First order phase transitions - PhD students aren't always wrong

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Plan of talk

Phase transitions, first and second order

Phase transitions on a computer (lattice models)

A problem (with simulations of first order transitions)

A solution

First and Second Order Transitions

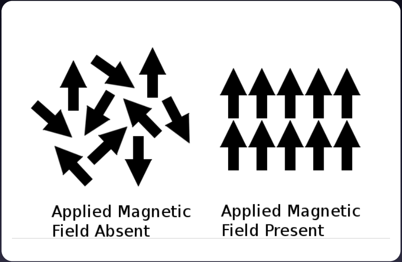
First-order phase transitions are those that involve a latent heat.

Second-order transitions are also called continuous phase transitions. They are characterized by a divergent susceptibility, an infinite correlation length, and a power-law decay of correlations near criticality.

Transitions - piccies

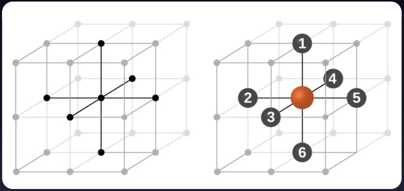
First order - melting

Second order - Curie



Transitions - on/in a computer

Spins interact with nearest neighbours



Low-T, like to align - ordered phase

High-T, disordered phase

Transitions - on/in a computer

Hamiltonian q-state Potts, $\sigma = 1 \dots q$

$$\mathcal{H}_q = -\sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j}$$

Evaluate a partition function, $\beta = 1/k_b T$

$$Z(\beta) = \sum_{\{\sigma\}} \exp(-\beta \mathcal{H}_q)$$

Derivatives of free energy give observables (energy, magnetization..)

$$F(\beta) = \ln Z(\beta)$$

Measure 1001 Different Observables

Order parameter

$$M = (q \max\{n_i\} - N)/(q-1)$$

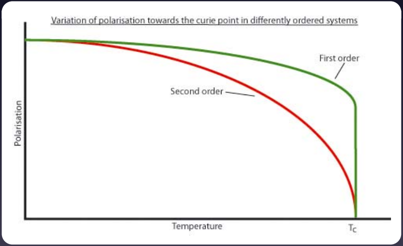
Per-site quantities denoted by $e = E/N$ and $m = M/N$

$$\begin{aligned} u(\beta) &= \langle E \rangle / N, \\ C(\beta) &= \beta^2 N[\langle e^2 \rangle - \langle e \rangle^2]. \end{aligned}$$

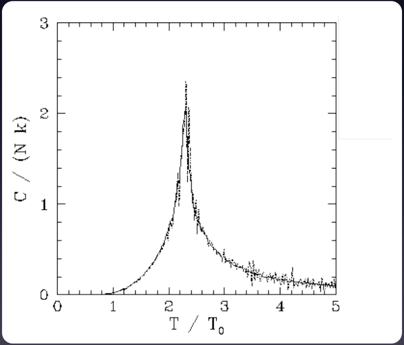
$$\begin{aligned} m(\beta) &= \langle |m| \rangle, \\ \chi(\beta) &= \beta N[\langle m^2 \rangle - \langle |m| \rangle^2] \end{aligned}$$

First and Second Order Transitions - Piccies

First order - discontinuities in magnetization, energy (latent heat)



Second order - divergences in specific heat, susceptibility



Continuous Transitions - Critical exponents

(Continuous) Phase transitions characterized by critical exponents

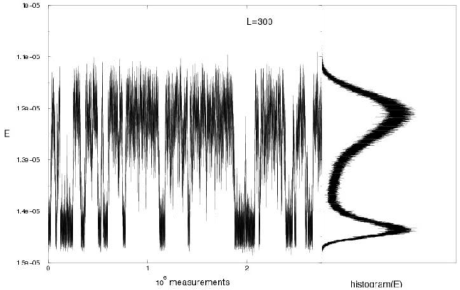
Define $t = |T - T_c|/T_c$

Then in general, $\xi \sim t^{-\nu}$, $M \sim t^{\beta}$, $C \sim t^{-\alpha}$, $\chi \sim t^{-\gamma}$

Can be rephrased in terms of the linear size of a system L

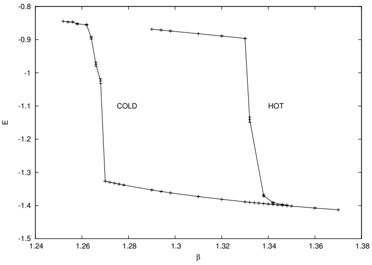
$\xi \sim L$, $M \sim L^{-\beta/\nu}$, $C \sim L^{\alpha/\nu}$, $\chi \sim L^{\gamma/\nu}$

What does a first order system look like (at PT) I?



What does a first order system look like (at PT) II?

Hysteresis



1st Order FSS: Heuristic two-phase model

A fraction W_o in q ordered phase(s), energy e_o

A fraction $W_\mathrm{d} = 1 - W_\mathrm{o}$ in disordered phase, energy e_d

Ignore transits

1st Order FSS: Energy moments

Energy moments become

$$\langle e^n \rangle = W_\mathrm{o} e_\mathrm{o}^n + (1 - W_\mathrm{o}) e_\mathrm{d}^n$$

And the specific heat then reads:

$$C_V(\beta, L) = L^d \beta^2 \left(\left\langle e^2 \right\rangle - \langle e \rangle^2 \right) = L^d \beta^2 W_\mathrm{o} (1 - W_\mathrm{o}) \Delta e^2$$

Max of $C_V^{\mathrm{max}} = L^d \left(\beta^\infty \Delta e / 2 \right)^2$ at $W_\mathrm{o} = W_\mathrm{d} = 0.5$

Volume scaling

1st Order FSS: Specific Heat peak shift

Probability of being in any of the states

$$W_o \sim q \exp(-\beta L^d f_o)\,,\;\; W_d \sim \exp(-\beta L^d f_d)$$

Take logs, expand around β^∞

$$\begin{aligned} \ln(W_o/W_d) &= \ln q + \beta L^d (f_d - f_o) \\ &= \ln q + L^d \Delta e(\beta - \beta^\infty) \end{aligned}$$

Solve for specific heat peak $W_o = W_d$, $\ln(W_o/W_d) = 0$

$$\beta^{C_V^{\max}}(L) = \beta^\infty - \frac{\ln q}{L^d \Delta e} + \dots$$

1st Order FSS: summary

Peaks grow as L^d

Transition point estimates shift as $1/L^d$

Strong First Order Transition

Plaquette Ising model

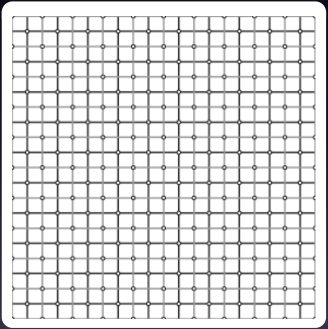
$$\mathcal{H} \;=\; -\sum_{\Box} \sigma_i \sigma_j \sigma_k \sigma_l$$

Only inaccurate (yours truly...) determination of transition point

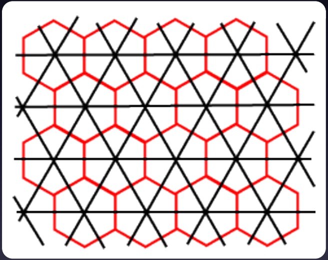
Same for dual model - only inaccurate (yours truly ...) determination of transition point

Duality - geometric

Square lattice - self dual



Triangle - hexagon dual



Duality - spin models

Spins on orginal lattice $\leftrightarrow$ spins on dual lattice

High-T $\leftrightarrow$ Low-T

$$\tanh \beta = e^{-2\beta^*}$$

Ising, square lattice

$$\begin{aligned} Z(\beta) &\simeq (1 + N \tanh(\beta)^4 + \ldots) \\ Z(\beta^*) &\simeq (1 + N \exp(-2\beta^*)^4 + \ldots) \end{aligned}$$

Duality - plaquette spin model

Plaquette Ising model

$$\mathcal{H} = -\sum_{\Box} \sigma_i \sigma_j \sigma_k \sigma_l$$

Dual to this

$$\mathcal{H}_{dual} = -\sum_{\langle ij \rangle_x} \sigma_i \sigma_j - \sum_{\langle ij \rangle_y} \tau_i \tau_j - \sum_{\langle ij \rangle_z} \sigma_i \sigma_j \tau_i \tau_j \,,$$

Exercise for a starting PhD student (Marco Mueller)

Simulate 3*d* plaquette model and dual

Do a better job than, ahem, before at determining transition point of both

Obtain consistent estimates of transition point

A Problem

Determine critical point(s) $L = 8 \ldots 27$, periodic bc, $1/L^3$ fits

Original model:

$$\beta^{\infty} = 0.549994(30)$$

Dual model:

$$\beta^{\infty}_{dual} = 1.31029(19)$$

$$\beta^{\infty} = 0.55317(11)$$

Estimates are about 30 error bars apart

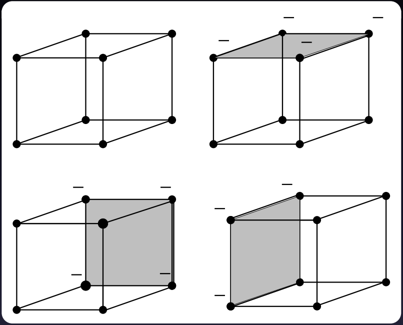
(Non) Solutions

Blame the student (yours truly....)

Blame the student (yours truly....)

Think - What is special about plaquette model?

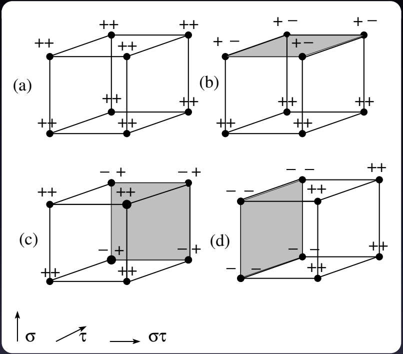
Groundstates: Plaquette



Degeneracy 2^{3L}

$$\mathcal{H} = -\sum_{\square} \sigma_i \sigma_j \sigma_k \sigma_l$$

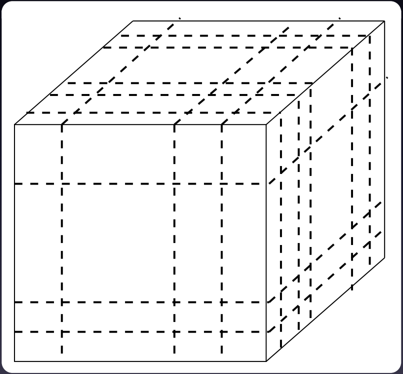
Groundstates: Dual



Degeneracy 2^{3L}

$$\mathcal{H}_{dual} = -\sum_{\langle ij \rangle_x} \sigma_i \sigma_j - \sum_{\langle ij \rangle_y} \tau_i \tau_j - \sum_{\langle ij \rangle_z} \sigma_i \sigma_j \tau_i \tau_j \,,$$

Typical Ground state



1st Order FSS with Exponential Degeneracy

Normally q is constant

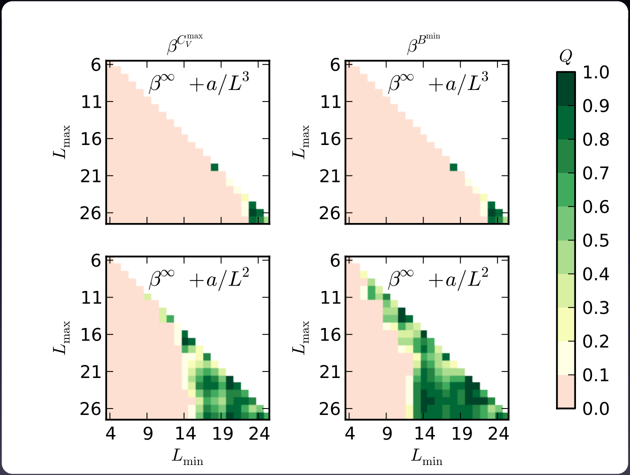
Suppose instead $q \propto e^{L}$ ($q = e^{(3 \ln 2) L}$)

$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{\ln q}{L^{d} \Delta e} + \dots$$

becomes

$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{3 \ln 2}{L^{d-1} \Delta e} + \dots$$

Quality of fits



Forcing a fit to $1/L^3$ gives much poorer quality

Conclusions

Standard 1st order FSS: $1/L^3$ corrections in 3D

Exponential degeneracy: $1/L^2$ corrections in 3D

PhD students are not always wrong

References

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