New model of magnetism with a tricritical point

A study using mean field theory, Metropolis Monte Carlo, and Wang-Landau Sampling

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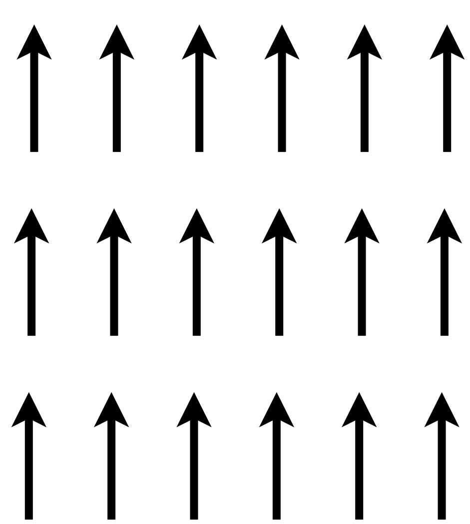
Outline

- Background
  - Magnetic phase transitions
  - My model: 1Dx1D geometry
  - Tricritical points
- Mean field theory results
- Metropolis Monte Carlo results
- Wang-Landau sampling results
- Future directions

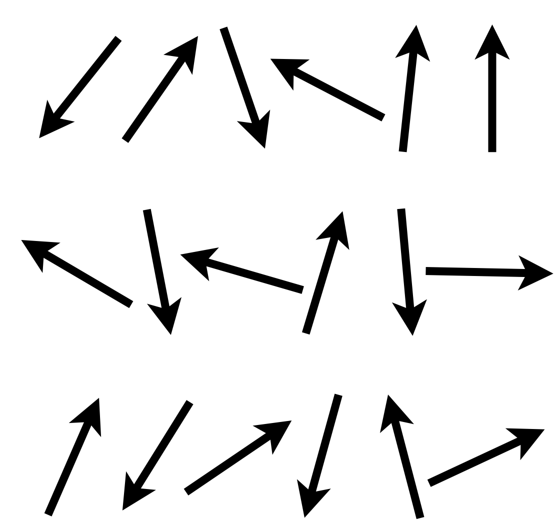
Phase Transitions:

- major goal of condensed matter physics: understanding phase transitions (PTs)
- important class of PTs: magnetic phase transitions
- some materials have a Curie temperature below which they are ferromagnetic (e.g. Iron has a $T_{Curie} = 1043$ K)
- magnetic moments of electrons align

$T < T_{Curie}$

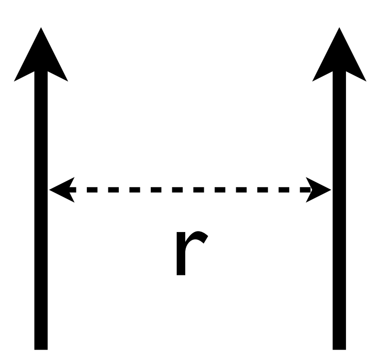


$T > T_{Curie}$



Ferromagnetism:

- magnetic moments
  - electron’s spin and orbital angular momentum
- electrons are fermions
  - obey Pauli exclusion principle
- neighboring electrons with same spin
  - antisymmetric spatial wf, increase r
  - reduces electrostatic energy



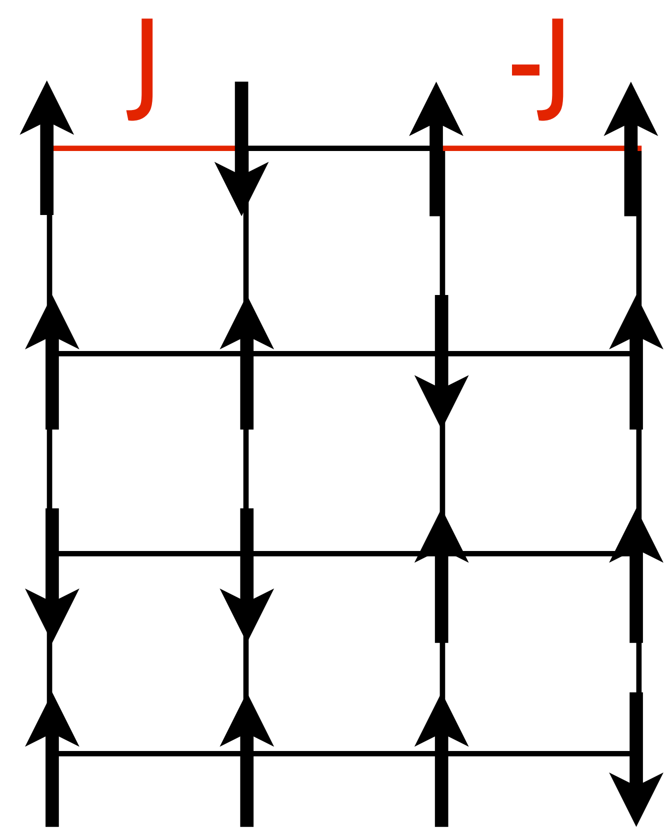
$$E = \frac{ke^2}{r}$$

Ising Model:

- model for magnetic PTs
- parameter J models Coulomb interaction
- 1D chain: no PT at finite T
- 2D lattice: shows PT at finite T!

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

$$S_i = +1, -1$$

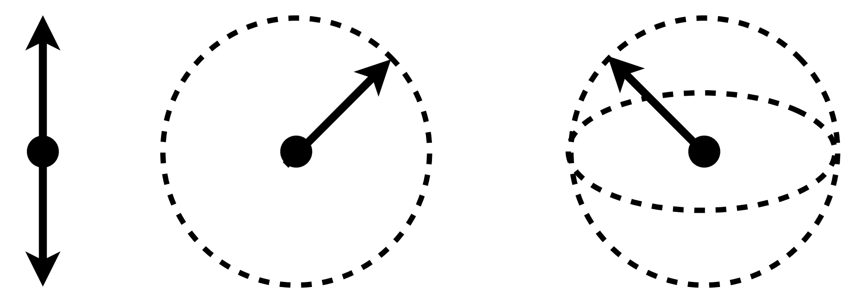


[1] Ising, Ernst. "Beitrag zur theorie des ferromagnetismus." Zeitschrift für Physik A Hadrons and Nuclei 31.1 (1925): 253-258.

[2] “Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition” Lars Onsager, Phys. Rev. 65, 117 (1944)

Magnetic PTs:

- existence and character of PTs is highly dependent upon:
  - lattice dimension (d)
  - symmetry of the degrees of freedom
- my model: 1D Ising chains coupled to perpendicular 1D Ising chains?
  - idea inspired by new quantum model of a magnetic material



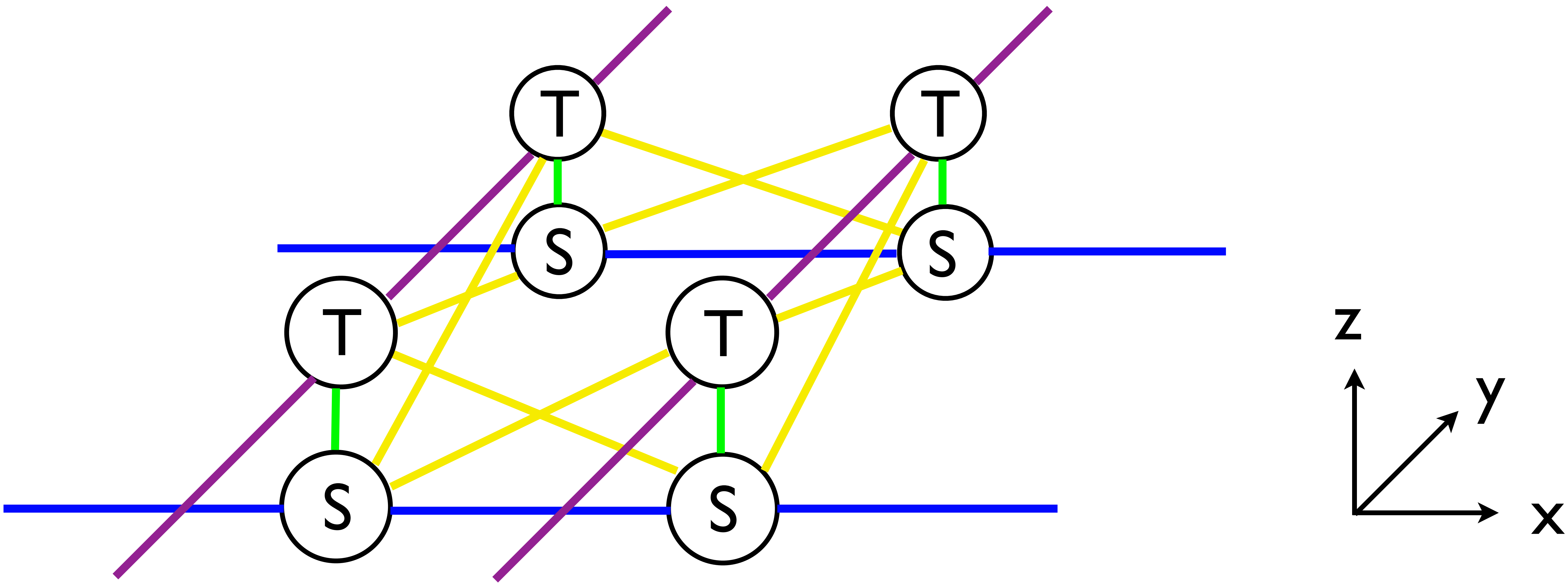
	Ising	XY	Heisenberg
d=1	No	No	No
d=2	Yes	KT	No
d=3	Yes	Yes	Yes

[3] “Organometalliclike localization of 4d-derived spins in an inorganic conducting niobium suboxide,” K.-W. Lee and W. E. Pickett, Phys. Rev. B91, 195152 (2015).

My Model:

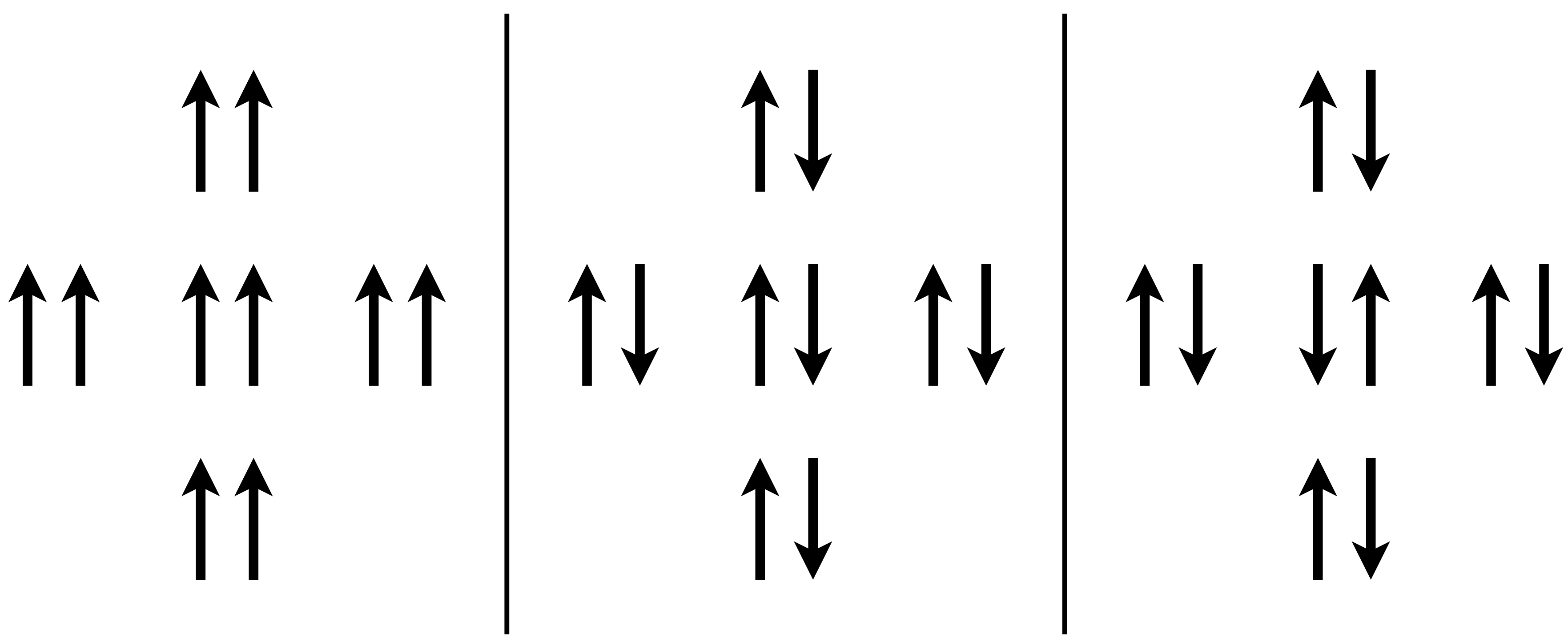
- S & T = {+1,-1}
- square lattice
- periodic boundary conditions

$$E = -J_x \sum_{\mathbf{r}} S_{\mathbf{r}} S_{\mathbf{r}+\hat{\mathbf{x}}} - J_y \sum_{\mathbf{r}} T_{\mathbf{r}} T_{\mathbf{r}+\hat{\mathbf{y}}} - J_K \sum_{\mathbf{r}} S_{\mathbf{r}} T_{\mathbf{r}} - J_{K'} \sum_{\mathbf{r}} [S_{\mathbf{r}}(T_{\mathbf{r}-\hat{\mathbf{y}}} + T_{\mathbf{r}+\hat{\mathbf{y}}}) + T_{\mathbf{r}}(S_{\mathbf{r}-\hat{\mathbf{x}}} + S_{\mathbf{r}+\hat{\mathbf{x}}})]$$



Model Details:

- 3 ordered phases



FM **AFM** **AFM-2**

$J_{k'}<0.5$ $J_{k'}>0.5$

Additional Motivation:

- Blume-Capel model: S = {+1, 0, -1}

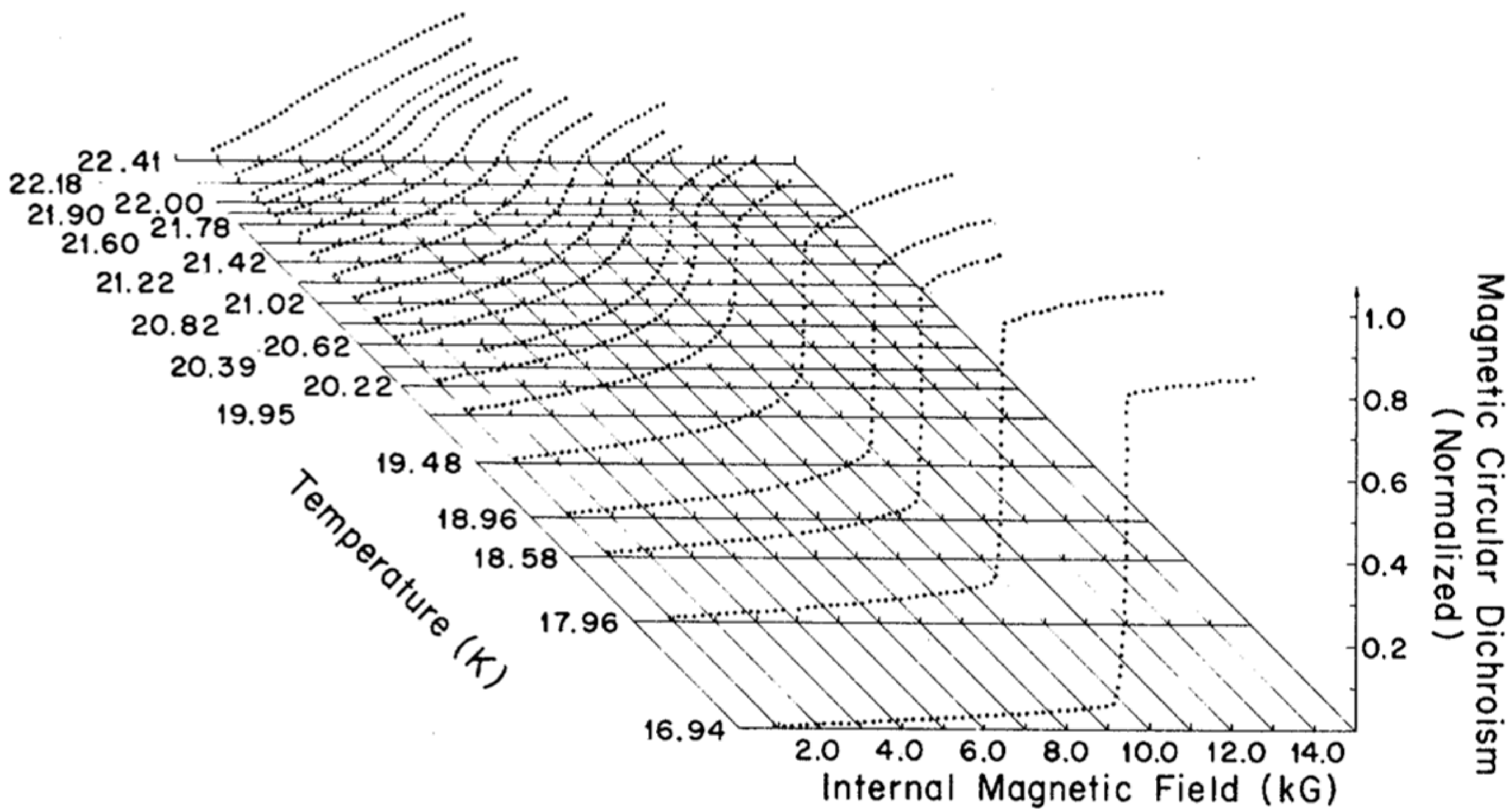
$$E_{\text{Blume-Capel}} = -J \sum_{<ij>} S_i S_j + \Delta \sum_i S_i^2$$

- hand waving argument: $S_i = -T_i$ acts like a spin 0 ?
- BC model contains tricritical point (TCP)
  - point where PT switches from 2nd order to 1st order
- only a few other classical spin models with tricritical points
- TCP first discovered experimentally in Helium-3/Helium-4 mixtures in 1967 [4]

[4] Graf, E. H., D. M. Lee, and John D. Reppy. "Phase Separation and the Superfluid Transition in Liquid He 3-He 4 Mixtures." Physical Review Letters19.8 (1967): 417.

TCPs in real magnetic materials:

- $FeCl_2$
- AFM to PM phase transition



[5] Griffin, J. A., and S. E. Schnatterly. "Optical Measurement of the Magnetic Tricritical Behavior of Fe Cl 2." Physical Review Letters 33.26 (1974): 1576.

Mean field theory (Ising):

- reduce many-body problem to one-body problem
- one site feels “mean-field” from surrounding spins
- for Ising model:

$$E = -J \sum_{\langle ij \rangle} S_i S_j$$

$$m \equiv \langle S_i \rangle$$

$$S_i = m + (S_i - m) \equiv m + \delta S$$

$$E_{MF} = -(Jzm) \sum_i S_i$$

$$m = \frac{1}{Z} \sum_{\text{configurations}} m_c e^{-\beta E_{MF,c}}$$

$$m = \tanh(\beta J z m)$$

$$\longrightarrow \boxed{T_C = \frac{Jz}{k_B}}$$

Mean field theory:

- for my model:

$$m_1 \equiv < S_r >$$

$$m_2 \equiv < T_r >$$

$$E^{MF} = -(2J_x m_1 + 4J_{K'} m_2) \sum_r S_r - (2J_y m_2 + 4J_{K'} m_1) \sum_r T_r - J_K \sum_r S_r T_r$$

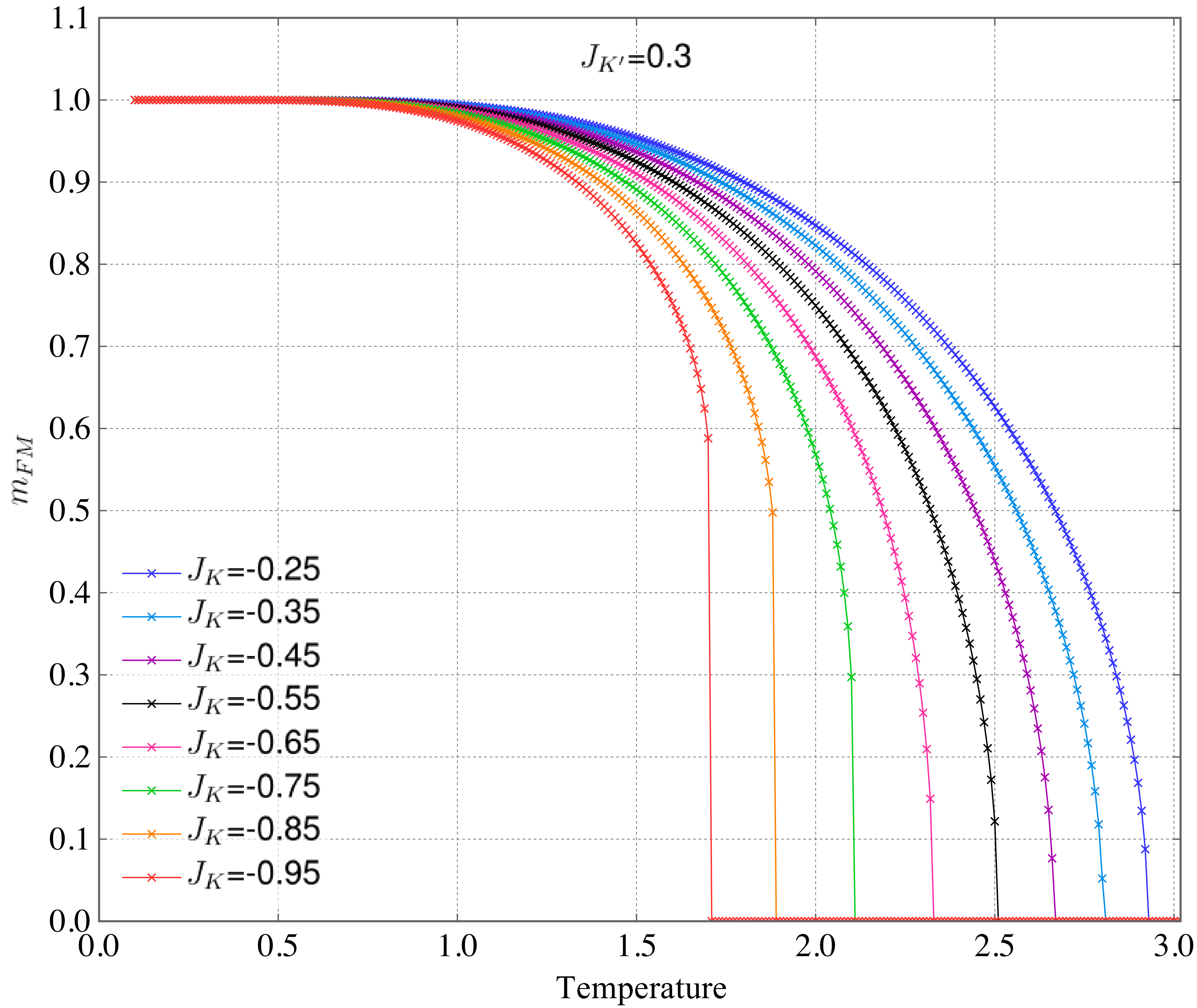
$$m_{FM} = m_1 = m_2$$

$$m_{AFM} = m_1 = -m_2$$

$$m_{FM} = \frac{\sinh\left(4\beta m_{FM}(J_{x,y} + 2J_{K'})\right)}{\cosh\left(4\beta m_{FM}(J_{x,y} + 2J_{K'})\right) + e^{-2\beta J_K}}$$

$$m_{AFM} = \frac{\sinh\left(4\beta m_{AFM}(J_{x,y} - 2J_{K'})\right)}{\cosh\left(4\beta m_{AFM}(J_{x,y} - 2J_{K'})\right) + e^{2\beta J_K}}$$

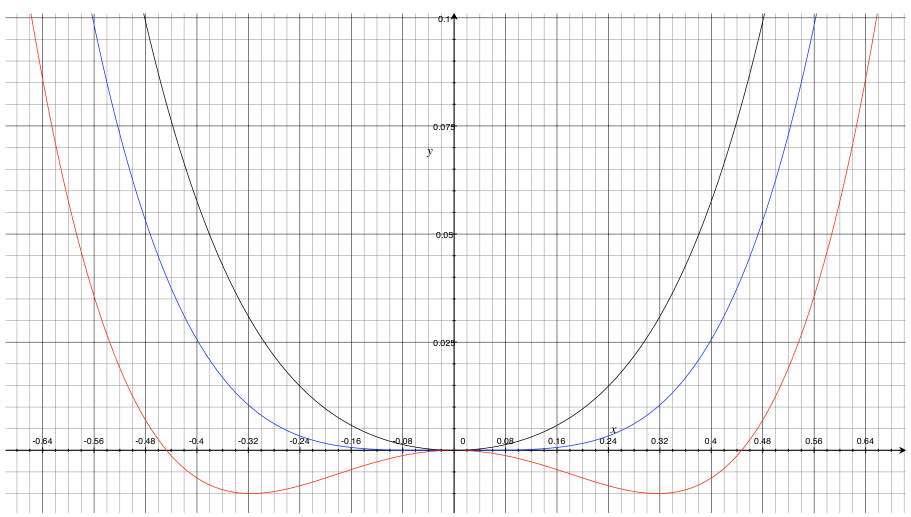
Mean field theory:



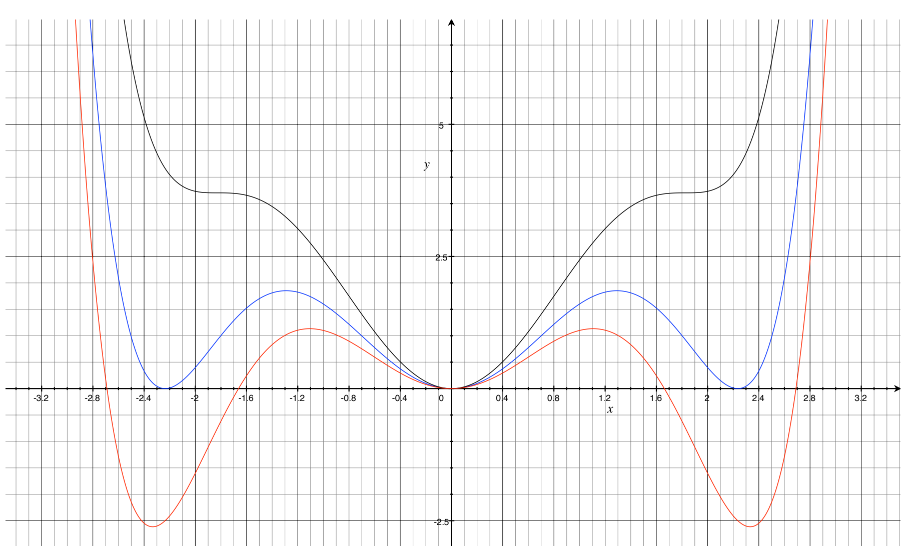
Landau theory of PTs:

- expand free energy in power series of order parameter
- since F(m) = F(-m), only even powers are needed
- minimum of free energy gives equilibrium state

$$f(m) = a + bm^2 + cm^4 + dm^6 + O(m^8)$$



- 2nd order PT: T_C occurs when $c>0$ and $b=0$



- 1st order PT: T_C occurs when $c<0$ and $c^2=4bd$
- TCP: $c=0$

Variational MFT:

- based on Gibbs-Bogoliubov-Feynman inequality

$$Z \geq Z_{MF} e^{-\beta\langle E-E_{MF}\rangle_{MF}}$$

- derived expression for free energies (FM and AFM)

$$\frac{F_{FM}}{N} = -k_B T \ln\left[2e^{J_K/k_B T}\right] - k_B T \ln\left[\cosh\left(\frac{2m_{FM}}{T}(2J_{x,y}+4J_{K'})\right) + e^{-2J_K/k_B T}\right] + m_{FM}^2(2J_{x,y}+4J_{K'})$$

$$\frac{F_{AFM}}{N} = -k_B T \ln\left[2e^{J_K/k_B T}\right] - k_B T \ln\left[1 + e^{-2J_K/k_B T}\cosh\left(\frac{2m_{AFM}}{T}(2J_{x,y}-4J_{K'})\right)\right] + m_{AFM}^2(2J_{x,y}-4J_{K'})$$

- expanded in power series and applied Landau theory
- 2nd order critical lines: quadratic coefficient = 0 (b=0)

$$T_{C,FM} = \frac{4(J_{x,y}+2J_{K'})}{1+e^{\frac{-2J_K}{T_{C,FM}}}} \qquad T_{C,AFM} = \frac{4(J_{x,y}-2J_{K'})}{1+e^{\frac{2J_K}{T_{C,AFM}}}}$$

Variational MFT:

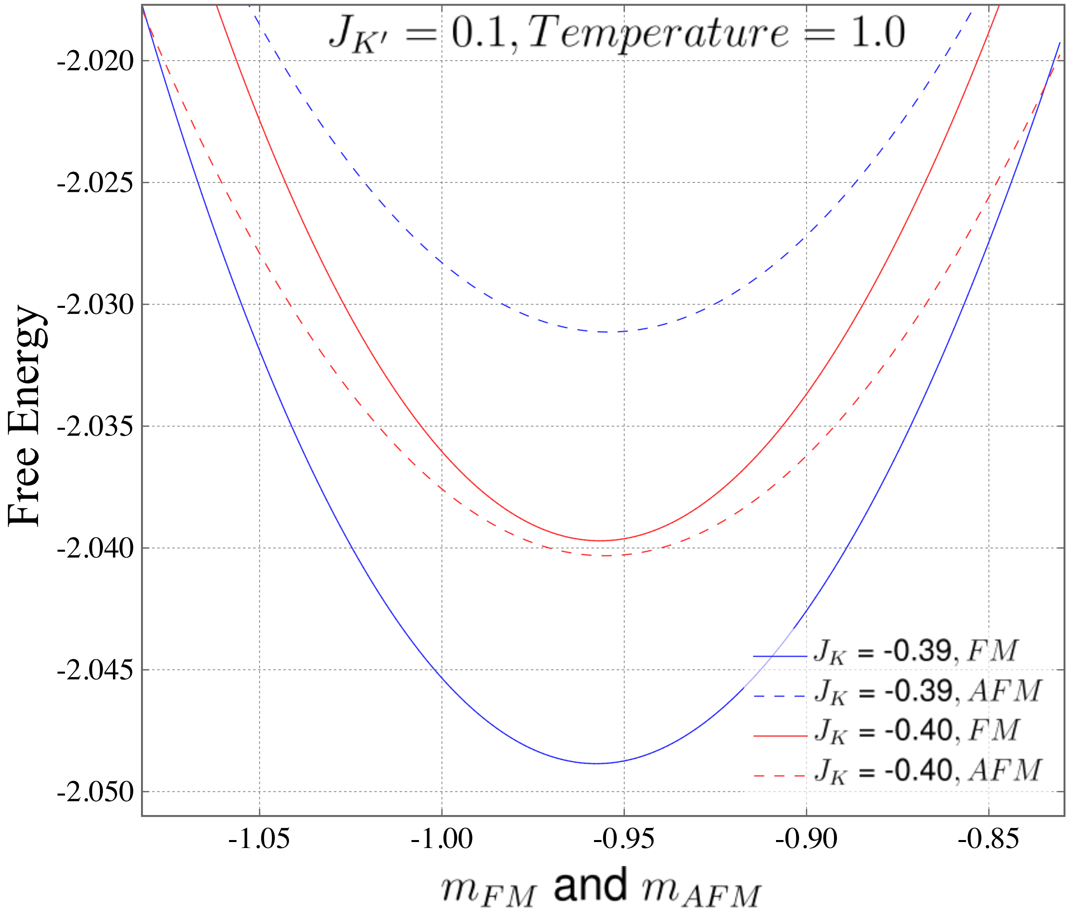
- TCP: set the quartic coefficient = 0 (c=0)

$$T_{TCP,FM} = \frac{-2J_K}{ln(2)} \qquad T_{TCP,AFM} = \frac{+2J_K}{ln(2)}$$

- TCP occurs when c=0 and b=0

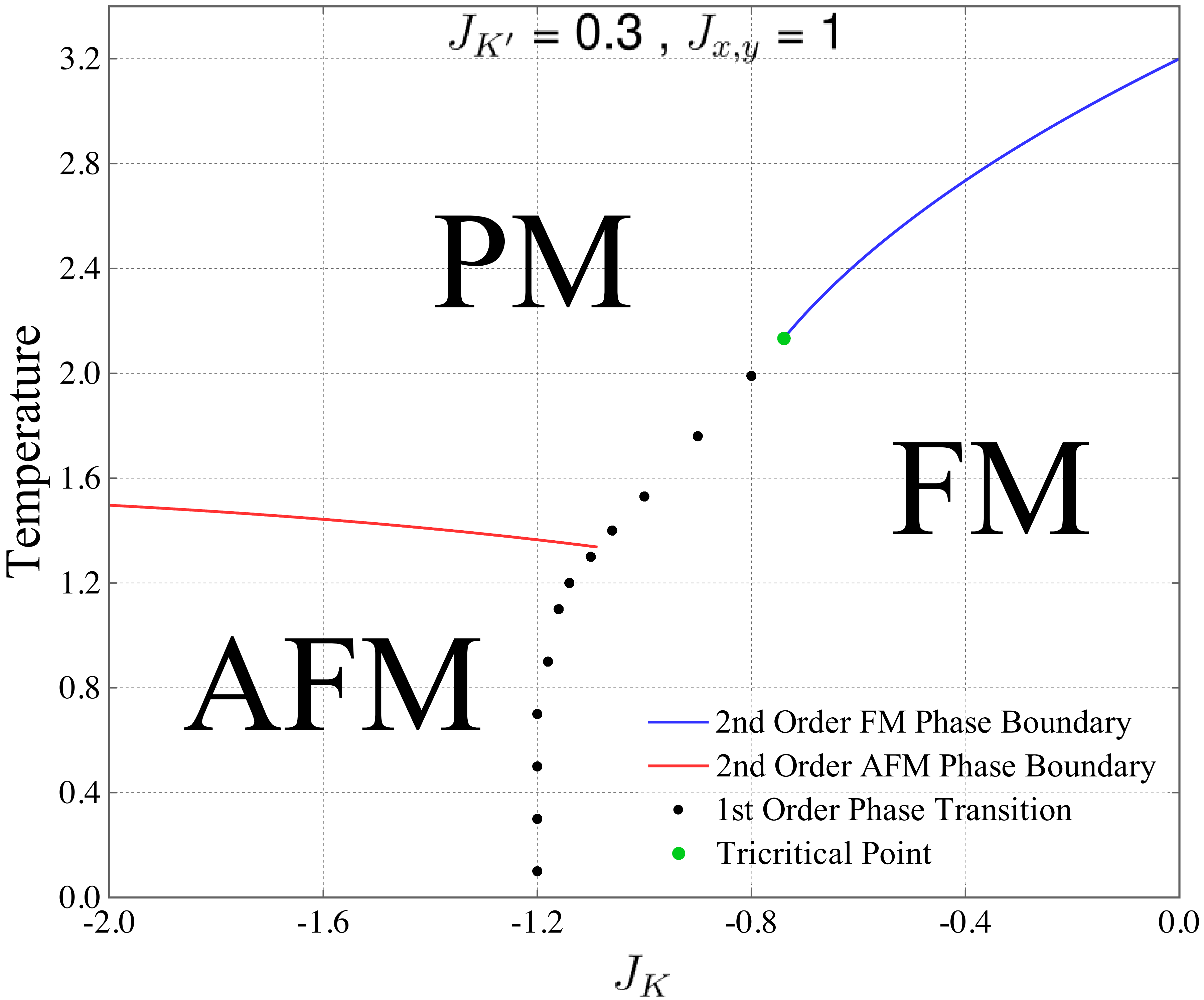
$$T_{\text{tricritical}} = \frac{4(J_{xy} + 2J_{K'})}{3}$$

$$J_{\text{K,tricritical}} = \frac{-2\ln(2)(J_{xy} + 2J_{K'})}{3}$$



- first order critical temperatures can be determined graphically

MFT Phase Diagram:



Monte Carlo background:

- in thermal equilibrium, states in our system obey a Boltzmann distribution

$$P_i = \frac{e^{-\beta E_i}}{Z}$$

- distribution not directly accessible
- solution: create a Markov chain of states that ultimately samples the Boltzmann distribution
  - detailed balance- guarantees existence of stationary distribution
  - ergodicity- guarantees uniqueness of stationary distribution

MC implementation:

- Metropolis Monte Carlo (MCC) Code in C++
- initially, random spin configuration on lattice
- suggest a spin to flip and calculate energy change
- accept or reject based upon Metropolis condition

$$W(A \to B) = 1 \text{ when } E_B \leq E_A$$

$$W(A \to B) = e^{\frac{-(E_B - E_A)}{k_B T}} \text{ when } E_B > E_A$$

- "thermalize" lattice until stationary distribution is reached
- make measurements by sampling the distribution

$$m_{FM} = |\frac{1}{2N} \sum_i \sum_j (S_{ij} + T_{ij})| \qquad m_{AFM} = |\frac{1}{2N} \sum_i \sum_j (-S_{ij} + T_{ij})|$$

T_C from MC:

- correlation length diverges at T_C but lattice is finite
- scaling theory is used to determine quantities in the thermodynamic limit
- Binder cumulant, U_L, is independent of L at T_C (t=0)

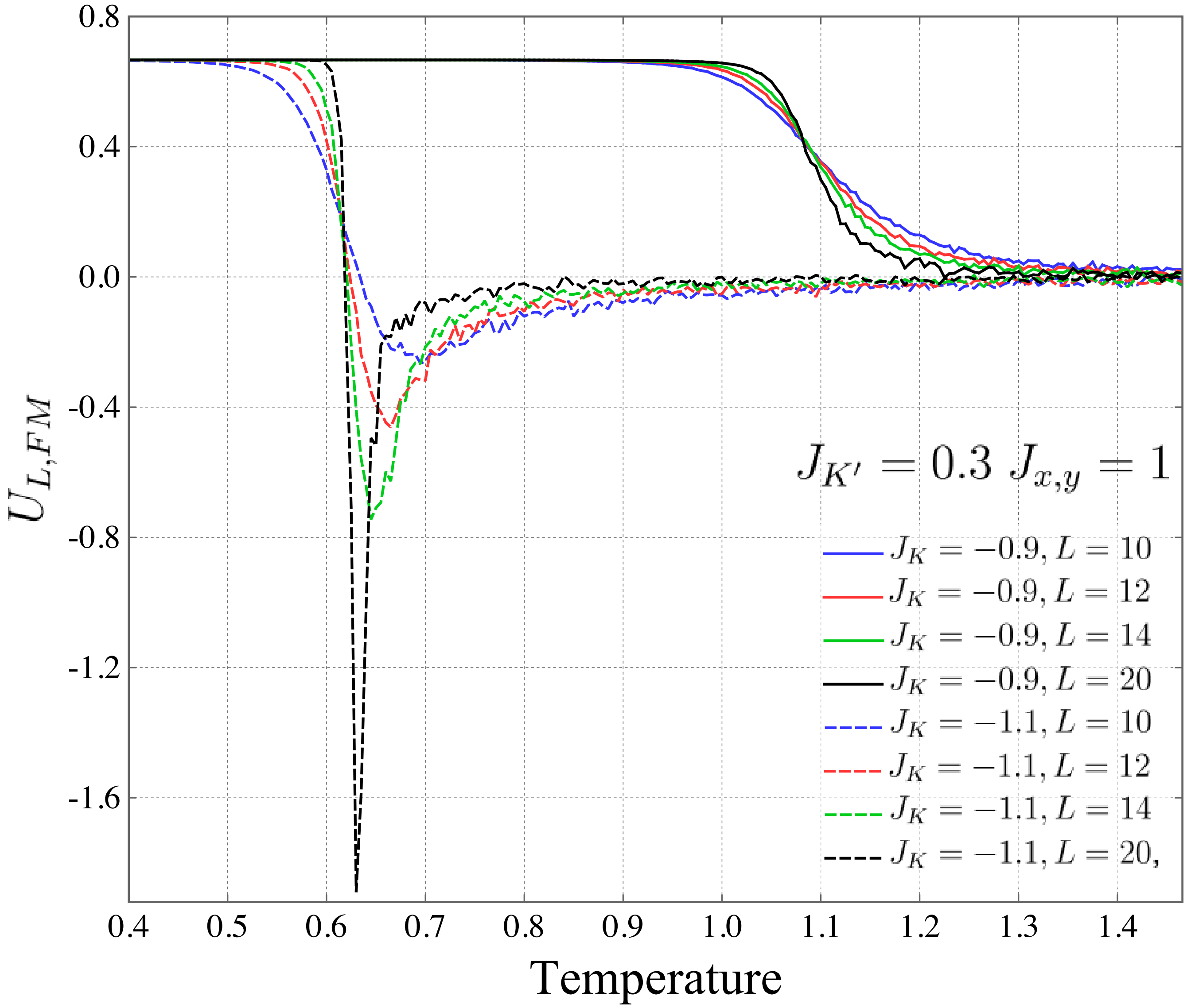
$$U_L = 1 - \frac{< m^4 >}{3 < m^2 >^2}$$

$$M = L^{\frac{-\beta}{\nu}} g_M(tL^{\frac{1}{\nu}})$$

$$\frac{< M^4 >_L}{< M^2 >_L^2} = \frac{L^{\frac{-4\beta}{\nu}} g_{M^4}(tL^{\frac{1}{\nu}})}{(L^{\frac{-2\beta}{\nu}} g_{M^2}(tL^{\frac{1}{\nu}}))^2} = g(tL^{\frac{1}{\nu}})$$

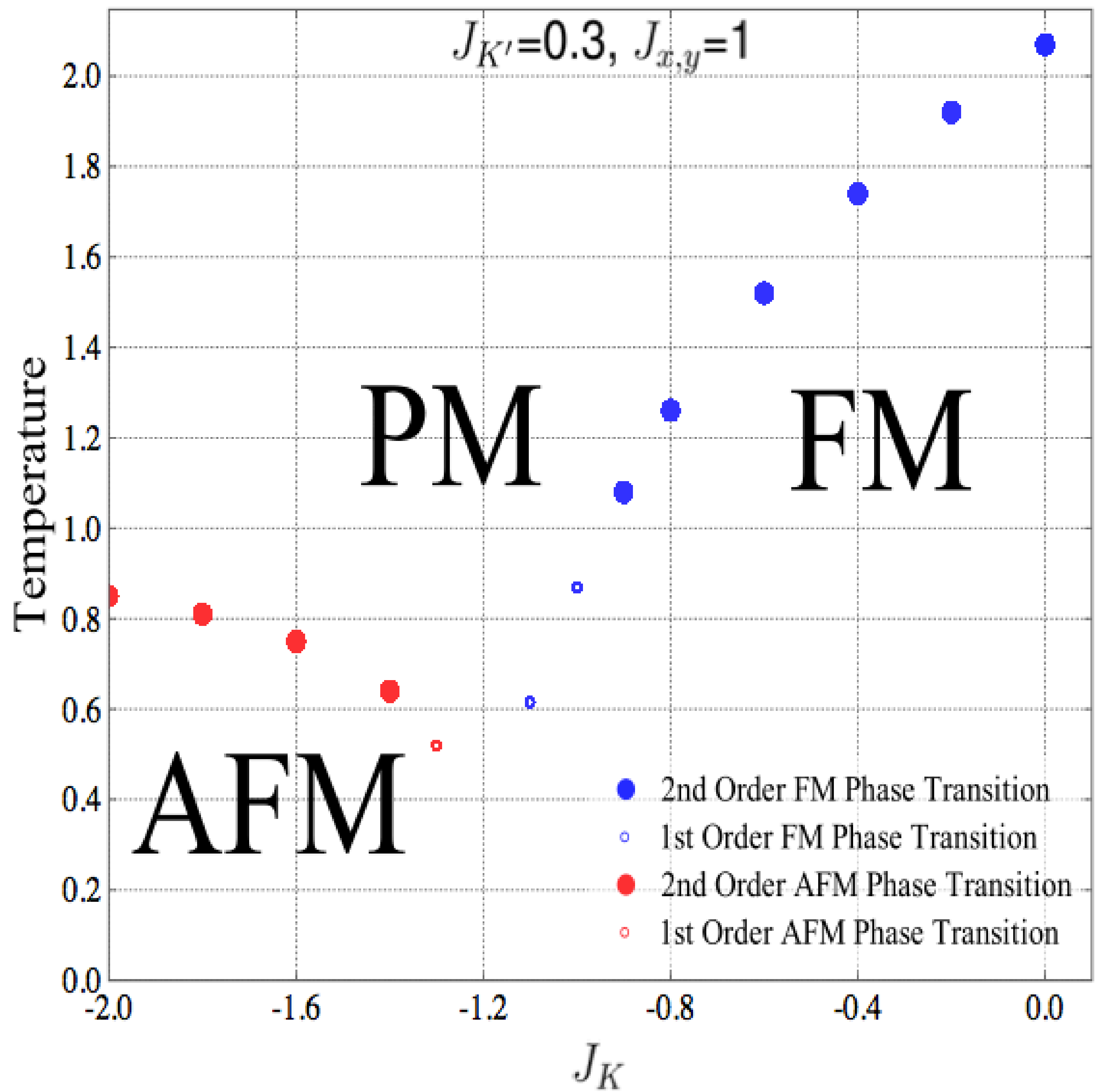
1st v. 2nd Order in MC:

- Binder cumulant can distinguish 1st and 2nd order PT
- 2nd order PT: U=2/3 at low T and U=0 at high T, always between those two values
- 1st order PT: minimum below 0, deeper for larger L



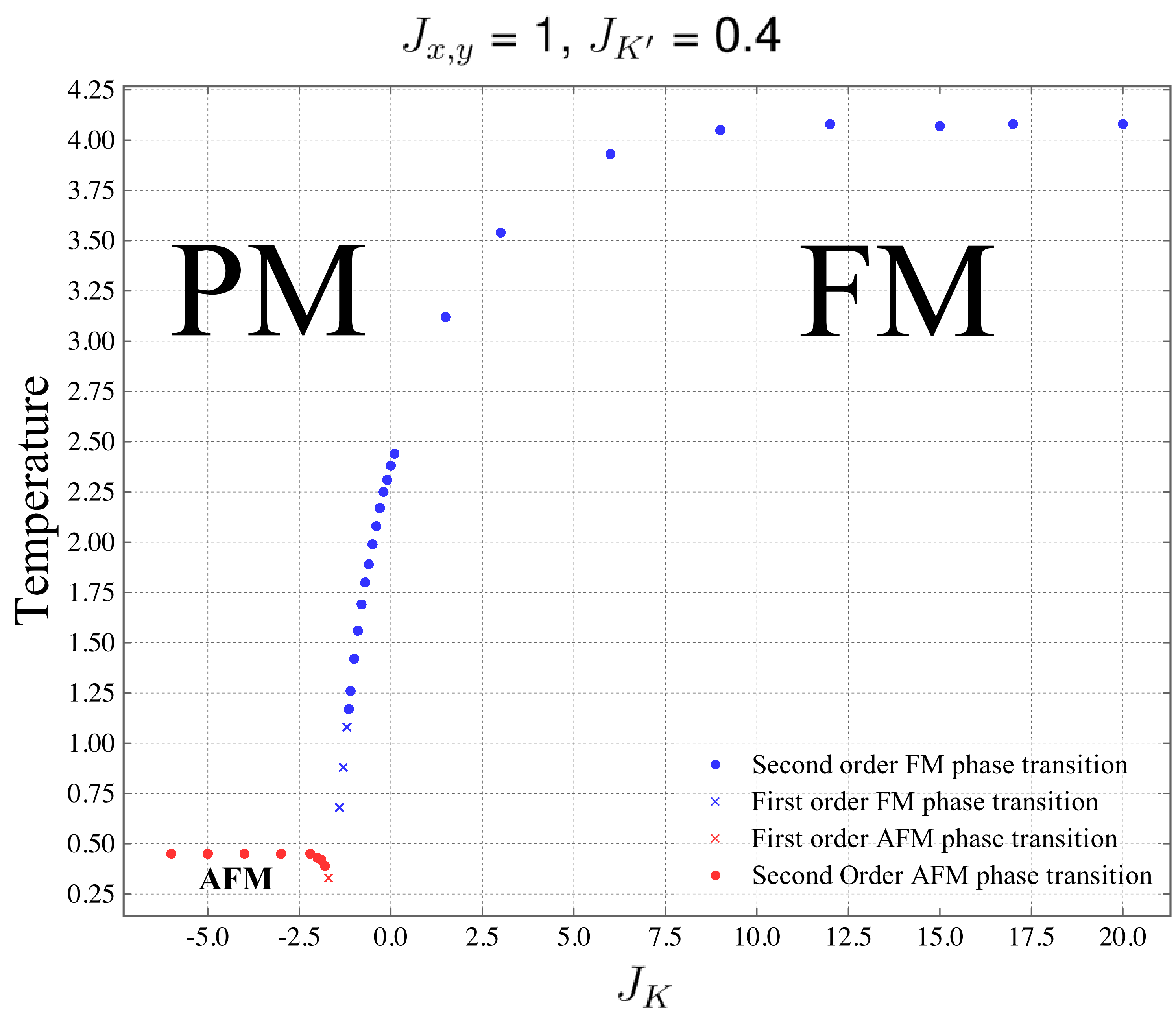
[6] K.Vollmayr, J.D.Reger, M.Scheucher, K.Binder Z. Phys. B91, 113-125 (1993).

Monte Carlo Phase Diagram:



Sanity check:

- check: large, positive J_K causes pair of S and T spins to align
- becomes the 2D Ising model with $J_{Ising,effective} = J_{x,y} + 2\ J_{k'}$
- 2D Ising Model: $T_{c,Ising} = 2.269\ J_{Ising}$
- $J_{k'} = 0.4$, $J_{x,y}=1$, and large positive J_k: expect $T_{c,\ chains} = 4.08$



Wang-Landau sampling:

- MMC suffers from:
  - critical slowing down at 2nd order PTs
  - long tunneling time between coexisting phases at 1st order PTs
- MMC gives canonical distribution at one temperature
- Wang-Landau sampling (2001) solves these problems by calculating the temperature-independent density of states (DOS)

[7] Wang, Fugao, and D. P. Landau. "Efficient, multiple-range random walk algorithm to calculate the density of states." Physical review letters 86.10 (2001): 2050.

Wang-Landau sampling:

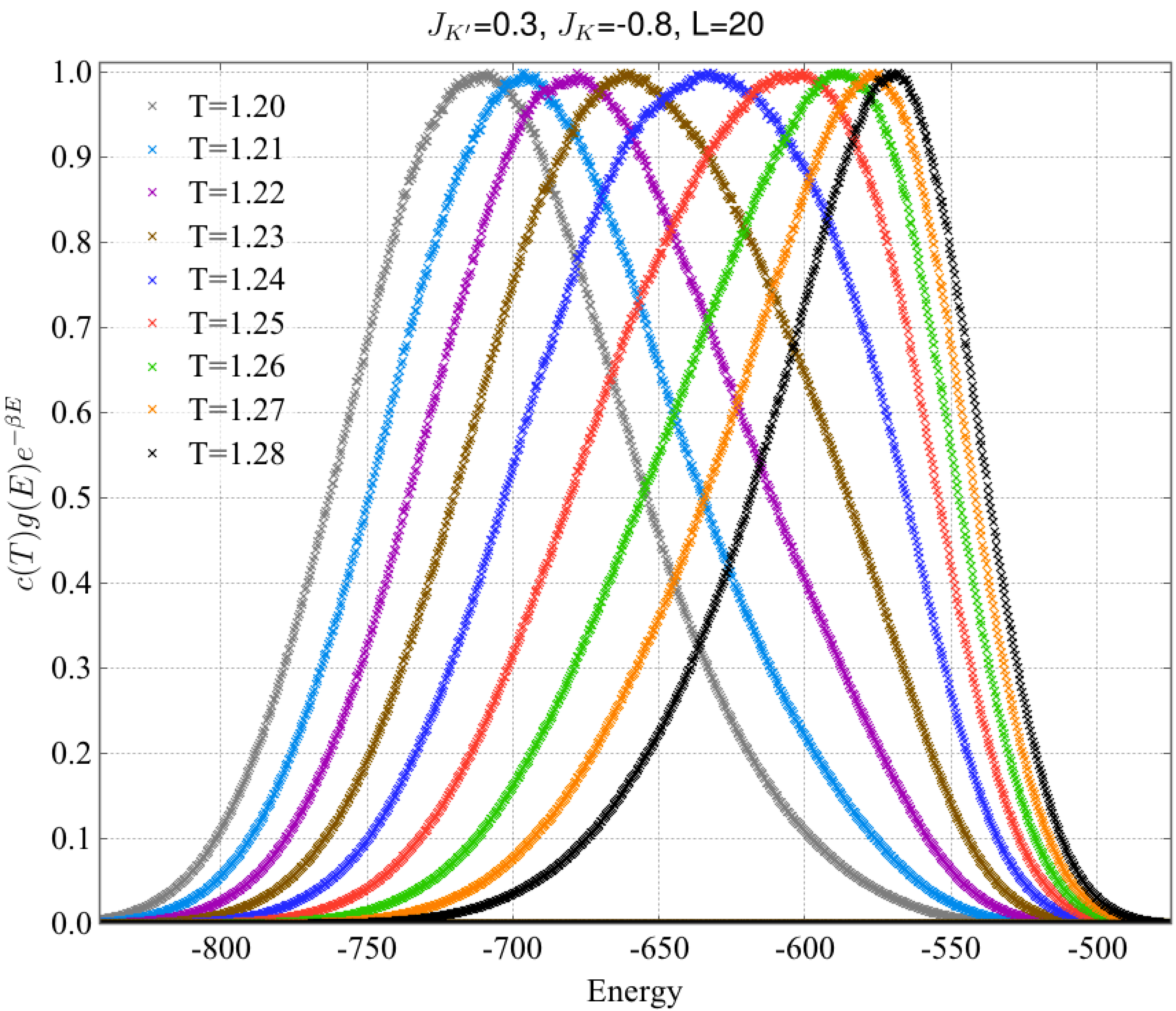
- performs random walk in energy space with acceptance probability proportional to $1/p(E_{new})$
  - a flat histogram will be produced
- WLS violates detailed balance in the beginning of the algorithm
- As algorithm converges to true DOS, detailed balance is satisfied

$$Z = \sum_{\text{configurations}} e^{-\beta E_{\text{configuration}}} = \sum_E g(E) e^{-\beta E}$$

$$P(E,T) = g(E) e^{\frac{-E}{k_B T}}$$

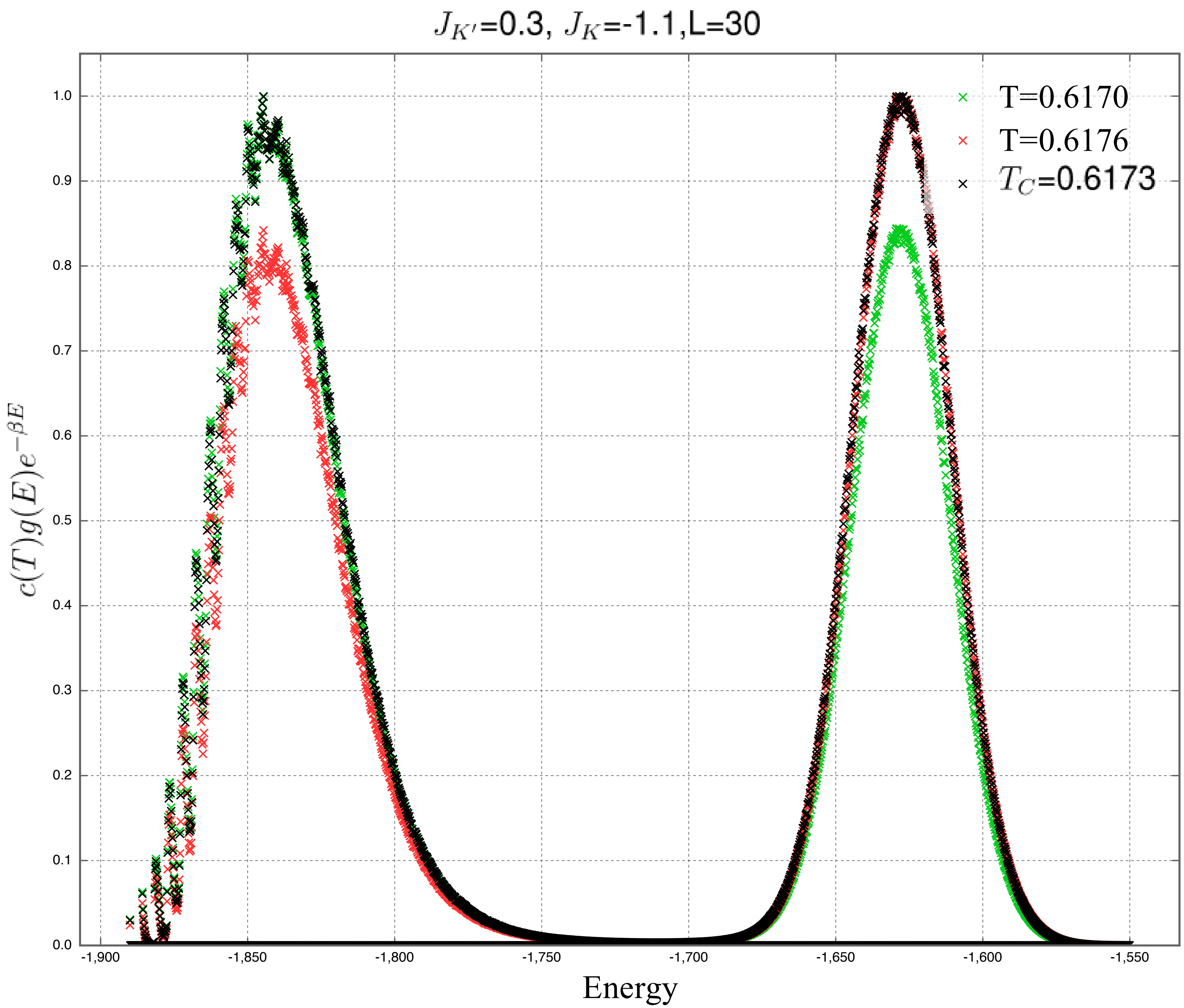
Wang-Landau sampling:

- Canonical distribution (CD) across a 2nd order PT



Wang-Landau sampling:

- Double peaked (equal height) CD at 1st order T_C



Future Directions:

- AFM-2 phase, vary other parameters (J_x and J_x)
- tricritical exponents
- new: use similar methods to explore isentropes in disordered classical spin models
- phase transitions in my classical model are driven by thermal fluctuations
- new: what would happen if we added quantum fluctuations?
- quantum tricritical points (T=0)
- QMC

Thanks for listening!