Degeneracy and first order phase transitions

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Des Johnston (bad guy)
Coventry, April 2016

Plan of talk

Mea Culpa

A family of $3D$ Ising models motivated by random surface simulations

A problem with the 1st order FSS for a plaquette $3D$ Ising model in this family

A solution

Mea Culpa I

Wolfhard has been interested in first order transitions for a *very* long time

Volume 105A, number 3 PHYSICS LETTERS 8 October 1984

FIRST ORDER IN 2D DISCLINATION MELTING

W. JANKE and H. KLEINERT
Institut für Theorie der Elementarteilchen, Freie Universität Berlin, Arnimallee 14, 1000 Berlin 33, West-Germany

Received 24 April 1984

We present a Monte Carlo study of a 2D gas of crystal disclinations and find a first-order melting transition.

Prejudice: first order transitions poor cousins of second order. Fewer different numbers to measure....and harder to do so.

Mea Culpa II

Even sharing an office with Wolfhard in 1989 wasn't enough to change my opinion

Though there were some distractions......

Only enlightened by recent work

The Hamiltonian(s) of Interest

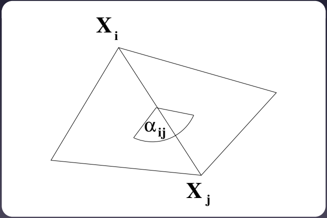
The Gonihedric action

- Savvidy "Gonihedric" Hamiltonian

$$
\begin{aligned}
H &= \sum_{ij} |X^{\mu}(i) - X^{\mu}(j)|\theta_{ij} \\
\theta_{ij} &= ||\pi - \alpha_{ij}||
\end{aligned}
$$

Gonia: angle

Hedra: face

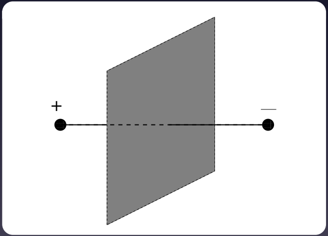


Spins Cluster Boundaries as Surface Models

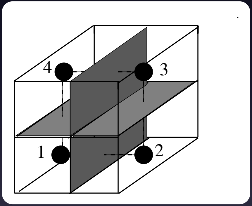
Spin cluster boundaries $\leftrightarrow$ surfaces

Edge spins: $U_{ij} = -1$

Vertex spins: $\sigma_i \sigma_j = -1$



Counting configurations with spins (areas and intersections)



Ising/Surface correspondence

Allow energy from areas, edges and intersections (*A. Cappi, P Colangelo, G. Gonella and A. Maritan*)

$$H = \sum (\beta_A n_A + \beta_C n_C + \beta_I n_I)$$

$$\beta_A = 2J_1 + 8J_2, \quad \beta_C = 2J_3 - 2J_2, \quad \beta_I = -4J_2 - 4J_3$$

$$H \quad = \quad J_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \sigma_i \sigma_j + J_3 \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l$$

Gonihedric $\rightarrow$ Tune Out Area Term

One parameter family of “Gonihedric” Ising models (Savvidy, Wegner)

$$\mathcal{H}^{\kappa} = -2\kappa \sum_{\langle i,j \rangle} \sigma_i \sigma_j + \frac{\kappa}{2} \sum_{\langle\langle i,j \rangle\rangle} \sigma_i \sigma_j - \frac{1-\kappa}{2} \sum_{\Box} \sigma_i \sigma_j \sigma_k \sigma_l$$

$\kappa = 0$ pure plaquette

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

The Dual ($\kappa = 0$)

An anisotropically coupled Ashkin-Teller model

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

Standard duality relation

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

Known: First Order Transition

Strong first order transition

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

Only inaccurate (Metropolis, yours truly, bad ...) determination of transition point

Same for dual model - (Metropolis, yours truly, bad ...) determination of transition point

“Standard” First Order Transitions

The q-state Potts model

Hamiltonian

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

Evaluate the partition function, derivatives give observables

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

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

Critical points shift as $1/L^d$

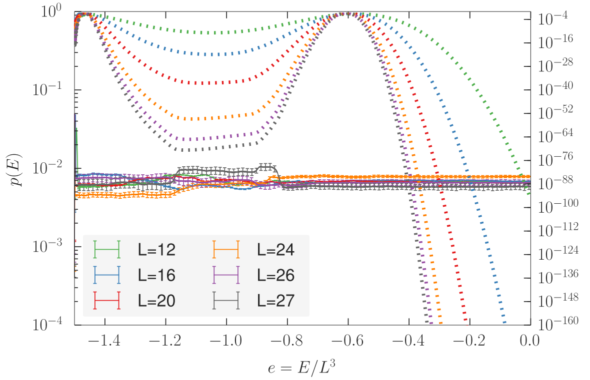
Except …

Fixed boundaries ($1/L$ leading term)

$$Z(\beta) = \left[e^{-\beta(L^d f_d + L^{d-1}\tilde{f}_o)} + q e^{-\beta(L^d f_o + L^{d-1}\tilde{f}_d)} \right] [1 + \ldots]$$

A Problem

Plaquette Model: Careful Multicanonical Simulations



Multicanonical histograms

Scaling of the Plaquette Model and Dual

Determine critical point(s) $L = 8 \ldots 27$, periodic bc, $1/L^3$ fits - a nice exercise for a PhD student (Marco)

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

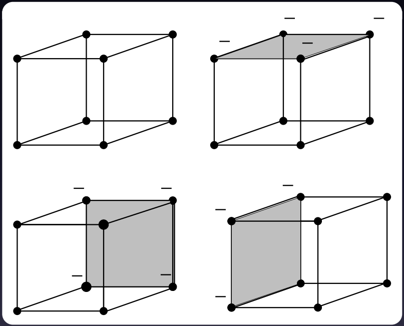
Potential Solutions

Blame the student (yours truly, bad....)

Incorrect, try again (good guys)

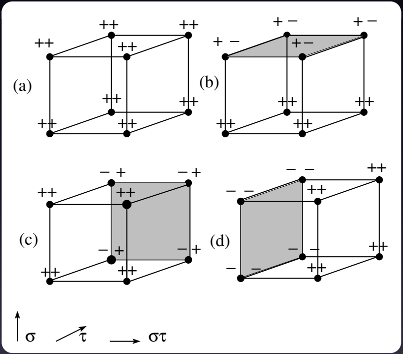
What is special about plaquette model?

Groundstates: Plaquette



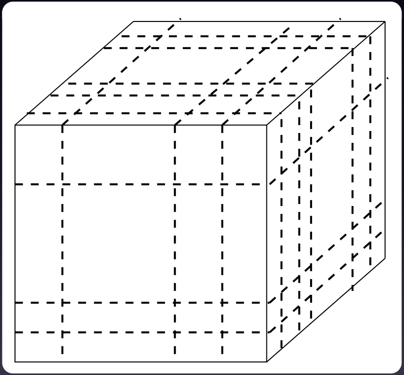
Persists into low temperature phase: degeneracy 2^{3L}

Groundstates: Dual



Dual degeneracy

Ground state



1st Order FSS with Exponential Degeneracy

Normally q is constant

Suppose instead $q \propto e^L$

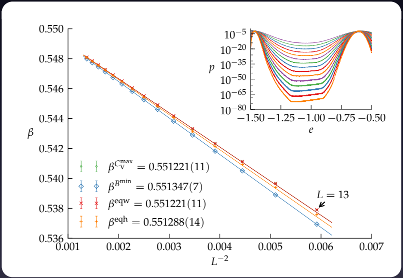
$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{\ln q}{L^d \Delta e} + \ldots$$

becomes

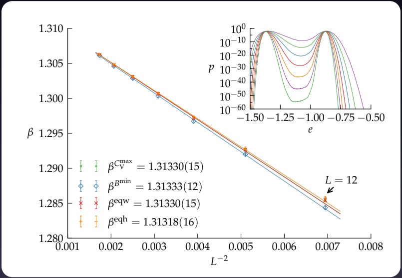
$$\beta^{C_V^{\max}}(L) = \beta^{\infty} - \frac{1}{L^{d-1} \Delta e} + \ldots$$

FSS

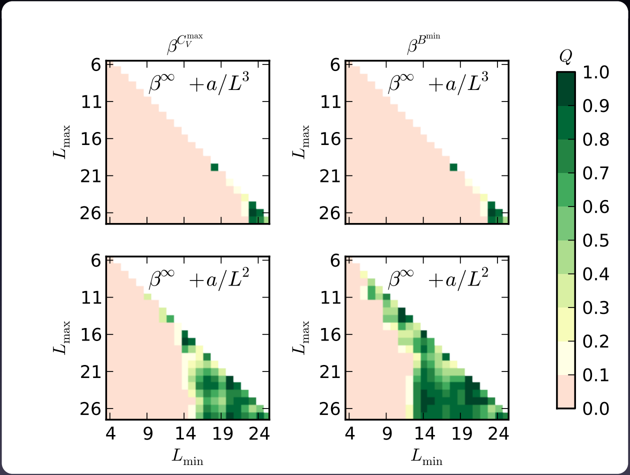
Plaquette Hamiltonian fits



Dual Hamiltonian fits



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

Fixed BC: $1/L$ (surface tension)

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

References

G.K. Savvidy and F.J. Wegner, Nucl. Phys. B **413**, 605 (1994).

M. Mueller, W. Janke and D. A. Johnston, Phys. Rev. Lett. **112** (2014) 200601.

M. Mueller, D. A. Johnston and W. Janke, Nucl. Phys. B **888** (2014) 214; Nucl. Phys. B **894** (2015) 1.

Marco's poster