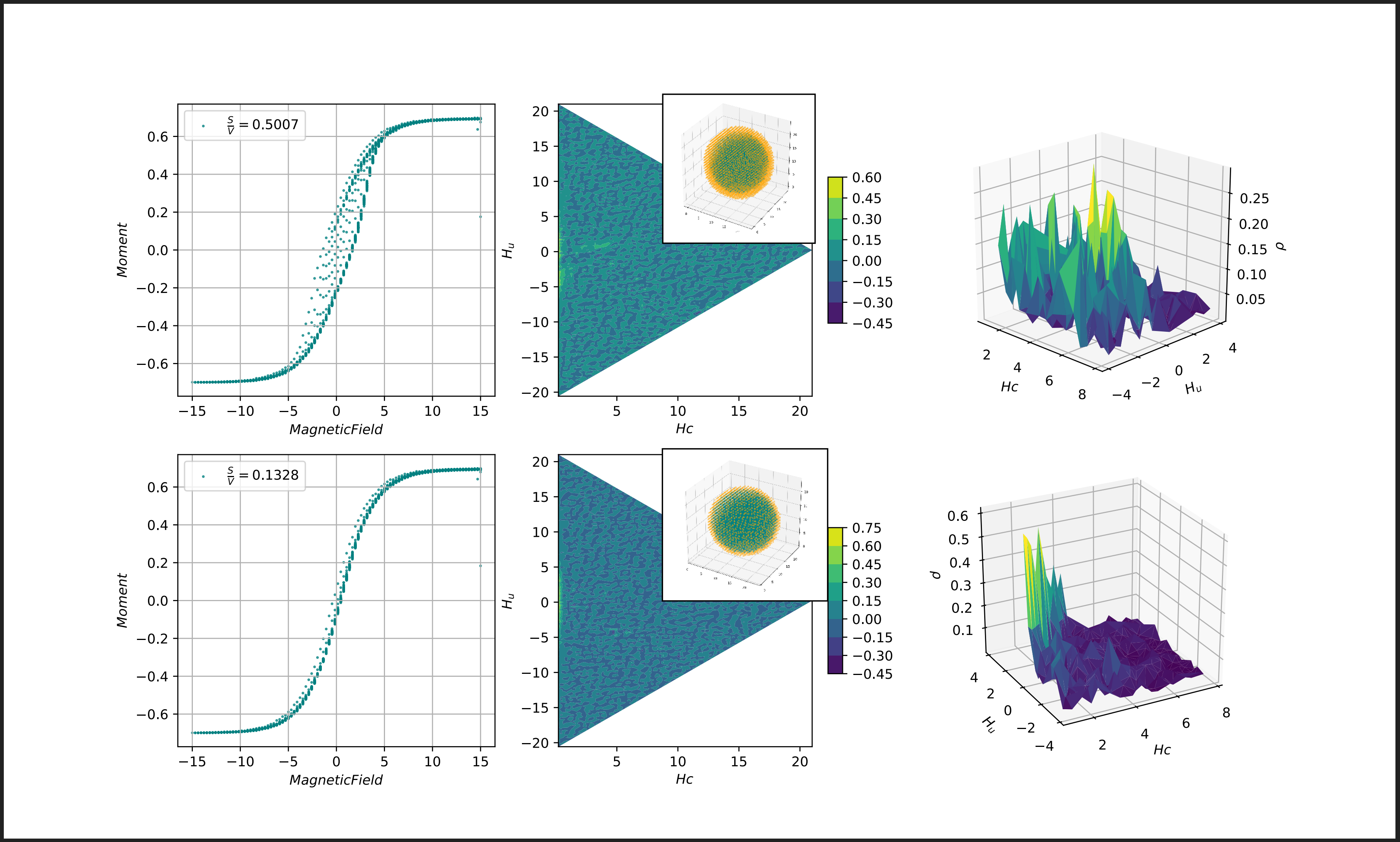
LAB DATA MEASURED BY ALEXANDER CARDONA



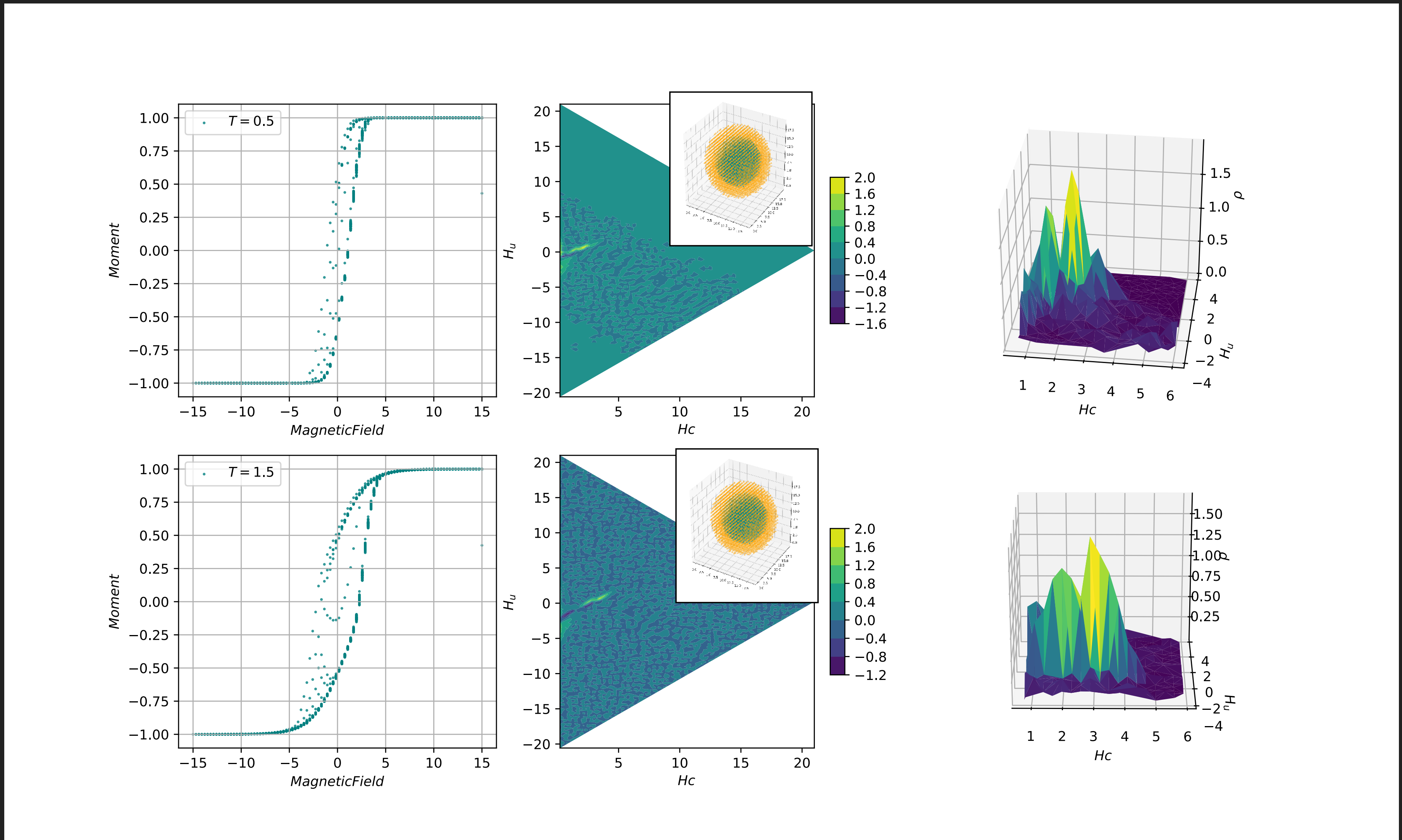
TAKE TWO CASES, DIFERRENT RELATIONS OF S/V



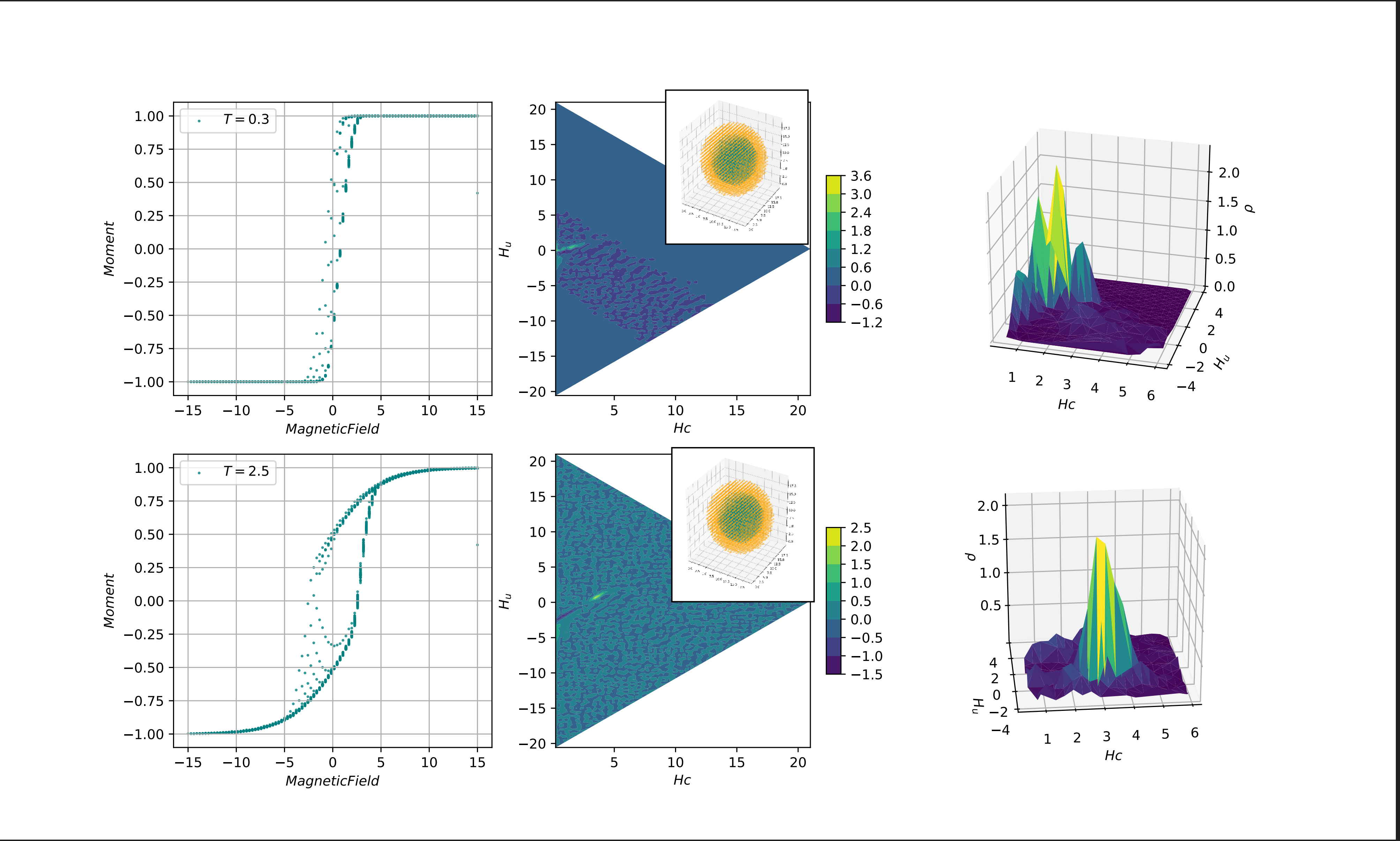
FERRO-ANTIFERRO SINGLE DOMAIN



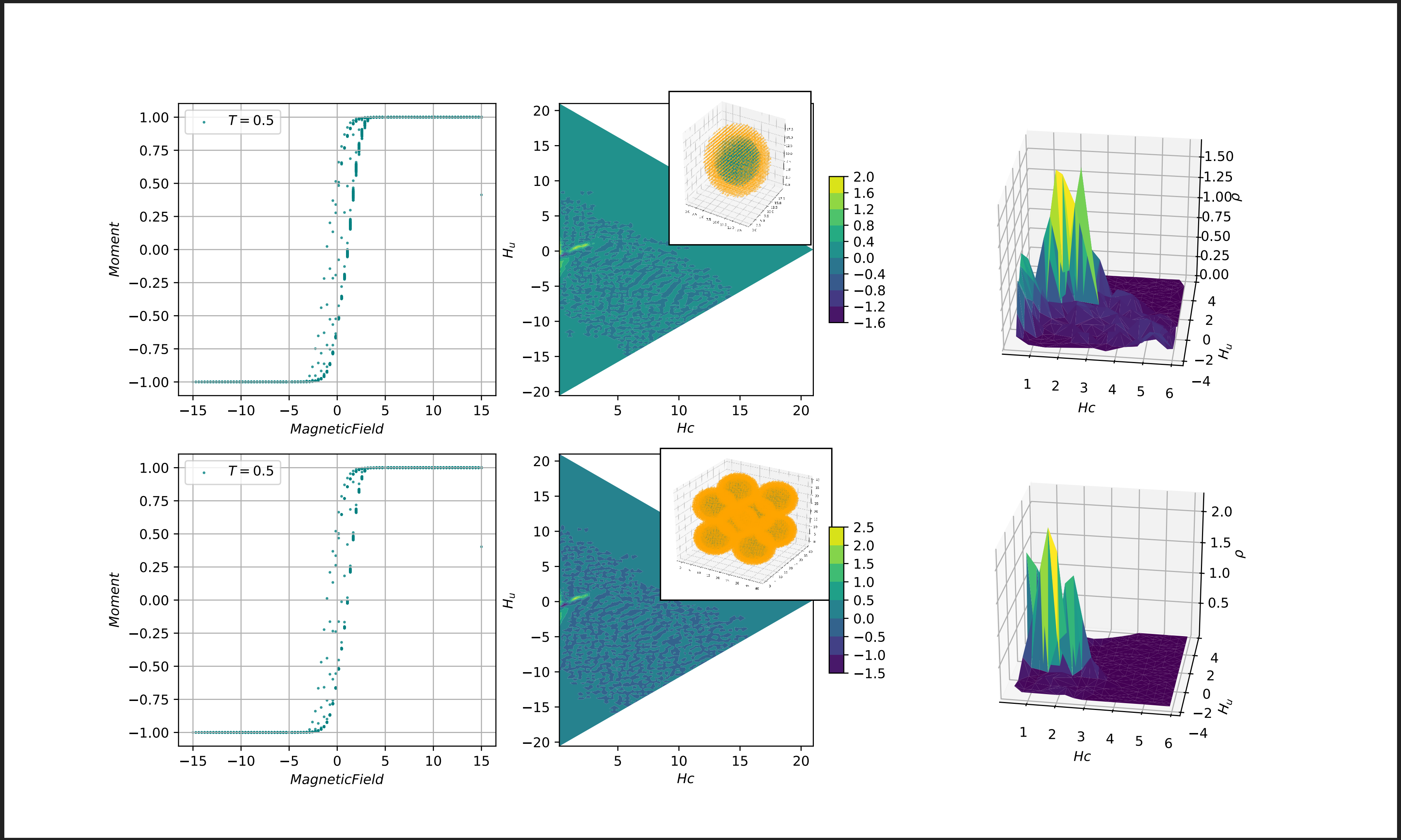
BIG CORE ANTIFERRO



POLES SEPARATION TEMPERATURE



POLES SEPARATION TEMPERATURE



INCREASING THE NUMBER OF PARTICLES

CONCLUSIONS

- Metropolis algorithm is an useful tool for optimization of non-convex problems, as it’s the minimization of the energy of a system in the canonical ensemble
- The Ising model makes an important contribution to the explanation of the physical phenomena that involves magnetic materials.
- FORC diagrams shows the core, shell and interface domains.
- There is a limit on the size of the particles, at which the magnetic properties depends on the size.
- Temperature is a key feature for being able to see domains.

MOST GENERAL METROPOLIS ALGORITHM [2]

1. **INITIALIZATION:** CHOOSE INITAL POINT x_0 AND AN ACCEPTANCE PROBABILITY DISTRIBUTION $g(x_i|x_{i-1})$.
2. **GENERATE:** A CANDIDATE FOR THE NEXT SAMPLE $g(x_i|x_{i-1}) \rightarrow x_i$
3. **CALCULATE:** THE ACCEPTANCE RATIO $\alpha = \frac{f(x_i)}{f(x_{i-1})}$
4. **ACCEPT OR REJECT:** GENERATE A RANDOM NUMBER $u \sim [0,1]$. IF $u \leq \alpha \Rightarrow x' = x_i$

   ELIF $u > \alpha \Rightarrow x' = x_{i-1}$
5. **REPEAT :** 2-3 UNTIL ACCOMPLISH CONDITION

GENERAL CANONICAL ENSEMBLE METROPOLIS ALGORITHM.

1. **INITIALIZATION:** CREATE THE SYSTEM IN A RANDOM MICRO-STATE

2. **GENERATE:** CHOOSE A RANDOM ELEMENT OF THE SYSTEM WITH AN UNIFORM DISTRIBUTION S

3. **CALCULATE:** CHANGE THE STATE OF THE ELEMENT S , COMPUTE THE ENERGY AND CALCULATE $p_x = \frac{1}{Z} e^{-\frac{E_S}{K_b T}}$

4. **ACCEPT OR REJECT:** IF S REDUCE THE ENERGY ACCEPT THE NEW MICRO STATE. ELSE IF $u \sim [0,1]$, $u \leq p_x \Rightarrow ACCEPT$. ELSE REJECT.

5. **REPEAT 2-3 UNTIL ENERGY CONVERGES.**

ACKNOWLEDGEMENTS

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- To Juan Gabriel Ramirez, for taking time to help me be prepare for this talk and being exigent in order to be a better physicist
- To the nano-magnetism lab for the disposal of all the resources needed for the develop of this work

REFERENCES

- 1. N. Metropolis; A.W. Rosenbluth; M.N. Rosenbluth; A.H. Teller & E. Teller (1953). "Equation of State Calculations by Fast Computing Machines". Journal of Chemical Physics. 21 (6): 1087–1092. Bibcode:1953JChPh..21.1087M.
- 2. W. K. Hastings, Monte Carlo sampling methods using Markov chains and their applications, Biometrika, Volume 57, Issue 1, April 1970, Pages 97–109, https://doi.org/10.1093/biomet/57.1.97
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- 4.Heslop, D., Dekkers, M. J., Kruiver, P. P., & Van Oorschot, I. H. M. (2002). Analysis of isothermal remanent magnetization acquisition curves using the expectation-maximization algorithm. *Geophysical Journal International*, *148*(1), 58-64.
- 5.Soares, J. M., Cabral, F. A. O., de Araújo, J. H., & Machado, F. L. A. (2011). Exchange-spring behavior in nanopowders of CoFe 2 O 4–CoFe 2. *Applied Physics Letters*, *98*(7), 072502.