Disorder Effects on Quantum and Classical 1st Order Phase Transitions

Michael Aizenman
Princeton University

Celebrating Giovanni, with deep appreciation ...

Mechanics: Classical, Statistical and Quantum
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Talk outline

Part I - Random Field Ising Model (RFIM)

i. Ground states and Gibbs equilibrium states of the RFIM

ii. Heuristics of the Imry-Ma rounding phenomenon & sketch of the proof (following an earlier work with J. Wehr ‘89/90)

Part II - QPT₁

i. Corresponding questions for Quantum Spin / Particle System

ii. Outline of the proof of the rounding of QPT₁

(joint work with R. Greenblatt and J.L. Lebowitz (PRL ‘09, JMP ‘12)

Part III - Back to RFIM, at its critical dimension

Does the RFIM exhibit a phase transition in D=2 dimensions?

Explain a conjecture [MA] which we are now in the process of disproving.

work in progress with J. Hanson (grad. st.) and L. Geisinger
Part I. The Imry-Ma phenomenon in the context of the RFIM

- It is a known theorem (explained below) that in low dimensional models of statistical mechanics 1st-order phase transitions are unstable with respect to the introduction of arbitrarily weak disorder in the field conjugate to the order parameter.

- This effect of disorder-induced fluctuations occurs regardless of the presence of thermal fluctuations, i.e., is ‘observable’ already at $T = 0$.

- The main conclusion extends to all $T \geq 0$ (although it ceases to be of relevance at high temperatures).

- The rounding effect occurs generally in dimensions $d \leq d_c$, with:
  - $d_c = 4$ for systems with continuous symmetry (in distributional sense)
  - $d_c = 2$ in the more general case (including the discrete-symm.-breaking of the RFIM).

We shall introduce the phenomenon in the context of the Random Field Ising Model, focusing initially on the model’s ground state.
Ground States of the RFIM

For a graph $G$, configurations $\sigma \in \{-1, 1\}^G$, and $\Lambda \subset G$, let:

$$H_\Lambda(\sigma) = \sum_{\{x,y\} \subset G, \text{dist}\{x,y\} = 1} (\sigma_x - \sigma_y)^2 + \sum_{x \in \Lambda, y \in \Lambda^c, \text{dist}\{x,y\} = 1} (\sigma_x - \hat{\sigma}_y)^2 - \sum_x (h + \varepsilon \eta_x)\sigma_x$$

with $\{\eta_x\}_{x \in G}$ - iid Gaussian random variables ($N(0, 1)$), and $h = 0$.

**Def:** $\sigma \in \{-1, 1\}^\Lambda$ is a **ground state config.** for $H_\Lambda$ (with the b.c. $\hat{\sigma}$) if

$$H_\Lambda(F\sigma) - H_\Lambda(\sigma) \geq 0 \quad \text{for all finite flips } F.$$

**Q 1:** With $G = Z^d$, for what dimensions $(d)$ is the $(h = 0)$ ground state **a.s. unique** at arbitrarily small $\varepsilon > 0$?

( Remark: note the **localization / delocalization** aspect of the problem)

**Q 2:** Repeat the question with $\{\sigma\}$ replaced by $O(N)$ spin variables $\{\hat{\sigma}\}$, and the random fields $\{\eta\}$ by $\{\hat{\eta}\}$ – of rotation invariant distribution.

**Q 3:** Ditto, with $\{\hat{\sigma}\}$ replaced by quantum spin variables $\{\hat{S}\}$. 
Heuristics of the Imry - Ma phenomenon

In minimizing $H_\Lambda(\sigma) = \sum_{x,y}(\sigma_x - \sigma_y)^2 - \sum_x(h + \varepsilon \eta_x)\sigma_x$

there is competition between:

1. **the effect of the boundary conditions** –
   ignoring the b.c. raises the energy by $|\partial \Lambda| \approx L^{d-1}

2. **the local potential** –
   its contribution to the energy of a uniform config. is $O(\sqrt{|\Lambda|}) \approx L^{d/2}$

The marginal dimension here is $d_c = 2$:

$$
\begin{align*}
    d > 2 : & \quad (1) \text{ wins } \quad (L^{d-1} \gg L^{d/2}) \\
    d < 2 : & \quad (2) \text{ wins } \quad (L^{d-1} \ll L^{d/2}) 
\end{align*}
$$

In 2D: at each scale the probability that the local field wins is scale independent ...

$\implies$ eventually (2) wins also in that case.

In the presence of continuous symmetry, the b.c. bound is lowered:

$L^{d-1} \implies L^{d-2}$ (soft modes allow easier decoupling from the boundary).
**Thm. 1** (J. Imbrie ‘84): *For $d > 2$ and $\varepsilon$ small enough, at a.e. $\eta$ the infinite-volume ground states corresponding to the (+) and (-) boundary conditions are distinct.*

**Thm. 2** (Aiz.-Wehr ‘89): *For $d \leq 2$ at any $\varepsilon > 0$ the ground state is a.s. unique.*

Remarks (excuse the repetition):

- Both statements were extended to **positive temperature Gibbs states**
  (Theorem 1 by Bric.-Kup. ‘87, and Theorem 2 in A-W ‘89, which applies to all $T \geq 0$).

- Thm. 2 (in its proper gen.) has an extension to systems with **continuous symmetry**
  for which the threshold dim. goes up to $d = 4$ (A-W ‘89).

- Thm. 2 was recently extended also to **quantum systems**
  (Greenblatt-Lebowitz-Aiz.)

- The above works have settled some **lively debates** (see REFs on p.7 and p.14)
  (Imry-Ma, Parisi- Sourlas, and more recent discussions of QPT$_1$).
References


Further Refs - Quantum Phase Transitions (QPT):


Mandelbrot Percolation:


Sketch of the proof of Thm. 2 (A-W)

With \( \Lambda \equiv [-L, L]^d \subset \Gamma \subset \mathbb{Z}^d \), let \( \mathcal{E}_\Gamma^\pm(\epsilon, \eta) := \min_\sigma H_{\Gamma}^{\pm b.c.}(\sigma) \)
and let \( m_\Gamma^\pm(\cdot; \epsilon, \eta) \) denote the minimizing configurations.

A simplifying short-cut (for RFIM) - by an FKG monotonicity argument:

1. for each \( \eta \) the limit exists: \[ m^\pm(x; \epsilon, \eta) := \lim_{\Gamma \to \mathbb{Z}^d} m_\Gamma^\pm(x; \epsilon, \eta) \]
2. \( m^+(\cdot) \geq m^-(\cdot) \), and the ground state is unique if and only if

(order parameter:) \[ b(\epsilon) := \mathbb{E} \left( m^+(x; \epsilon, \cdot) - m^-(x; \epsilon, \cdot) \right) = 0 \quad (\forall x \in \mathbb{Z}^d) \]

To prove Theorem 2 (by contradiction) consider

\[ G_\Lambda(\epsilon, \eta_\Lambda) := \lim_{\Gamma \to \mathbb{Z}^d} \mathbb{E} \left( [\mathcal{E}_\Gamma^+(\epsilon, \eta) - \mathcal{E}_\Gamma^+(\epsilon, \eta|_{\Lambda^c})] - [\mathcal{E}_\Gamma^-(\epsilon, \eta) - \mathcal{E}_\Gamma^-(\epsilon, \eta|_{\Lambda^c})] \mid \eta_\Lambda \right) \]

where \( \eta|_{\Lambda^c} \) denotes \( \eta \) modified to vanish in \( \Lambda \), i.e., \( \eta|_{\Lambda^c} := \eta \text{ I}[\Lambda^c] \).

\( G_\Lambda(\epsilon, \eta_\Lambda) \) represents the contribution of the Random Field within \( \Lambda \) to the difference between the ground state energies of the (+) vss. (−) boundary conditions.
This quantity has the **potentially contradictory properties**:

1. \[ |G_\Lambda(\varepsilon, \eta_\Lambda)| \leq 4 |\partial \Lambda| = C_d \, L^{d-1} \]

2. \[ \frac{\partial}{\partial \eta_x} G_\Lambda(\varepsilon, \eta_\Lambda) = \varepsilon \mathbb{E} \left[ \left( m^+(x; \varepsilon, \eta) - m^-(x; \varepsilon, \eta) \right) | \eta_\Lambda \right] \geq 0 \quad \text{(in a weak sense)} \]

\((m^\pm(x; \varepsilon, \eta))\) are covariant under translations, continuous & piecewise differentiable in \(\eta\)

with: \[ \mathbb{E} \left( \frac{\partial}{\partial \eta_x} G_\Lambda(\varepsilon, \eta_\Lambda) \right) = b(\varepsilon) \equiv \text{our order parameter} \]

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**Proposition** [de-concentration of measure] (Aiz.-Wehr + corr. by Bovier (\(\delta\)))

Under the above conditions (2.), for \(\{\eta_x\}\) iid with finite moments \(\mathbb{E} \left( |\eta\sigma|^{2+\delta} \right) < \infty\):

\[ \lim_{L \to \infty} \mathbb{E} \left( \exp \left\{ \frac{t}{\sqrt{|\Lambda|}} \left[ G_\Lambda(\varepsilon, \eta_\Lambda) - \mathbb{E} (G_\Lambda) \right] \right\} \right) \geq \exp \left\{ t^2 \tilde{b}^2 / 2 \right\} \]

with \(\tilde{b} \neq 0\) whenever \(b(\varepsilon) \neq 0\)

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\[ \Rightarrow \text{For} \quad d/2 \geq d - 1 \quad \text{almost surely} \quad m^+(x; \varepsilon, \eta) = m^-(x; \varepsilon, \eta) \quad \ldots \ldots \]

(i.e. \(d \leq 2\))

Q.E.D. (Thm. 2)
Part II. QPT \(_1\) (joint work with R. Greenblatt and J.L. Lebowitz)

The results presented next apply to quantum systems on homogeneous \(d\) dimensional graphs, such as \(\mathbb{Z}^d\). Associated with each site \(x \in \mathbb{Z}^d\) is a quantum system whose state space is isomorphic to a common finite dimensional Hilbert space \(\mathcal{H}_0\). The local systems are coupled through a Hamiltonian which for a finite region \(\Gamma \subset \mathbb{Z}^d\), with free boundary conditions, takes the form

\[
H^{h,\varepsilon,\eta}_{\Gamma,0} = \sum_{A \subset \Gamma} Q_A + \sum_{x \in \Gamma} (h + \varepsilon \eta_x) \kappa_x
\]

Here \(Q_A\) is an operator which acts on the quantum degrees of freedom in \(A\) (i.e. an operator acting in \(\bigotimes_{x \in A} \mathcal{H}_x\)).

- The interaction is assumed to be translation invariant (\(Q_{T_x A} = U_x^\dagger Q_A U_x\), with \(T_x\) denoting translations on the lattice and \(U_x\) the corresponding unitary operators), and of finite range (i.e., \(Q_A = 0\) for all sets with \(\text{diam } A > R\), at some finite \(R\)).

- **Disorder** enters through the random coefficients \(\eta_x\), whose variance is fixed at 1.

- The terms which \(\eta_x\) multiply are assumed to be of the form \(\kappa_x \equiv U_x^\dagger \kappa_0 U_x\), with \(\kappa_0\) an operator which acts on a finite cluster of sites, whose size may be greater than 1.

- Hamiltonians with other boundary conditions (\(B\)): \(H^{h,\varepsilon,\eta}_{\Gamma,B}\), are defined analogously, in particular the **periodic boundary conditions** (\(B = \text{per}\)) which are our default choice.
Examples
The Quenched Free Energy

The finite volume partition function is

$$Z_{\Gamma,B}(h, \beta, \epsilon; \eta) := \text{Tr} \exp(-\beta H_{\Gamma,B}^{h,\epsilon \eta}),$$

and the corresponding Gibbs state is

$$\langle \ldots \rangle_{\Gamma,B}^{h,\beta,\epsilon}(\eta) := \frac{\text{Tr} \left( \ldots e^{-\beta H_{\Gamma,B}^{h,\eta}} \right)}{Z_{\Gamma,B}(h, \beta, \epsilon; \eta)}.$$

When deemed obvious from the context, some of the subscripts may be omitted.

The free energy for a finite system is

$$F_{\Gamma,B}(h, \beta, \epsilon; \eta) := \frac{-1}{\beta} \log Z_{\Gamma}(h, \beta, \epsilon; \eta),$$

In particular, for square domains $\Gamma_K = [-K, K]^d \cap \mathbb{Z}^d$ with the periodic b.c., we denote

$$F_{K}^{h}(\eta) \equiv F_{\Gamma_K,\text{per}}(h, \beta, \epsilon; \eta).$$

The free energy density, per unit volume, is

$$\mathcal{F}_{\Gamma,B}(h, \beta, \epsilon; \eta) := \frac{F_{\Gamma,B}(h, \beta, \epsilon; \eta)}{|\Gamma|}.$$
‘Self averaging’ for the quenched free energy density

**Proposition 1.** If $\eta$ form a translation invariant and ergodic process, then for any $\beta \in [0, \infty]$ there is a full measure set $\mathcal{N}$ of field configurations for which

$$F(h, \beta, \epsilon) := \lim_{L \to \infty} F_{\Gamma_L, B}(h, \beta, \epsilon; \eta)$$

exists for all $h$ and is independent of $\eta$ and the boundary conditions $B$.

- $F(h, \beta, \epsilon)$ is concave in $h$.

- $\beta = \infty$ corresponds to the ground state energy: for almost every $\eta$ the limit

$$F(h, \infty, \epsilon) := \lim_{\beta \to \infty} F(h, \beta, \epsilon)$$

exists and is equal to the limit of the energy densities of the finite volume ground states of the random Hamiltonian (whose value is independent of the boundary conditions). I.e., for the free energy the limits $\beta \to \infty$ and $L \to \infty$ are interchangeable.

- The uniqueness of the free energy density does not extend to uniqueness of the Gibbs states, or ground states in case $\beta = \infty$. The question which our results address is whether the different Gibbs states (or ground states) of the given Hamiltonian can differ in their mean magnetization, that is in the volume averages of $\langle \kappa_x \rangle$. 

Two related perspectives

- **Thermodynamics**: a 1st order phase transition is associated with the discontinuity of the first derivative of the free energy with respect to one of its parameters. By default, this parameter will be denoted here by \( h \).

- **Stat. Mech manifestation**: 1st order phase transition is expressed in the non-uniqueness, among the infinite volume Gibbs equilibrium states, of the bulk density of some extensive quantity.

Our discussion concerns the case when the quantity in question is the one \( \kappa_x \) whose coupling parameter in \( H \) is the field \( h \) which is randomized by the disorder.
The general results - thermodynamic statement

**Theorem 3** Assuming the variables \( \eta_x \) are i.i.d. with abs. cont. distribution and finite \((2+\delta)\) moments for any such system in dimension \( d \leq 2 \) the quenched free energy density \( \mathcal{F} \) is differentiable in \( h \) at all \( h, \epsilon \neq 0, \) and \( \beta \leq \infty \).

For \( \beta < \infty \), the abs. cont. assumption can be relaxed, requiring instead that the distribution of \( \eta \) has no isolated point masses, or alternatively that the system satisfies the weak FKG property with respect to \( \kappa \).

**Theorem 4** For such systems with \( H_0 \) having the **continuous symmetry** (of rotations in the spin state space) and the random terms being iid with rotation invariant distribution, the quenched free energy density \( \mathcal{F} \) is differentiable in \( \vec{h} \) at \( \vec{h} = \vec{0} \) (for any \( \epsilon \neq 0 \) and \( \beta \leq \infty \)) in all dimensions \( d \leq 4 \).
Differentiability of $\mathcal{F}$ means No Long Range Order

The basis of the Thermo $\Leftrightarrow$ Stat Mech connection is the relation

$$\frac{\partial \mathcal{F}_\Gamma^h}{\partial h} = \langle \bar{\kappa}_\Gamma \rangle^h_{\Gamma,B}(\eta).$$

Convexity arguments then imply:

**Proposition 2.** Under the assumptions of Proposition 1, for any set of the parameters $(\beta, h, \varepsilon)$ at which $\mathcal{F}$ is differentiable in $h$,

$$\lim_{L \to \infty} \left\langle \frac{1}{|\Gamma_L|} \sum_{x \in \Gamma_L} \kappa_x \right\rangle^h_{\Gamma_L, B}(\eta) = \frac{\partial \mathcal{F}}{\partial h} \quad (\ast)$$

for a.e. realization of the disorder $\eta$, and any choice of the boundary conditions $B$.

Furthermore, also:

$$\lim_{K \geq L \to \infty} \langle \bar{\kappa}_{\Gamma_L} \rangle^h_{\Gamma_K, B}(\eta) = \frac{\partial \mathcal{F}}{\partial h}.$$
Elements of the proof

(lesson: keep to thermodynamics, do not probe the states [no ‘metastases’] )

- The proof utilized Thermodynamic bounds on the free energy ‘second difference’ (in the field $h$, and disorder $\eta_L$):

$$\hat{G}_{\Lambda,K}^\delta(\eta_\Lambda) := \mathbb{E} \left( \left( F_K^{h+\delta}(\eta) - F_K^{h+\delta}(\eta_{\Lambda^c}) \right) - \left( F_K^{h-\delta}(\eta) - F_K^{h-\delta}(\eta_{\Lambda^c}) \right) \right) \bigg| \eta_\Lambda$$

where $\mathbb{E}(\cdot|\eta_\Lambda)$ is the conditional average over the random terms outside $\Lambda$, and $F_K$ refers to the free energy with the periodic boundary conditions (this choice of b.c. assures translation covariance, which is used in the argument).

- The quantum version of $G_L(\eta_\Lambda)$ is constructed with the double limit

$$\lim_{\delta \downarrow 0} \lim_{K \to \infty} \hat{G}_{L,K}^\delta(\eta_L)$$

which is proven to exists ($\forall \eta_\Lambda$). This quantity has the properties we desire of $G_L(\eta_L)$

- The basic estimate which allows to extend the classical analysis is:

$$\left| \log \text{Tr} \ e^C - \log \text{Tr} \ e^D \right| \leq \|C - D\|$$

(for pairs of Hermitian matrices $C, D$ of the same finite size)
Part III. A Puzzle concerning Phase Transition in two dimensions

Thm. 2 implies that for \( d = 2 \), at a.e. \( \eta \), and any fixed \( x \in \mathbb{G} \):

\[
\Delta m_L(x; \varepsilon, \eta) := m^+_L(x; \varepsilon, \eta) - m^-_L(x; \varepsilon, \eta) \rightarrow 0 \quad \text{as } L \rightarrow \infty.
\]  

(1)

**Q 2:** At what rate does \( \mathbb{E}(\Delta m_L(0; \varepsilon)) \) decay?

An easy observation (via a percolation argument): at sufficiently high \( \varepsilon \)

\[
\mathbb{E}(\Delta m_L(0; \varepsilon)) \leq A e^{-\mu L}.
\]

**Previously conjectured (MA):** For the 2D RFIM, there exists \( \varepsilon_0 > 0 \) such that for all \( \varepsilon < \varepsilon_0 \):

\[
\mathbb{E}(\Delta m_L(0; \varepsilon)) \geq \frac{C}{L^\alpha},
\]

with \( \alpha \equiv \alpha(\varepsilon) \leq 1 \).

We now think (and are in the process of proving) that this is incorrect, and exponential decay occurs at arbitrarily small \( \varepsilon > 0 \) (joint work with J. Hanson, and L. Geisinger).
Mandelbrot percolation (‘74) - as an allegory for boundary sensitivity

Dyadic blocks removed independently, with probability \((1 - p)\), regardless of the scale

\[ p = 0.707 \]

\[ p = 0.888 \]

Theorem (CCD) In any \(d > 1\), the model has thresholds \(0 < p_1 < p_2 < 1\)

for \textit{survival} (at \(p > p_1\)) and for \textit{percolation} (at \(p \geq p_2\)).

Q: Does influence propagation in the 2D RFIM resemble at low \(\varepsilon\) such fractal Swiss cheese?

(A renormalization argument now says NO)  

Grazie Giovanni for inspiration!
Thank you for your attention!
A puzzling gap in the theory of quantum fluctuations

Of particular relevance for us is the conclusion that when $\mathcal{F}$ is differentiable there is only one possible limit for the mean value of the volume averaged quantity:

$$\lim_{L \to \infty} \left\langle \frac{1}{|\Gamma_L|} \sum_{x \in \Gamma_L} \kappa_x \right\rangle^h_{\Gamma_L,B} (\eta) = \frac{\partial \mathcal{F}}{\partial h}$$

which by Proposition 1 is independent of the boundary conditions.

For classical systems more can be said: if $\mathcal{F}$ is differentiable not only do the Gibbs state averages of $\bar{\kappa}_\Gamma$ converge, but the distribution of this quantity with respect to the Gibbs state collapses onto a point (in the limit $\Lambda \nearrow Z^d$).

Such a stronger statement concerning quantum fluctuations is not known to be true. Nevertheless, Equation (*) holds also for the quantum systems.