Numerical test of the Cardy-Jacobsen conjecture in the site-diluted Potts model in three dimensions

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Outline of the Talk

- Effect of the disorder on a first order phase transition ($D = 2$).
  - The Aizenman-Wehr theorem ($D = 2$).
  - The Cardy-Jacobsen conjecture ($D > 2$).

- The three-dimensional diluted Potts model with $Q = 4$ and 8 states:
  - Numerical Simulations.
  - Observables.
  - Scaling near a tricritical point.
  - Our results: Testing the Cardy-Jacobsen conjecture.

- Conclusions.
Effect of Quenched disorder on first order phase transitions.

Some examples:
1. Tilt ordering.
2. Ferroelectrics.
3. Random block copolymers.
4. Topological phases in correlated electron systems.
5. Surface waves.
7. Liquid crystals.

Aizenman and Wehr Theorem
In **TWO** dimensions the slightest concentration of impurities switches the transition from first order to second order.
The Cardy-Jacobsen conjecture ($D > 2$) (I).


The models

- **RFIM:** $\mathcal{H} = -J \sum_{<i,j>} s_i s_j - \sum_i h_i s_i - H \sum_i s_i$. $h^2_R$ is the variance of the random fields $\{h_i\}$. (see Natterman and Belanger reviews in *Spin Glasses and Random Fields* (A.P. Young editor)).

- **DAFF:** $\mathcal{H} = +J \sum_{<i,j>} \epsilon_i \epsilon_j s_i s_j - H \sum_i s_i$. (see Fernandez et al. PRB 84, 100408(R) (2011)).

- **Q-states diluted Potts model:** $\mathcal{H} = - \sum_{<i,j>} \epsilon_i \epsilon_j \delta_{s_i, s_j}$. $\epsilon_i = 1$ with probability $p$. In addition $w \propto p$. 
The Cardy-Jacobsen conjecture \((D > 2)\) (II).

CJ mapping in the limit of a strong first order phase transition (FOT)

<table>
<thead>
<tr>
<th>Strong FOT</th>
<th>Random Field</th>
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<tbody>
<tr>
<td>(\Sigma/kT_c)</td>
<td>(J/kT)</td>
</tr>
<tr>
<td>((L/kT_c)w)</td>
<td>(h_{RF}/kT)</td>
</tr>
<tr>
<td>((T - T_c)L)</td>
<td>(HM)</td>
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For the \(Q \gg 1\) diluted Potts Model

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<tbody>
<tr>
<td>(w \log Q)</td>
<td>(h_{RF})</td>
</tr>
<tr>
<td>(\log Q)</td>
<td>(J)</td>
</tr>
<tr>
<td>(t \log Q)</td>
<td>(H)</td>
</tr>
</tbody>
</table>
The critical exponents are:

- \( y_p = y_{h_R/J}^{\text{RFIM}} = \frac{1}{\nu^{\text{RFIM}}} \).
- \( y_T = y_H^{\text{RFIM}} - \theta = \frac{1}{2} (D - \theta + 2 - \eta^{\text{RFIM}}) \).
- The latent heat vanishes with \( \beta^{\text{RFIM}} \).
- The surface tension exponent \( \mu \) is given by \( \mu = D - \theta - 1 \) (modified Widom law).
The Cardy-Jacobsen conjecture \((D > 2)\) (IV).

RG behavior (Cardy & Jacobsen)

Phase diagram

Some previous work:

- Tricritical point. Mercaldo et al. PRE 73, 026126 (2006); Fernandez et al. PRL 100, 57201 (2008).
Simulations Details

Simulations

- We have used the Extended Microcanonical Approach (Martín-Mayor, PRL 98, 137207 (2007)).
- Spin Update: Swendsen-Wang and Metropolis.
- $12 \leq L \leq 64$ and $0.6 \leq p \leq 1$.
- 500 samples on each lattice size.
- $Q = 8$. However we have reanalyzed our old $Q = 4$ data.

Ibercivis Citizen Computer

- Boinc based volunteer platform.
- Stable and open infrastructure.
- Around $10^5$ cores and $2 \times 10^5$ users.
- $3 \times 10^6$ CPU hours [2.4 GHz single CPU].
- More information www.ibercivis.com
We compute $\beta_c^L$ using the Maxwell rule.

In addition:

$$\Delta e = e_d - e_o; \quad \Sigma(L) = \frac{N}{2L^{D-1}} \int e^d_L(\beta_c^L) \, de \left( \langle \hat{\beta} \rangle e - \beta_c^L \right)$$
Behavior of the Maxwell construction ($Q = 8$ and $L = 48$) varying the dilution:
Control Variates

- We want to improve $A$ using its correlations with $B$ (Fernandez et al., PRE 79, 051109 (2009)).

- If $\langle B \rangle = 0$, we can define $\hat{A} \equiv A + \alpha B$, so $\langle \hat{A} \rangle = \langle A \rangle$. But depending on $\alpha$: $\text{var}(\hat{A}) < \text{var}(A)$. The optimal value being:

$$\alpha_{\text{opt}} = \frac{\text{cov}(A, B)}{\sqrt{\text{var}(A)\text{var}(B)}}$$

\[
\begin{align*}
\beta_c' = \beta_c + \alpha (p_i - p), & \quad p_i = N_i/N, \quad p = 0.95 \\
\chi^2/\text{dof} = 5.4/3
\end{align*}
\]
Close to the tricritical point at \((p_t, T_t = T_c(p_t))\)

\[ O(L, p_t + \delta p, T_t + \delta T) = L^x G(L^y u_T, L^y u_p), \]

- \(u_T = f_T(\delta T, \delta p)\) and \(u_p = f_p(\delta T, \delta p)\).

The Maxwell construction enforces \(u_T = 0\) (with accuracy of order \(O(L^{-D})\)), so \(u_p \propto \delta p\).

\[ O(L, p, \text{Maxwell}) = L^x \left( \tilde{G}(L^y(p - p_t)) + O(L^{y_T - D}) \right) . \]

So, the Maxwell construction allows us to employ standard FSS, with an effective scaling-corrections exponent \(\omega = D - y_T\).

Notice that \(u_Q = 1/\log Q\) is irrelevant with exponent \(-\theta\). However, numerically \(\theta \approx \omega\).
The RFIM value of $\theta = 1.469(20)$ has been used.
Fixing $\beta y_p = 0.0119(4)$: $\omega = 1.53(5)(3)$ ($\chi^2$/d.o.f. = 14/15).
Results (III): Testing C-J Conjecture

- From the Latent Heat:
  \[ \beta y_p = 0.0022(48)(3) \text{ and } \omega = 1.36(8)(1). \]
  Fixing \( \beta y_p = 0.0119(4) \):
  \[ \omega = 1.53(5)(3). \]
  \[ y_T = D - \omega \text{ so } y_T = 1.47(8). \] [Mercaldo et al: \( y_T = 1.49(9) \).]

- From the Surface Tension:
  \[ y_p = 0.775(46)(1) \text{ fixing } \omega = 1.36(8)(1). \]
  \[ y_p = 0.779(41)(4) \text{ fixing } \omega = 1.53(5)(3). \]
  \[ \alpha = (2y_p - D + \theta)/y_p = 0.030(10). \]
  By fitting \( \Sigma(L, \rho_t^{L,2L}) = A_Q L^{\theta-2} (1 + B_Q L^{-\omega}) \) using \( \omega = 1.5(1) \) we obtain \( \theta = 1.52(11)(2). \)

- RFIM values:
  \[ \theta = 1.469(20) \text{ and } \beta/\nu = 0.0119(4). \]
  \[ 0.73 \leq 1/\nu \leq 1.12. \]
  \[ y_H - \theta = 1.52(2); \omega = 1.48(2). \]
  Experimentally \( \alpha \simeq 0 \text{ (maybe a log div.).} \)
Conclusions

- We have presented a finite size scaling study of the 3D $Q = 4$ and 8 diluted Potts model.
- We have used the citizen computer IBERCIVIS (www.ibercivis.com) for the equivalent of $3 \times 10^6$ CPU hours.
- We have run the extended microcanonical method.
- By considering leading scaling corrections we have shown that the Universality class for the tricritical point is that of the RFIM such as was predicted by Cardy and Jacobsen.