Markov Chain Monte Carlo Simulations for the 2D Ising Model

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Final Presentation for PHYS 382: Advanced Physics Laboratory

OVERVIEW

- Model phase transitions and observe critical phenomena in the 2D Ising Model using Markov-chain Monte Carlo simulations.
- Measure thermodynamic quantities, such as magnetization, magnetic susceptibility, specific heat and correlation length
- Obtain values for critical exponents as well as the critical temperature T_C , and verify with known theoretical values

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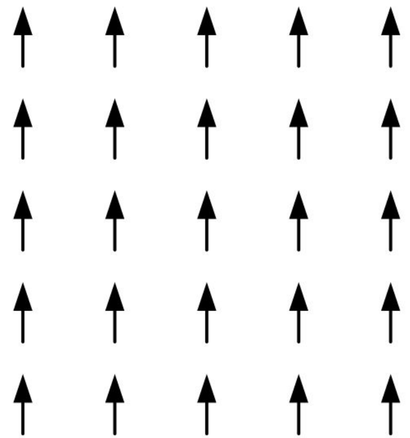
BACKGROUND

ISING MODEL

- **mathematical model** that describes an array of magnetic dipole moments with 2 possible spin states
- One of the simplest models to exhibit a **phase transition** at a critical temperature
- Above critical temperature, **thermal fluctuations** disrupt aligned spins and cause them to randomly flip



Ground state of 5x5 Ising Model

STATISTICAL MECHANICS

Gibbs Distribution

- probability of finding a macroscopic system in a microscopic state of energy E is given by:

$$P(\text{state}) \propto e^{-\frac{E}{k_B T}}$$

- Useful thermodynamic quantities (specific heat and susceptibility) can be derived using the **partition function**:

$$\mathcal{Z} = \sum_i e^{-\beta E_i}$$

$$c_V = \frac{\beta}{T}\left[\langle E^2\rangle_T - \langle E\rangle_T^2\right]$$

$$\chi = \beta\left[\langle M^2\rangle_T - \langle M\rangle_T^2\right]$$

CRITICAL EXPONENTS & IDENTITIES

Critical Exponent	Definition	Theoretical Value
α	$C_v \propto \lvert t\rvert^{-\alpha}$	0
β	$\lvert M\rvert \propto \lvert t\rvert^{\beta}$	1/8
γ	$\chi \propto \lvert t\rvert^{-\gamma}$	7/4
δ	$\lvert M\rvert \propto \lvert B\rvert^{\delta}$	15
ν	$\xi \propto \lvert t\rvert^{-\nu}$	1
η	$\langle\sigma(0)\sigma(x)\rangle \propto \lvert x\rvert^{d-2+\eta}$	1/4

Rushbrooke's Identity: $\alpha + 2\beta + \gamma = 2$

Widom's Identity: $\delta - 1 = \gamma/\beta$

Josephson's Identity: $2 - \alpha = d\nu$

Fisher's Identity: $\gamma = (2-\eta)\nu$

Theoretical critical exps and identities in the **infinite lattice-size limit**

6 critical exps, 4 identities
$\rightarrow$ **2 independent variables**

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METHOD

METHOD: MONTE CARLO SIMULATIONS

- **Markov Chain Monte Carlo simulation**, lattice-size N x N
- 0.01 intervals from **T=0** to **T=4.6**
- Initializes with a **random spin configuration** at each temperature step
- Evolves by **invoking spin transitions at calculated probability**, and determines the corresponding energy and magnetization of the system
- Designate set number of **burn-in steps** to allow system to converge (reach the **global minimum of the Gibbs Distribution**)

METHOD: ANNEALING AND CONVERGENCE

- To help with **convergence**, we implement code to **anneal** both the **magnetic field** and **temperature**.
- **“Cool down"** these quantities in order to avoid test points from **getting stuck in local minimum of the Gibbs distribution**, and help them reach the global minimum where the **value converges correctly**.

METHOD: OBTAINING ERROR VALUES

- Obtain error values for C_V and susceptibility (χ) by **binning** our data collection steps **at each temperature** to obtain C_V and χ values, then calculating the **sample standard deviation S** of those values.
- 50,000 data collection steps , bin size of 100 steps $\longrightarrow$ **500 bins**
- Final standard deviation obtained by implementing following correction:

$$\sigma_{\text{population}} = \sigma_{\text{sample}} \frac{\sqrt{N_{\text{sample}} - 1}}{\sqrt{N_{\text{population}}}} = \sigma_{\text{sample}} \frac{\sqrt{499}}{\sqrt{50000}}$$

$$\Rightarrow \boldsymbol{\sigma_{\text{population}} \approx 0.1 \times \sigma_{\text{sample}}}$$

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ANALYSIS

ANALYSIS: PRIMER

Nonlinear Weighted Fits

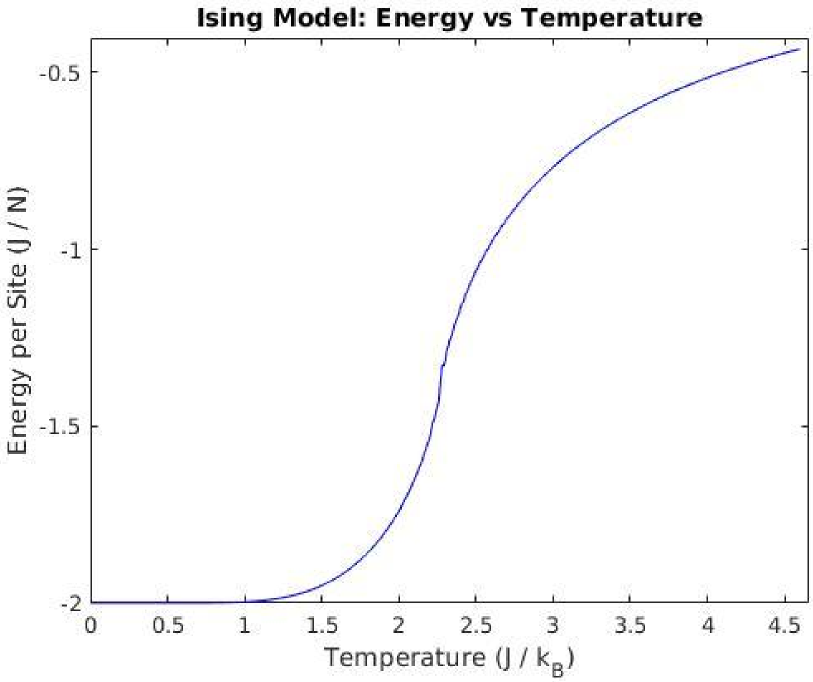
- MATLAB's Weighted Nonlinear Regression Model Fitter
- Hougen-Watson Algorithm
- Weights assigned using instrumental weighting

Chi-Squared Analysis

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{x_i - x_{curve}}{\sigma_i} \right)^2$$

Good Fit: $\chi^2 \cong 1$

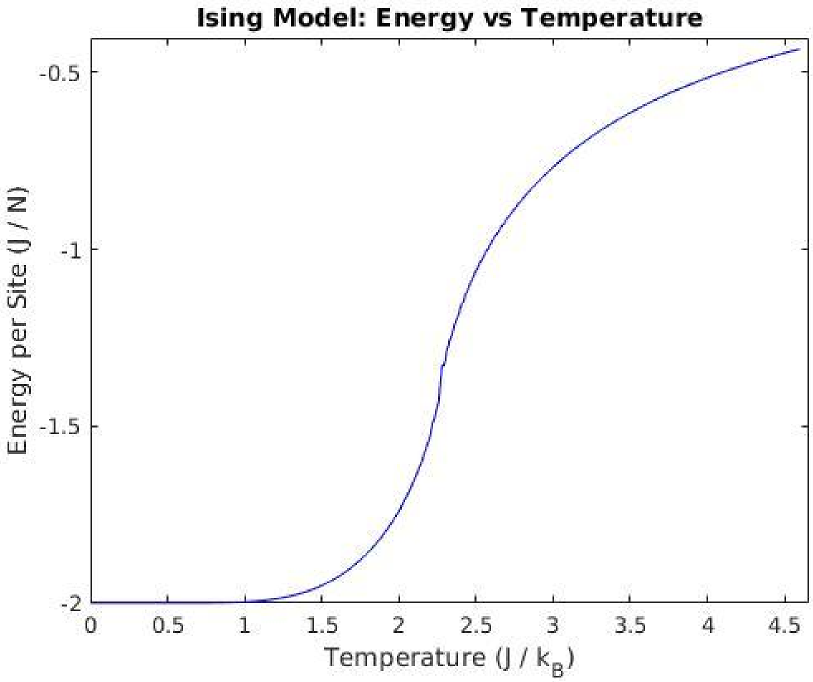
ANALYSIS: ENERGY

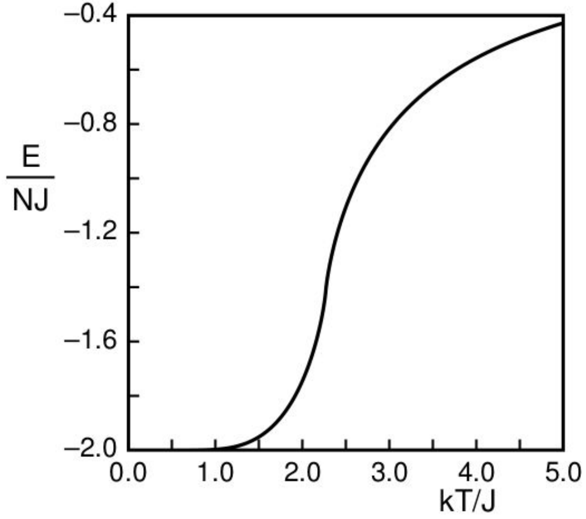


Energy vs. Temperature curve for N=100 lattice, no ext. B field.

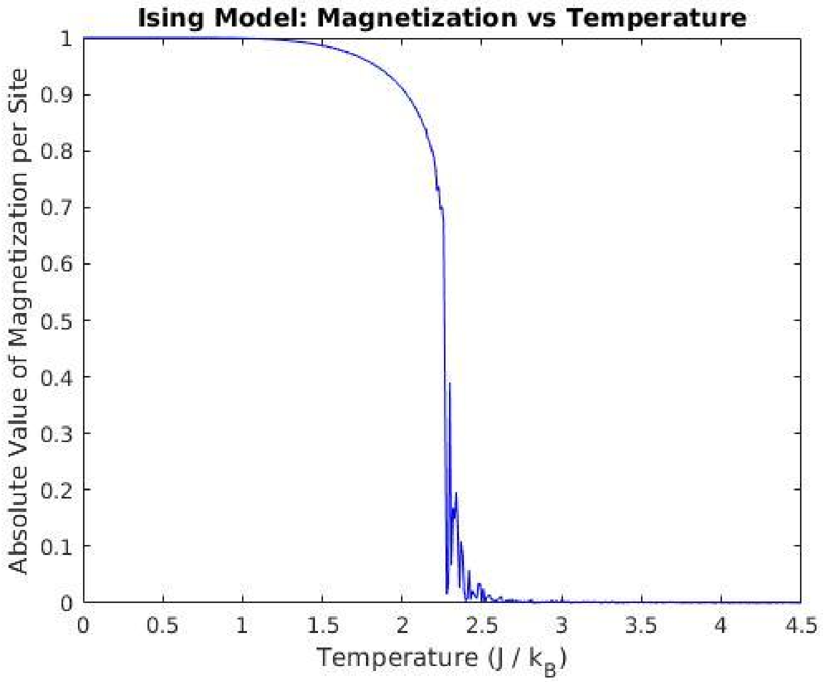
Complex elliptical function

ANALYSIS: ENERGY





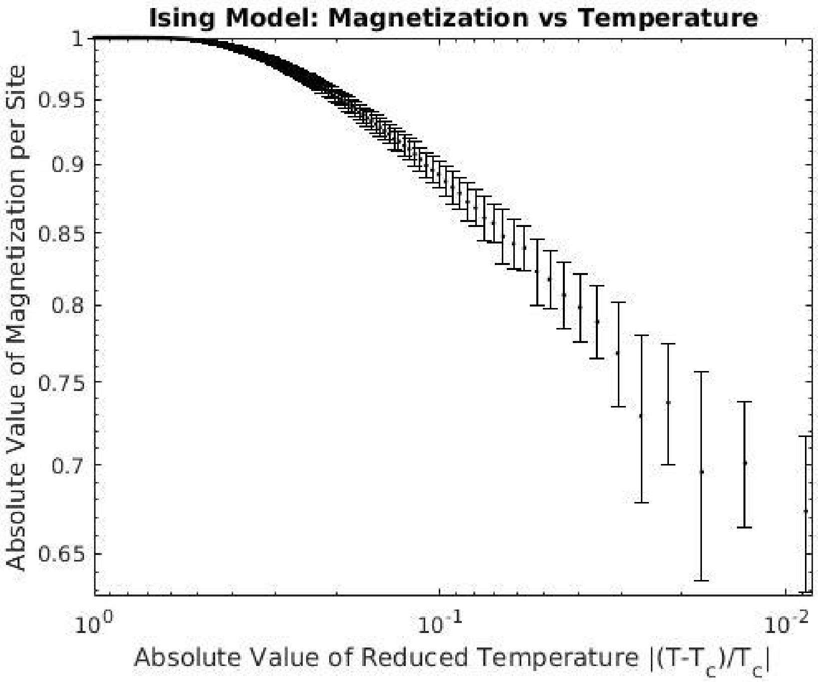
ANALYSIS: MAGNETIZATION



Magnetization vs. Temperature curve for N=100 lattice, no ext. B field.

Drops sharply at critical temperature

ANALYSIS: MAGNETIZATION

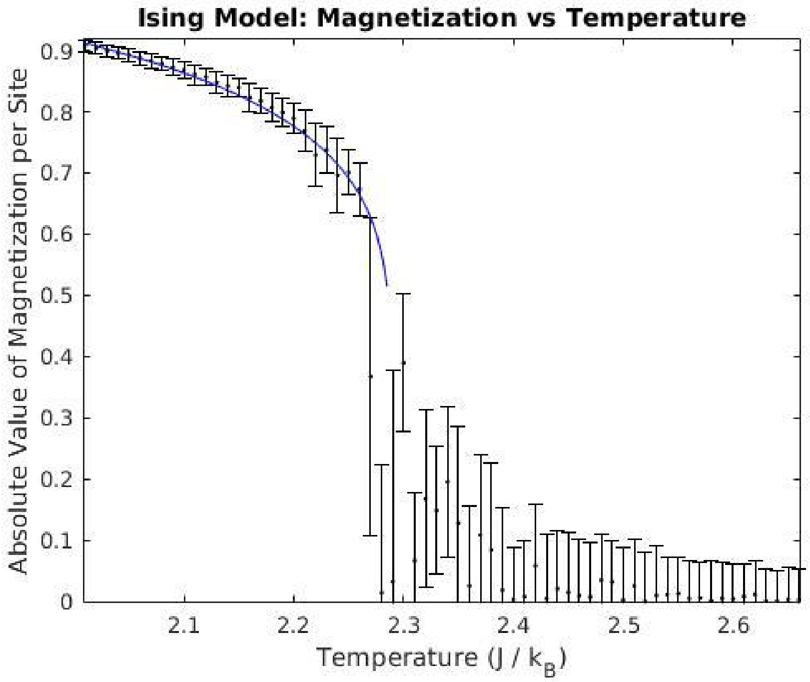


Power law verification via log-log plot

$$|M| \propto |t|^{\beta} \text{ where } t = \frac{T - T_c}{T_c}$$

Fit function used: $|M| = A\left|\frac{T - T_c}{T_c}\right|^{\beta}$

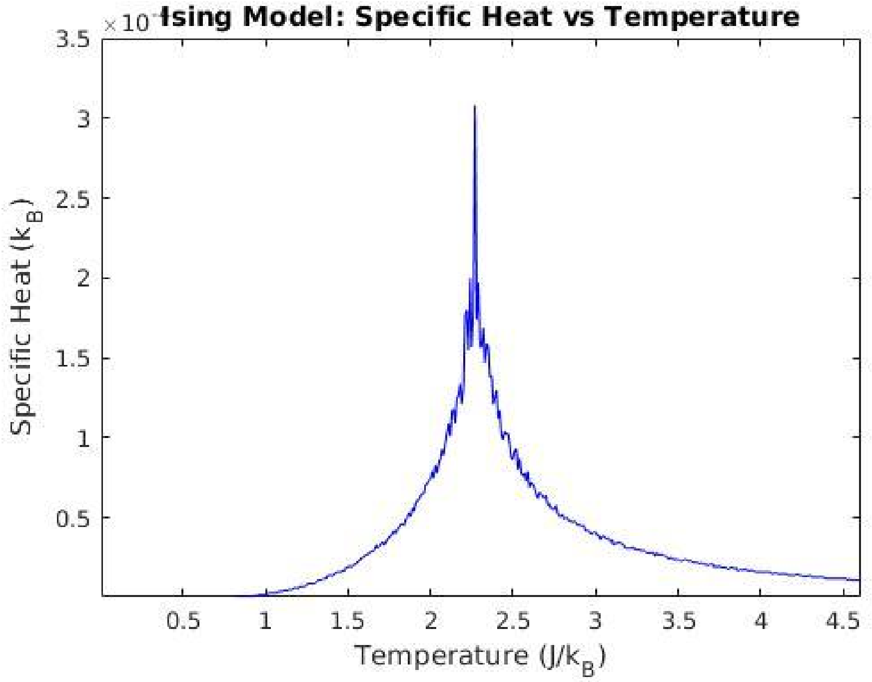
ANALYSIS: MAGNETIZATION



Fit function used: $|M| = A\left|\frac{T - T_c}{T_c}\right|^{\beta}$

Parameter	Value
A	1.230 ± 0.036
T_c	2.29 ± 0.002
β	0.127 ± 0.005
Chi^2/DoF	0.4001

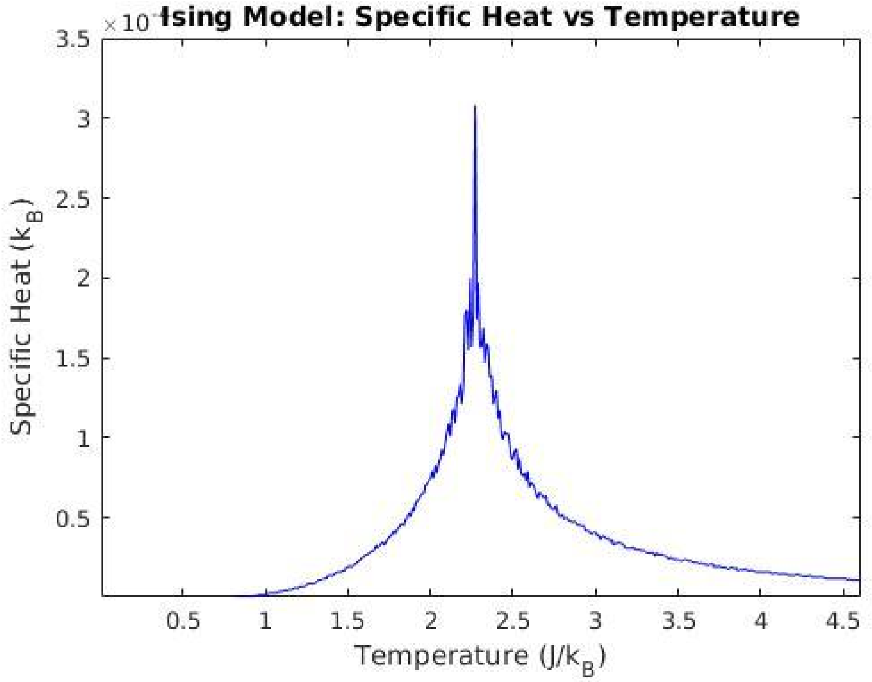
ANALYSIS: SPECIFIC HEAT



Specific Heat vs. Temperature curve for N=100 lattice, no ext. B field.

Sharply diverges at critical temperature

ANALYSIS: SPECIFIC HEAT

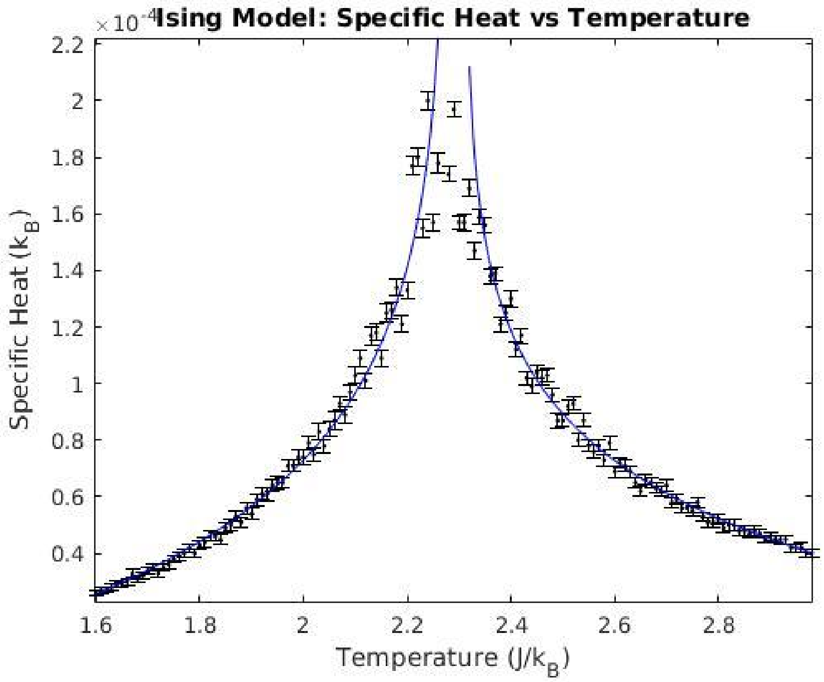


Logarithmic divergence verification via log-linear plot

$$\mathrm{C_V} \propto |t|^{-\alpha} \Rightarrow \boldsymbol{\alpha = 0}$$

Fit function used: $A \ln\left|\frac{T - T_c}{T_c}\right| + C_{\mathrm{V},0}$

ANALYSIS: SPECIFIC HEAT

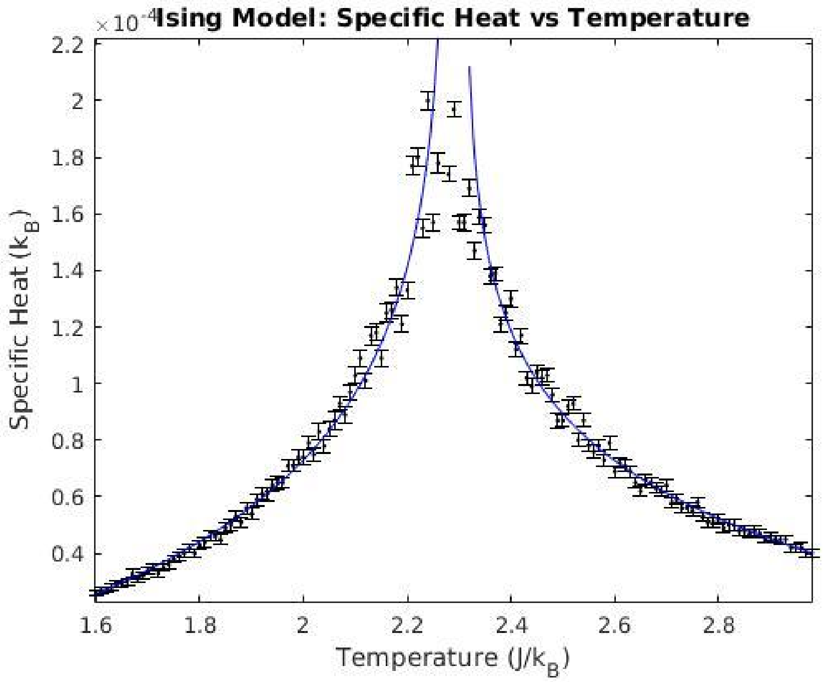


Fit function used: $A \ln\left|\frac{T - T_c}{T_c}\right| + C_{\mathrm{V},0}$

Parameter	Value
A	(-5.28 ± 0.14) E -5
T_{c1}	2.276 ± 0.008
$C_{\mathrm{V},0}$	(-3.85 ± 0.13) E -5
$\mathrm{Chi}^2/\mathrm{DoF}$	1.363

C_V Weighted Fit Parameters **below** T_c

ANALYSIS: SPECIFIC HEAT

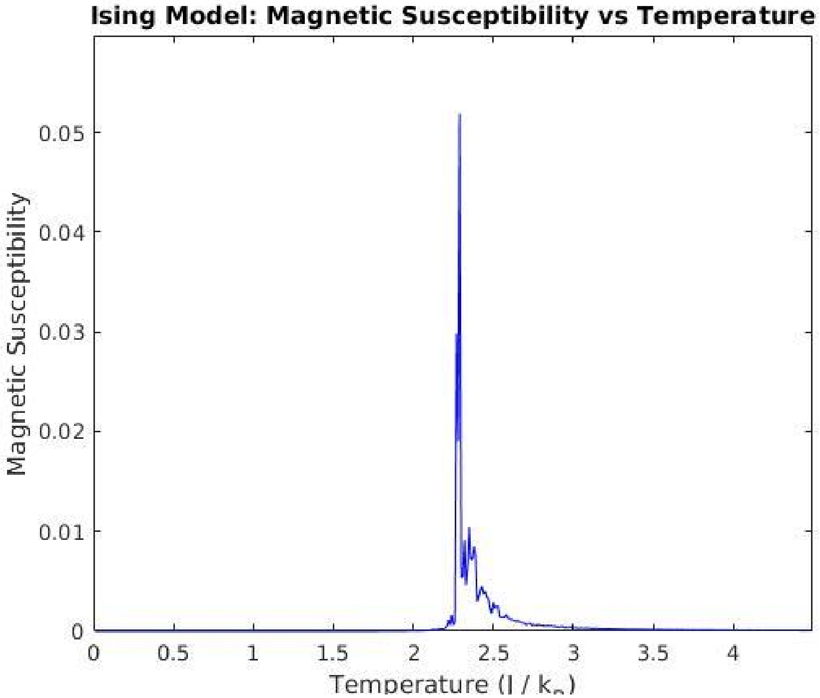


Fit function used: $A \ln\left|\frac{T - T_c}{T_c}\right| + C_{V,0}$

Parameter	Value
A	(-3.9 ± 0.1) E -5
T_{c2}	2.312± 0.004
$C_{V,0}$	(-7.8 ± 0.13) E -6
Chi^2/DoF	1.416

C_V Weighted Fit Parameters **above** T_c

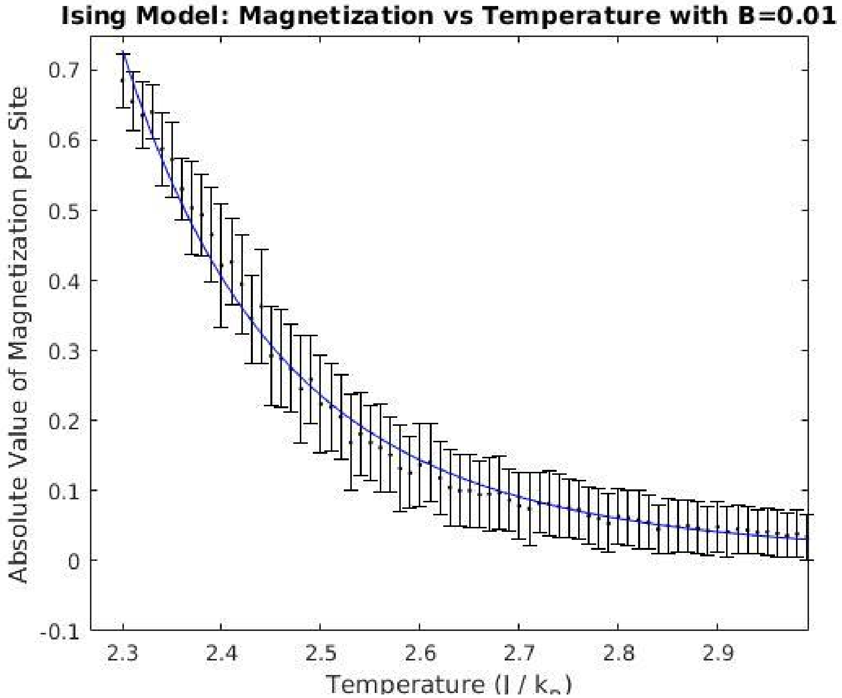
ANALYSIS: SUSCEPTIBILITY



Susceptibility vs. Temperature curve for N=100 lattice, no ext. B field.

Sharply diverges at critical temperature

ANALYSIS: SUSCEPTIBILITY



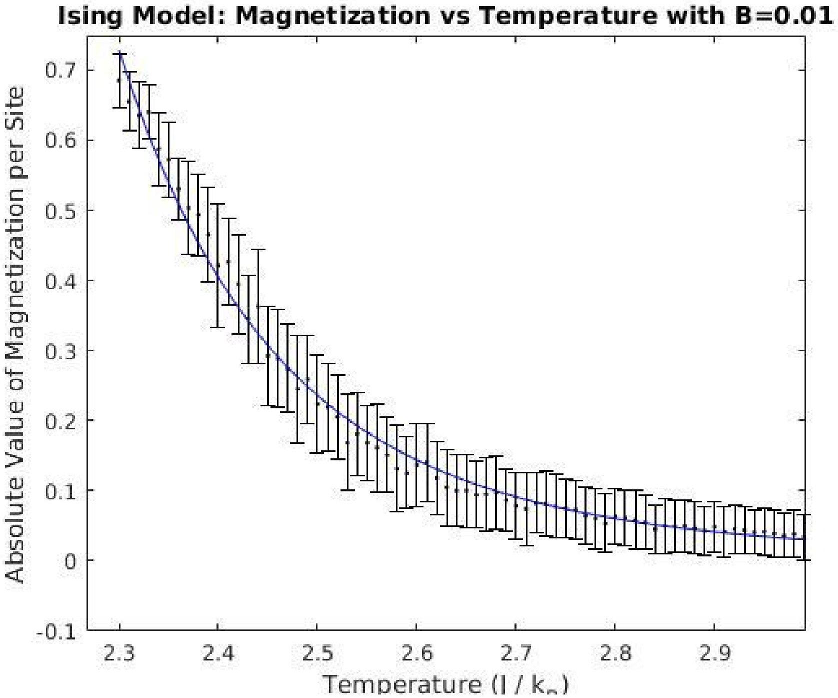
Difficult to fit due to large errors

Handout Technique to extract γ:

Apply small magnetic field to system

$$\chi = \frac{\partial M}{\partial \mathrm{B}} \Rightarrow M \approx \chi \mathrm{B} \propto |t|^{-\gamma}\mathrm{B} \propto |t|^{-\gamma}$$

ANALYSIS: SUSCEPTIBILITY

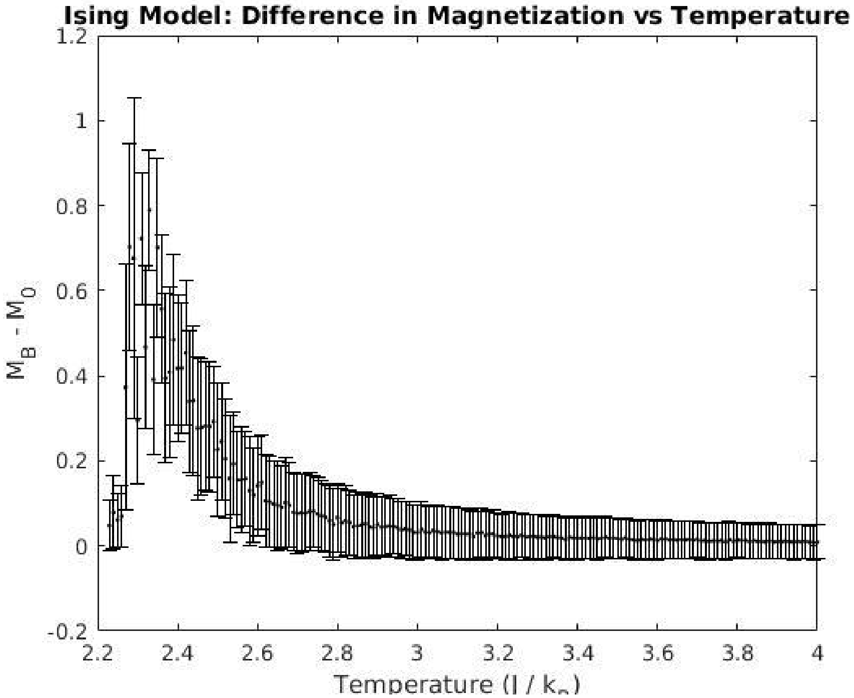


Fit function used: $M = A\left|\frac{T - T_c}{T_c}\right|^{-\gamma}$

Parameter	Value
A	12.6 ± 28.4
T_c	0.95 ± 1.39
γ	8.05 ± 7.67
$\mathrm{Chi}^2/\mathrm{DoF}$	0.177

Huge uncertainties - need better method

ANALYSIS: SUSCEPTIBILITY (NEW METHOD)



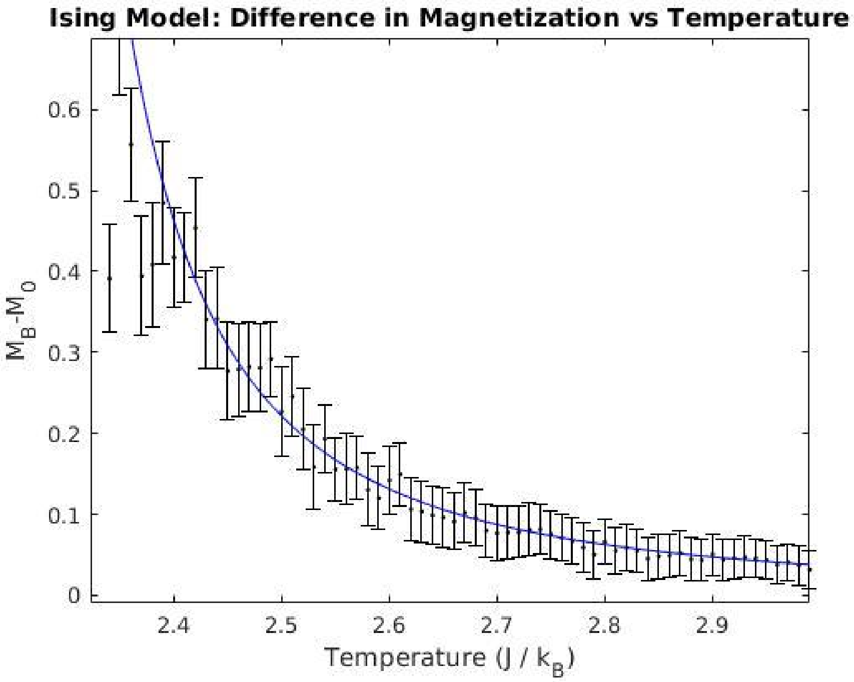
New method to extract γ:

Compare magnetic and nonmagnetic systems

$$\chi = \frac{\partial M}{\partial \mathrm{B}} \approx \frac{\Delta M}{\Delta \mathrm{B}} = \frac{M_1 - M_0}{B_1 - B_0}$$

$$\chi \propto \Delta M \Rightarrow \Delta M \propto |t|^{-\gamma}$$

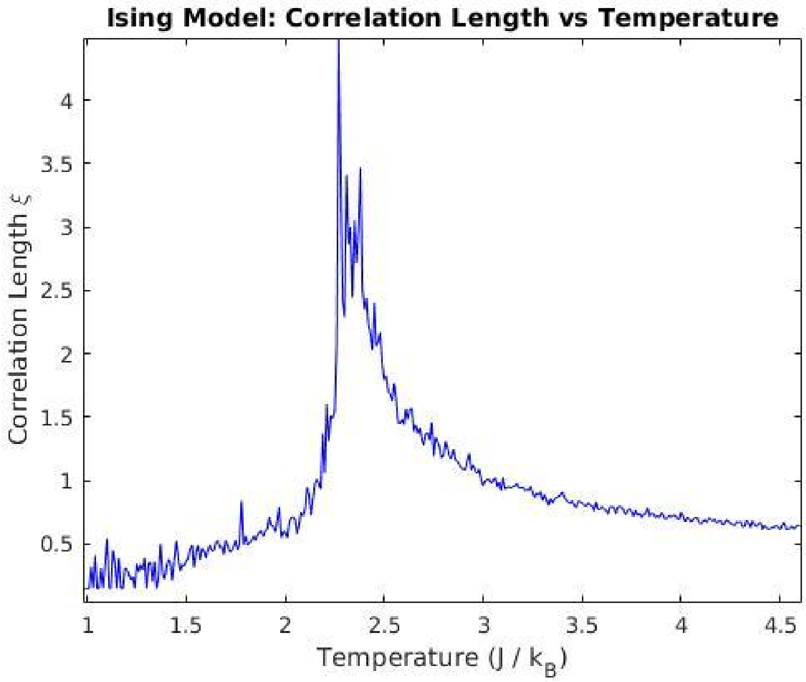
ANALYSIS: SUSCEPTIBILITY (NEW METHOD)



Fit function used: $\Delta M = A\left|\frac{T - T_c}{T_c}\right|^{-\gamma}$

Parameter	Value
A	(6.07 ± 0.21) E -3
T_c	2.21 ± 0.13
γ	1.78 ± 0.06
$\mathrm{Chi}^2/\mathrm{DoF}$	0.1735

ANALYSIS: CORRELATION LENGTH



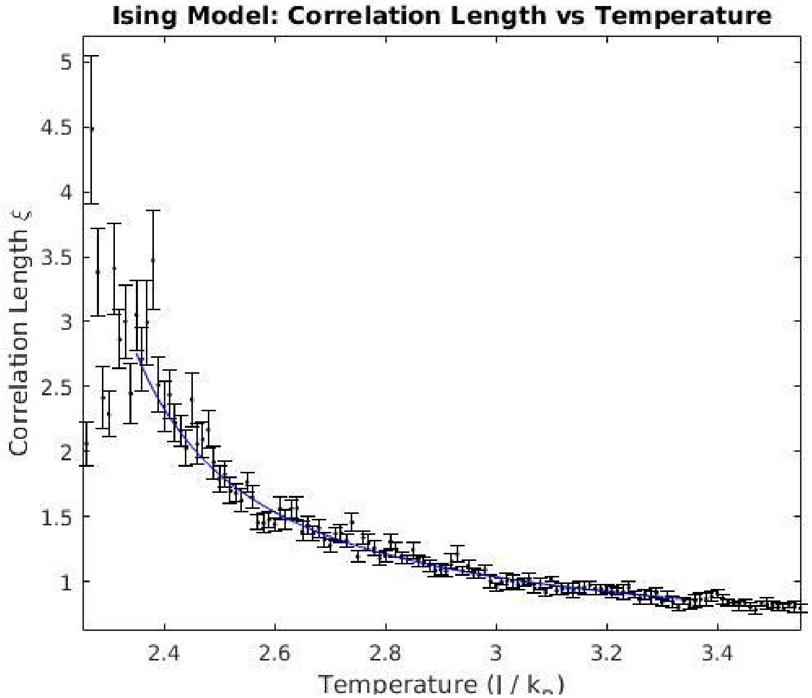
For a given spin state, spin correlation decreases as distance increases

Characterized by correlation length, ξ:

$$\langle \sigma(0)\sigma(x) \rangle \propto e^{-x/\xi}$$

$$\text{where } \xi \propto |t|^{-\nu}$$

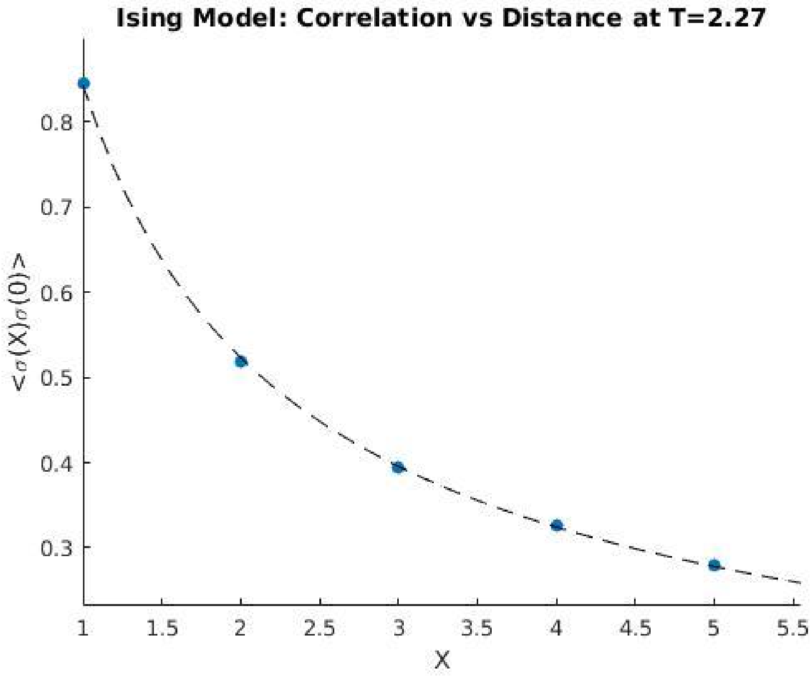
ANALYSIS: CORRELATION LENGTH



Fit function used: $\xi = A\left|\frac{T - T_c}{T_c}\right|^{-\nu} + \xi_0$

Parameter	Value
A	0.27 ± 0.156
T_c	2.14 ± 0.10
ν	0.94 ± 0.42
ξ_0	0.41 ± 0.22
$\mathrm{Chi}^2/\mathrm{DoF}$	1.0652

ANALYSIS: CORRELATION LENGTH



Relation used to obtain η:

$$\langle \sigma(0)\sigma(x)\rangle \propto \frac{1}{|x|^{d-2+\eta}}$$

Fit Function Used: $\langle \sigma(0)\sigma(x)\rangle = A|x|^{-\eta}$

Parameter	Value
A	0.884 ± 0.003
η	0.690 ± 0.005

ANALYSIS: CRITICAL TEMPERATURE

Parameter	Experimentally Obtained T_c
Magnetization (M)	2.29 ± 0.02
Specific Heat ($C_{v,\text{left}}$)	2.28 ± 0.08
Specific Heat ($C_{v,\text{right}}$)	2.31 ± 0.04
Susceptibility (χ)	2.21 ± 0.13
Correlation Length (η)	2.14 ± 0.10

Exact Value: $T_c = \dfrac{2}{\ln(1+\sqrt{2})} \approx 2.269$

ANALYSIS: CRITICAL EXPONENTS

Crit. Exp.	Definition	Theoretical Value	Experimental Value
α	$\mathrm{C_v} \propto \lvert\mathrm{t}\rvert^{-\alpha}$	0	0
β	$\lvert\mathrm{M}\rvert \propto \lvert\mathrm{t}\rvert^{\beta}$	0.125	0.127 ± 0.005
γ	$\chi \propto \lvert\mathrm{t}\rvert^{-\gamma}$	1.75	1.78 ± 0.06
ν	$\xi \propto \lvert\mathrm{t}\rvert^{-\nu}$	1	0.94 ± 0.42
η	$\langle\sigma(0)\sigma(x)\rangle \propto \lvert x\rvert^{d-2+\eta}$	0.25	0.690 ± 0.005

ANALYSIS: IDENTITIES

$$\text{Rushbrooke's Identity: } \alpha + 2\beta + \gamma = 2$$
$$\text{Widom's Identity: } \delta - 1 = \gamma/\beta$$
$$\text{Josephson's Identity: } 2 - \alpha = d\nu$$
$$\text{Fisher's Identity: } \gamma = (2 - \eta)\nu$$

Identity	Left Hand Side	Right Hand Side
Rushbrooke's	1.892 ± 0.162	2
Widom's	14 *(theoretical)*	13.6 ± 2.0
Josephson's	2	1.88 ± 0.84
Fisher's	1.65 ± 0.15	1.23 ± 0.55

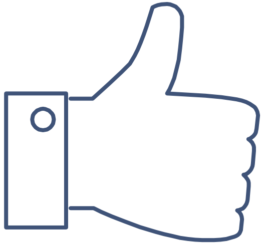
REFERENCES

Thompson, Jed. "Phys 381/282/504 Lab Handout: Two-Dimensional Ising Model." Yale University – Department of Physics. Spring 2017. Web.

"Standard Deviation." Standard Deviation | How and when to use the Sample and Population Standard Deviation - A measure of spread | Laerd Statistics. N.p., n.d. Web. 17 Apr. 2017.

Department of Physics. (n.d.). Lecture 6: Chi Square Distribution (c2) and Least Squares Fitting [PDF]. Ohio State University.

Weighted Nonlinear Regression Open Script. (n.d.). Retrieved April 17, 2017, from https://www.mathworks.com/help/stats/examples/weighted-nonlinear-regression.html



THANK YOU

Please feel free to ask any questions