The Random Ising Ferromagnet in a Transverse Field; the Simplest Model with Quantum Phase Transition

by

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Monte Carlo and Structure Optimization Methods for Biology, Chemistry, and Physics


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What is a quantum Phase Transition?

Quantum mechanics is "irrelevant" for critical phenomena except for $\xi = 0$.
Why are quantum Phase Transitions with disorder poorly understood?

Main reason:
Lack of a perturbative renormalization group, $\varepsilon$-expansion

$\Rightarrow$ Flow to strong coupling

- Probably no upper critical dimension
- Relation to Griffiths-McCoy singularities?

$\Rightarrow$ Numerics (Monte Carlo)
Simplest model

\[ H = - \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z - \sum h_i \sigma_i^z \]

\{ J_{ij}, h_i \} \text{ random.}

\text{n.b. discrete symmetry}

Ising model in a transverse field

We are interested in:

- (quantum) critical behavior
- Griffiths-McCoy singularities away from the critical point.
Dynamical Exponent (criticality)

Have to include dynamics at the start, even to get static exponents

\[ \xi_T \sim \xi^z \]

Pure System Space and time are equivalent so

\[ z = 1 \]

Exponents those of the \((d + 1)\)-dimensional classical model. (Elliott, Pfeuty 1970)

Random System Space and time are not equivalent so

\[ z \neq 1 \]

What is \(z\)?
Griffiths - McCoy Singularities
slow dynamics - gapless

1st understand gap in Pure Model

Let $\Delta = h/J$.

For $\Delta < \Delta_c, m \equiv \langle \sigma_i^z \rangle > 0, \Rightarrow$ Ferromagnet

For $\Delta > \Delta_c, m = 0, \Rightarrow$ Paramagnetic

Energy Gap

If $h = 0$ the two ground states

are degenerate.

For $h < h_c$ there is a tunneling splitting. Size $N$ need $N$-th order perturbation theory. Splitting $\sim (h/J)^N \sim \exp(-cN)$. Hence gap varies as follows:

$\Delta$ is the dynamical exponent.
$\nu$ is the correlation length exponent
Now look at the random case (paramagnetic phase)

Probability \( \sim e^{-\mu V} \) that a point is in a region of volume \( V \) which is "locally in the ferromagnetic phase"

This has a local gap \( \epsilon \sim e^{-cV} \)

Change variables

\[ \Rightarrow \text{density of states (power law)} \]

\[ P(\epsilon) \sim \epsilon^{-1 + \mu/c} \]

write \( \frac{\mu}{c} = \frac{d}{Z'(\Lambda)} \) continuously varying

In a region of size \( V = L^d \)
the lowest energy excitation is

\[ \epsilon_{\text{min}} \sim L^{-1/2'} \] (i.e. gapless)

so \( 2' \) is a (sort of) dynamical exponent

Note: analogy to 2-level systems in glasser
The average on-site, (imaginary) time dependent correlation function at $h_0 = 2$, or $\delta = \frac{1}{2} \ln(2) = 0.347$, in the paramagnetic phase. As expected one has a power law variation. The slope of the fit is $-0.48$. This is $1/z(\delta)$ so we find $z(0.347) = 2.1$. 
The average local susceptibility at $h_0 = \frac{3}{2}$, or $\delta = \frac{3}{2} \ln(2) = 0.549$, in the paramagnetic phase. Notice the clear divergence. The slope is $-0.39$ which gives $\frac{1}{\Delta}(0.549) = 0.61$. 

**Paramagnetic phase (d=1)**
\[ \langle 0^z | (t) 0^z | (0) \rangle \sim \frac{1}{T^d} \int \frac{dz}{z} \]

\[ \xi \sim T^{-1} + \frac{d}{z}, \quad c \sim T^d \frac{d}{z}, \]

Also, \( \xi \) diverges before critical point is reached if \( \xi'(h) > d \).

\( d = 1 \)  

This happens \( \frac{1}{\xi} \).  

Summary for Griffiths-McCoy Singularities

- Always expect correlations to decay with a power of time in a range about critical point.
- May or may not have a divergent \( \xi \) in a range about critical point.
- Like a line of critical points, continuously varying exponent \( \xi' \) as far as time correlations are concerned.
- Effects much less strong for continuous symmetry.
Exact results in $d=1$

- $\lim_{h \to h_c} z'(h) = \infty$
  - Hence $X$ diverges for a range of $h$ about $h_c$ [McCoy]

- $z = \infty$ (at criticality)
  - $\ln T \sim L^\gamma$ ($\nu = \frac{1}{2}$) rather than $\gamma \sim L^z$
    - Activated dynamical scaling

- $C_{av} \sim \frac{1}{\nu} \phi$
  - $C_{typ} \sim \exp[-\text{const} \, \nu^0]$ ($\nu = \frac{1}{2}$)
    - i.e. very broad distributions.

- $C_{av} \sim \exp(-\frac{\nu}{3\nu_{av}})$, $\bar{s}_{av} \sim \bar{s}^{-\nu_{av}}$ ($\nu_{av} = 2$)
  - $C_{typ} \sim \exp(-\frac{\nu}{3\nu_{typ}})$, $\bar{s}_{typ} \sim \bar{s}^{-\nu_{typ}}$ ($\nu_{typ} = 1$)
    - Different exponents for average and typical correlation functions.
slope = -0.38, Prediction \( 2-\phi, \phi = \frac{\sqrt{5}+1}{2} = 1.62 \)

\[ C_{av}(r) \]

\[ r \]

\[ h_0 = 1 \]

\(-d\) AT criticality
- Are these results special to $d=1$?

$\Rightarrow$ Investigate $d=2$ by Monte Carlo

(with C. Pich)

(Also Rieger & Kawashima)

(n.b. Senthil & Sachdev, for the percolation critical point)
Random Ising model in a transverse field

Hamiltonian

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x$$

where $h_i$ is the transverse field.

We took uniform distributions for $h$ and $J$

so that some fields are much smaller than the bonds in their vicinity and some are much bigger than the nearby bonds.

i.e. The disorder is Strong.

n.b. A ferromagnet, not a spin glass.

No frustration
Cluster Algorithm
(for spin system without frustration)

starting from a site draw bonds between parallel spins with probability
\[ p = 1 - e^{-2H} \]

\[ \Rightarrow \text{site-bond model} \]

Flip all spins in a cluster

Statistical weight same for each orientation of spins in cluster. Size of clusters ~ 5!!

weight of bond: \((1-p)e^H\)  \(\rightarrow\) same  \(\rightarrow\) weight of bond \(e^{-H}\)
Classical Model - 2+1 dimensions

Imaginary time \( 0 < \gamma < \beta \)

Time slices, width \( \Delta \gamma \)

- \( \Delta \gamma = 1 \) 3-d Ising model with perfectly correlated disorder
  Wolff algorithm (APY + C. Aich)
  Same universality class as \( \Delta \gamma \to 0 \)
  \( L \gamma = 1/T \)

- \( \Delta \gamma \to 0 \) Exact representation of quantum Hamiltonian
  Continuous imaginary time
  Cluster algorithm (Rieger + Kanashima)
  (cf. Beard + Wiese)

Anisotropic (finite-size) scaling since \( z \neq 1 \)
Improved Estimator for Correlation Functions

Conventionally:
1 if spins parallel
-1 if spins anti-parallel

⇒ variance = 1, if mean small.

Swendsen Wang improved estimator:
1 if spins in same SW cluster
0 otherwise

⇒ variance = mean, if mean small

# of statistically independent measurements for error = mean

Conventionally: \( \sim (\text{mean})^{-2} \)

Improved estimator: \( \sim (\text{mean})^{-1} \)
Advantages of Cluster Algorithms

- Reduces critical slowing down
- Improved estimator for correlation functions
- Deals with a very broad distribution of interactions
- Continuous imaginary time algorithm
Griffiths - McCoy Singularities in 2-d
Continuous imaginary time algorithm

\[ \uparrow d/\varepsilon'(h) \]

[Rieger + Hawashima]
Looks like \( \varepsilon' \to \infty \) \( \Rightarrow h \to h_c \)
(as in 1-d)
Monte Carlo (at criticality)

\[ d = 1, \ T_{cl} = T_c \]

\[ C_{av} (L/2) \]
\[ C_{typ} (L/2) \]

--- slope = -0.54
monte Carlo (at criticality)

$d=1$, $T_{cl}=T_c$

$i.e. \ C_{typ} \sim \exp\[-const. \ \sigma^2]\$

with $\sigma = \frac{1}{2}$ (agrees with exact soln of D. Fisher)
Monte Carlo (at criticality)

$d=2$, $T_{cl}=T_c$

$C_{av}(L/2)$
$C_{typ}(L/2)$

Slope $=-1.95$
Monte Carlo (at criticality)

$d = 2, \ T_{cl} = T_c$

\[ C_{typ} \sim e^{-\text{const.} \sigma / \Delta} \]

with $\sigma \approx \frac{1}{3}$  

[n.b. $\sigma = \frac{1}{2}$ in $d = 1$]
Conclusions

Quantum Phase Transitions with disorder
(discrete symmetry)

- Strong Griffiths-McCoy singularities away from critical point
- Critical Phenomena: distributions very broad—average and typical different — $\tilde{z} = \infty$
- Need experiments
  - magnetic $Li_{1-x} Ho_x YF_4$
  - Ferroelectrics?
  - Heavy fermions?
- Need better theoretical understanding
  
  cf. Motrunich, Mau, Huse, Fisher
  numerical RG