Layered systems at mean field criticality

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Motivation

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In spite of its success, the topic remained "quiet" for a while.

Important developments in the 90s:

- Interesting mathematical ideas - coarse graining, mesoscopic description, variational problems

- Precise description before the mean field limit
Cassandro, Presutti (1996), Bovier, Zahradnik (1997)

- Progress towards the study of phase transitions in the continuum
Lebowitz, Mazel, Presutti (1999)

Framework

System of ± 1 Ising spins on the lattice $\mathbb{Z} \times \mathbb{Z}$: $\{\sigma(x,i)\}$

- On each horizontal line $\{(x,i), x \in \mathbb{Z}\}$, we have a ferromagnetic Kac interaction:

$$-\frac{1}{2} J_\gamma(x,y)\sigma(x,i)\sigma(y,i),$$

$J_\gamma(x,y) = c_\gamma \gamma J(\gamma(x-y))$,

where $J(\cdot) \geq 0$ symmetric, smooth, compact support, $\int J(r)dr = 1$, $J(0) > 0$.

$\gamma > 0$ (scale parameter)

c_γ is the normalizing constant: $\sum_{y \neq x} J_\gamma(x,y) = 1$, for all x

Fix the inverse temperature at the mean field critical value $\beta = 1$:

Also in the Lebowitz-Penrose limit no phase transition is present

- Add a small nearest neighbor vertical interaction

$$-\epsilon\ \sigma(x,i)\sigma(x,i+1).$$

Question: Does it lead to phase transition?

Theorem 1

Given any $\epsilon > 0$, for any $\gamma > 0$ small enough $\mu_\gamma^+ \neq \mu_\gamma^-$, $\mu_\gamma^\pm$ the plus-minus DLR measures defined as the thermodynamic limits of the Gibbs measures with plus, respectively minus, boundary conditions.

A few comments or questions:

- When $\beta > 1$ a version of this theorem holds for $\epsilon = \gamma^A$ for any $A > 0$.

- The model goes back to a system of hard-rods proposed by Kac-Helfand (1960s)

- Related to a one-dimensional quantum spin model with transverse field.
(Aizenman, Klein, Newman (1993); Ioffe, Levit (2012))

- Highly anisotropic interactions in nature: graphite. Multilayered graphene

- What if we take $\epsilon(\gamma) \to 0$?

- If $\epsilon(\gamma) = \kappa\gamma^b$, for which b do we see a change of behavior in κ?

- Phase diagram in the limit $\gamma \to 0$?

Outline:

• Study the Gibbs measures for a "chessboard" Hamiltonian $H_{\gamma,\epsilon}$: some vertical interactions are removed.

• For $H_{\gamma,\epsilon}$ we have a two dimensional system with pair of long segments of parallel layers interacting vertically within the pair (but not with the outside) plus horizontal Kac.

• Preliminary step: look at the mean field free energy function of two layers and its minimizers; exploit the spontaneuous magnetization that emerges.

• This spontaneous magnetization used for the definition of contours (as in the analysis of the one dimensional Kac interactions below the mean field critical temperature).

• For the chessboard Hamiltonian, and after a proper coarse graining procedure, we are able to implement the Lebowitz-Penrose procedure and to study the corresponding free energy functional

• Peierls bounds (Theorem 2) for the weight of contours is transformed in variational problems for the free energy functional.

Coarse grained description and contours Length scales and accuracy:

$$\gamma^{-1/2}, \quad \ell_\pm = \gamma^{-(1\pm\alpha)}, \quad \zeta = \gamma^{a}, \qquad 1 \gg \alpha \gg a > 0.$$

$\gamma^{-1/2}$ • to implement coarse graining - procedure to define free energy functionals

ζ, ℓ_- and ℓ_+ • to define, at the spin level, the *plus/ minus* regions and then the contours

Partition each layer into intervals of suitable lengths $\ell \in \{2^n,\ n \in \mathbb{Z}\}$.

$$C_x^{\ell,i} = C_x^{\ell} \times \{i\} := ([k\ell, (k+1)\ell) \cap \mathbb{Z}) \times \{i\},\ \text{where } k = \lfloor x/\ell \rfloor$$

$\mathcal{D}^{\ell,i} = \{C_{k\ell}^{\ell,i}, k \in \mathbb{Z}\}$

empirical magnetization on a scale ℓ in the layer i

$$\sigma^{(\ell)}(x,i) := \frac{1}{\ell} \sum_{y \in C_x^{\ell}} \sigma(y,i).$$

To simplify notation take γ in $\{2^{-n}, n \in \mathbb{N}\}$. We also take $\gamma^{-\alpha}$, $\ell_\pm$ in $\{2^n, n \in \mathbb{N}_+\}$

• The "chessboard" Hamiltonian:

$$H_{\gamma,\epsilon} = -\frac{1}{2}\sum_{x\neq y,i} J_\gamma(x,y)\sigma(x,i)\sigma(y,i) - \epsilon\sum_{x,i}\chi_{i,x}\sigma(x,i)\sigma(x,i+1),$$

where

$$\chi_{x,i} = \begin{cases} 1 & \text{if } \lfloor x/\ell_+ \rfloor + i \text{ is even,} \\ 0 & \text{otherwise.} \end{cases}$$

If $\chi_{x,i} = 1$, we say that (x,i) and $(x,i+1)$ interact vertically; $v_{x,i}$ the site (x,j) which interacts vertically with (x,i).

• Theorem 1 will follow once we prove that the magnetization in the plus state of the chessboard Hamiltonian is strictly positive (by the GKS correlation inequalities).

• For $H_{\gamma,\epsilon}$ we detect a spontaneous magnetization $m_\epsilon > 0$ in the limit $\gamma \to 0$.
We use m_ϵ to define contours.

Natural guess for m_ϵ: minimizers of "mean field free energy function" of two layers.

(i) First take two layers of ± 1 spins whose unique interaction is the n.n.vertical one. (a system of independent pairs of spins)

- $\hat{\phi}_\epsilon(m_1, m_2)$ the limit free energy (as the number of pairs tends to infinity).

Proposition 1. $X_n = \{-1, 1\}^n$. For $i = 1, 2$, let $m_i \in \{-1 + \frac{2j}{n} \colon j = 1, \ldots, n-1\}$ and

$$Z_{\epsilon,n}(m_1, m_2) = \sum_{(\sigma_1,\sigma_2)\in X_n\times X_n} \mathbf{1}_{\{\sum_{x=1}^n \sigma_i(x) = nm_i \; i=1,2\}} e^{\epsilon \sum_{x=1}^n \sigma_1(x)\sigma_2(x)}.$$

There is a continuous and convex function $\hat{\phi}_\epsilon$ defined on $[-1, 1] \times [-1, 1]$, with bounded derivatives on each $[-r, r] \times [-r, r]$ for $|r| < 1$, and a constant $c > 0$ so that

$$-\hat{\phi}_\epsilon(m_1, m_2) - c\frac{\log n}{n} \leq \frac{1}{n} \log Z_{\epsilon,n}(m_1, m_2) \leq -\hat{\phi}_\epsilon(m_1, m_2).$$

(ii) Mean field free energy for two layers (reference in the L-P context):

- $\hat{f}_\epsilon(m_1, m_2) := -\frac{1}{2}\Big(m_1^2 + m_2^2\Big) + \hat{\phi}_\epsilon(m_1, m_2)$

Proposition 2. For any $\epsilon > 0$ small enough $\hat{f}_\epsilon(m_1, m_2)$ has two minimizers: $\pm m^{(\epsilon)} := \pm(m_\epsilon, m_\epsilon)$ and there is a constant $c > 0$ so that

$$|m_\epsilon - \sqrt{3\epsilon}| \leq c\epsilon^{3/2}.$$

Moreover, calling $\hat{f}_{\epsilon,\mathrm{eq}}$ the minimum of $\hat{f}_\epsilon(m)$, for any $\zeta > 0$ small enough:

$$\Big|\hat{f}_\epsilon(m) - \hat{f}_{\epsilon,\mathrm{eq}}\Big| \geq c\zeta^2, \quad \text{for all } m \text{ such that } \|m - m^{(\epsilon)}\| \wedge \|m + m^{(\epsilon)}\| \geq \zeta.$$

Partition $\mathbb{Z}^2$ into rectangles $\{Q_\gamma(k,j)\colon\, k,j \in \mathbb{Z}\}$, where

$$Q_\gamma(k,j) = \Big([k\ell_+, (k+1)\ell_+) \times [j\gamma^{-\alpha}, (j+1)\gamma^{-\alpha})\Big) \cap \mathbb{Z}^2 \text{ if } k \text{ is even}$$

$$Q_\gamma(k,j) = \Big([k\ell_+, (k+1)\ell_+) \times (j\gamma^{-\alpha}, (j+1)\gamma^{-\alpha}]\Big) \cap \mathbb{Z}^2 \text{ if } k \text{ is odd.}$$

Sometimes write $Q_{x,i} = Q_\gamma(k,j)$ if $(x,i) \in Q_\gamma(k,j)$.

Important features

- Spins in $Q_{x,i}$ do not interact vertically with the spins outside, i.e. $v_{x,i} \in Q_{x,i}$ for all (x,i).
- The $Q_\gamma(k,j)$ are squares if lengths are measured in interaction length units.
- The size of the rectangles in interaction length units diverges as $\gamma \to 0$.

The random variables $\eta(x,i)$, $\theta(x,i)$ and $\Theta(x,i)$ are then defined as follows:

- $\eta(x,i) = \pm 1$ if $\left|\sigma^{(\ell-)}(x,i) \mp m_\epsilon\right| \le \zeta$;
  $\eta(x,i) = 0$ otherwise.
- $\theta(x,i) = 1$, $[= -1]$, if $\eta(y,j) = 1$, $[= -1]$, for all $(y,j) \in Q_{x,i}$;
  $\theta(x,i) = 0$ otherwise.
- $\Theta(x,i) = 1$, $[= -1]$, if $\eta(y,j) = 1$, $[= -1]$,
  for all $(y,j) \in \cup_{u,v \in \{-1,0,1\}} Q_\gamma(k+u, j+v)$, block 3×3 of Q-rectangles
  with (k,j) determined by $Q_{x,i} = Q_\gamma(k,j)$.

plus phase: union of all the rectangles $Q_{x,i}$ s.t. $\Theta(x,i) = 1$,
minus phase: union of those where $\Theta(x,i) = -1$,
undetermined phase the rest.

$Q_\gamma(k,j)$ and $Q_\gamma(k',j')$ connected if (k,j) and (k',j') are $*$–connected,
i.e. $|k-k'| \vee |j-j'| \le 1$.

By choosing suitable boundary conditions: $\Theta = 1$ outside of a compact ($\Theta = -1$ recovered via spin flip).

Given such a σ, *contours* are the pairs $\Gamma = (\mathrm{sp}(\Gamma), \eta_\Gamma)$, where
$\mathrm{sp}(\Gamma)$ a maximal connected component of the undetermined region,
η_Γ the restriction of η to $\mathrm{sp}(\Gamma)$

Geometry of contours

$\mathrm{ext}(\Gamma)$ the maximal unbounded connected component of the complement of $\mathrm{sp}(\Gamma)$

$\partial_{\mathrm{out}}(\Gamma)$ the union of the rectangles in $\mathrm{ext}(\Gamma)$ which are connected to $\mathrm{sp}(\Gamma)$.

$\partial_{\mathrm{in}}(\Gamma)$ the union of the rectangles in $\mathrm{sp}(\Gamma)$ which are connected to $\mathrm{ext}(\Gamma)$.

- Θ is constant and different from 0 on $\partial_{\mathrm{out}}(\Gamma)$
- Γ is plus if $\Theta = 1$ on $\partial_{\mathrm{out}}(\Gamma)$; $\eta = 1$ on $\partial_{\mathrm{in}}(\Gamma)$. Analogously for minus contours.

$\mathrm{int}_k(\Gamma), k = 1, \ldots, k_\Gamma$ the bounded maximal connected components (if any) of the complement of $\mathrm{sp}(\Gamma)$,

$\partial_{\mathrm{in},k}(\Gamma)$ the union of all rectangles in $\mathrm{sp}(\Gamma)$ which are connected to $\mathrm{int}_k(\Gamma)$.

$\partial_{\mathrm{out},k}(\Gamma)$ is the union of all the rectangles in $\mathrm{int}_k(\Gamma)$ which are connected to $\mathrm{sp}(\Gamma)$.

- Θ is constant and different from 0 on each $\partial_{\mathrm{out},k}(\Gamma)$; write $\partial^{\pm}_{\mathrm{out},k}(\Gamma)$, $\mathrm{int}^{\pm}_k(\Gamma)$, $\partial^{\pm}_{\mathrm{in},k}(\Gamma)$ if $\Theta = \pm 1$ on the former; observe $\eta = \pm 1$ on $\partial^{\pm}_{\mathrm{in},k}(\Gamma)$, resp.

$$c(\Gamma) = \mathrm{sp}(\Gamma) \cup \bigcup_k \mathrm{int}_k(\Gamma).$$

Diluted Gibbs measures Let Λ be a bounded region which is an union of Q-rectangles. $\bar{\sigma}$ external condition s.t. $\eta = 1$ in $\partial_{\mathrm{out}}(\Lambda)$

Θ computed on $(\sigma_\Lambda, \bar{\sigma})$; $\partial_{\mathrm{in}}(\Lambda)$ union of all Q-rectangles in Λ connected to Λ^c.

The plus diluted Gibbs measure (with boundary conditions $\bar{\sigma}$):

$$\mu^{+}_{\Lambda,\bar{\sigma}}(\sigma_\Lambda) = \frac{e^{-H_{\gamma,\epsilon}(\sigma_\Lambda|\bar{\sigma})}}{Z^{+}_{\Lambda,\bar{\sigma}}} \mathbf{1}_{\{\Theta=1 \text{ on } \partial_{\mathrm{in}}(\Lambda)\}}.$$

where

$$Z^{+}_{\Lambda,\bar{\sigma}} = \sum_{\sigma_\Lambda} \mathbf{1}_{\{\Theta=1 \text{ on } \partial_{\mathrm{in}}(\Lambda)\}} e^{-H_{\gamma,\epsilon}(\sigma_\Lambda|\bar{\sigma})} =: Z_{\Lambda,\bar{\sigma}}(\Theta = 1 \text{ on } \partial_{\mathrm{in}}(\Lambda)),$$

Minus diluted Gibbs measure defined analogously.

Peierls estimates for the plus and minus diluted Gibbs measures

$$W_\Gamma(\bar\sigma) := \frac{Z_{c(\Gamma);\bar\sigma}(\eta = \eta_\Gamma \text{ on } \mathrm{sp}(\Gamma); \Theta = \pm 1 \text{ on each } \partial^{\pm}_{\mathrm{out},k}(\Gamma))}{Z_{c(\Gamma);\bar\sigma}(\Theta = 1 \text{ on } \mathrm{sp}(\Gamma) \text{ and on each } \partial^{\pm}_{\mathrm{out,k}}(\Gamma)\})},$$

where $Z_{\Lambda,\bar\sigma}(\mathcal{A})$ is the partition function in Λ with Hamiltonian $H_{\gamma,\epsilon}$, with boundary conditions $\bar\sigma$ and constraint $\mathcal{A}$.

Theorem 2 (Peierls bound)

There are $c > 0$, $\epsilon_0 > 0$ and $\gamma_\cdot : (0,\infty) \to (0,\infty)$ so that for any $0 < \epsilon \le \epsilon_0$, $0 < \gamma \le \gamma_\epsilon$ and any contour Γ with boundary spins $\bar\sigma$

$$W_\Gamma(\bar\sigma) \le e^{-c|\mathrm{sp}(\Gamma)|\gamma^{2a+4\alpha}}.$$

• Theorem 1 for the chessboard Hamiltonian follows easily from the Peierls bound (along the lines of the usual proof for n.n. Ising at low temperatures:)

Sketch

Let $\{\Lambda_n\} \nearrow \mathbb{Z}^2$ an increasing sequence of bounded Q-measurable regions

For γ small enough and all boundary conditions $\bar{\sigma}$ such that $\eta = 1$ on $\partial_{\text{out}}(\Lambda_n)$, one gets, by simple counting: (recall $a << 1$ and $\alpha << 1$)

$$\mu^+_{\Lambda_n,\bar{\sigma}}\Big[\Theta(0) < 1\Big] \leq \sum_{D \ni 0} |D| e^{-\frac{c}{2}|D|\gamma^{-1+2a+2\alpha}}$$

the sum over all connected regions D made of unit cubes with vertices in $\mathbb{Z}^2$, and

the sum vanishes in the limit $\gamma \to 0$.

• By the spin flip symmetry: there are at least two DLR measures.

• By ferromagnetic inequalities: $\mu^+_\gamma \neq \mu^-_\gamma$ in Theorem 1.

Reduction of Peierls bounds to a variational problem

- A Lebowitz-Penrose theorem for the spin model corresponding to $H_{\gamma,\epsilon}$.

(coarse graining procedure / free energy functional)

$$Z_{\Lambda,\bar{\sigma}}(\mathcal{A}) := \sum_{\sigma_\Lambda \in \mathcal{A}} e^{-H_{\gamma,\epsilon}(\sigma_\Lambda \,|\, \bar{\sigma})},$$

where $\bar{\sigma}$ is a spin configuration in the complement of Λ and $\mathcal{A}$ is a set of configurations in Λ defined in terms of the values of η_Λ.

- Coarse-grain on the scale $\gamma^{-1/2}$.

$M_{\gamma^{-1/2}}$ the possible values of the empirical magnetizations $\sigma^{(\gamma^{-1/2})}$, i.e.

$$M_{\gamma^{-1/2}} = \{-1, -1 + 2\gamma^{1/2}, ..., 1 - 2\gamma^{1/2}, 1\}$$

and

$$\mathcal{M}_\Lambda := \{m(\cdot) \in (M_{\gamma^{-1/2}})^\Lambda : \; m(\cdot) \text{ is constant on each } C^{\gamma^{-1/2},i} \subseteq \Lambda\}.$$

The free energy functional (on Λ with boundary conditions $\bar{m}$) defined on $[-1,1]^{\Lambda}$

$$\begin{aligned} F_{\Lambda,\gamma}(m|\bar{m}) &= \frac{1}{2}\sum_{(x,i)\in\Lambda} \hat{\phi}_\epsilon(m(x,i), m(v_{x,i})) \\ &- \frac{1}{2}\sum_{(x,i)\neq(y,i)\in\Lambda} J_\gamma(x,y)m(x,i)m(y,i) \\ &- \sum_{(x,i)\in\Lambda,\ (y,i)\notin\Lambda} J_\gamma(x,y)m(x,i)\bar{m}(y,i), \end{aligned}$$

Recall: $v_{x,i} \in \Lambda$ for each $(x,i) \in \Lambda$ since there are no vertical interactions between a Q–rectangle and the outside.

Theorem 3. There is a constant c so that

$$\log Z_\Lambda(\bar{\sigma};\mathcal{A}) \leq -\inf_{m\in\mathcal{M}_\Lambda\cap\mathcal{A}} F_{\Lambda,\gamma}(m|\bar{m}) + c|\Lambda|\gamma^{1/2}\log\gamma^{-1},$$

where $\bar{m}(x,i) = \bar{\sigma}^{\gamma^{-1/2}}(x,i)$, $(x,i) \notin \Lambda$. Moreover, for any $m \in \mathcal{M}_\Lambda \cap \mathcal{A}$

$$\log Z_\Lambda(\bar{\sigma};\mathcal{A}) \geq -F_{\Lambda,\gamma}(m|\bar{m}) - c|\Lambda|\gamma^{1/2}\log\gamma^{-1}.$$

Of course in the upper bound can replace $\mathcal{M}_\Lambda$ by $[-1,1]^{\Lambda}$.

Peierls bound. Sketch of the proof.

Upper bound for the numerator: must show that the excess free energy due to the constraint on $\eta = \eta_\Gamma$ is much larger than the error terms in Theorem 3.

• Important: to show that can restrict to infimum over smooth functions
i.e. $|m(x,i) - m^{\ell -}(x,i)| < c\gamma^\alpha$ far from the boundary of $\mathrm{sp}(\Gamma)$.
$\Delta_0 = \mathrm{sp}(\Gamma)$ minus internal boundaries

$$\inf_{m \in [-1,1]^\Lambda \cap \mathcal{A}} F_{\mathrm{sp}(\Gamma),\gamma}(m|\bar m) \quad \geq \quad \Phi_{\Delta_0} + \Phi_{\Delta_{\mathrm{in}}}(\bar m_{\sigma_{\mathrm{ext}}}) + \sum_k \Phi^+_{\Delta_k^+}(\bar m_{\sigma_{I_k^+}}) + \sum_k \Phi^-_{\Delta_k^-}(\bar m_{\sigma_{I_k^-}}),$$

where

$$\Phi_{\Delta_0} = \inf\left\{ F^*_{\Delta_0,\gamma}(m) \;\middle|\; m \in [-1,1]^{\Delta_0}, |m - m^{(\ell_-)}| \leq c\gamma^\alpha,\ \eta(\cdot;m) = \eta_\Gamma(\cdot), \right\}$$

and

$$F^*_{\Delta_0,\gamma}(m) \quad = \quad \sum_{(x,i)\in\Delta_0} \{-\frac{1}{2}m(x,i)^2 + \frac{1}{2}\hat\phi_\epsilon(m(x,i), m(v_{x,i}))\} + \frac{1}{4} \sum_{(x,i)\neq(y,i)\in\Delta_0} J_\gamma(x,y)(m(x,i) - m(y,i))^2, \quad (I)$$

We omit any details about the other terms (boundaries).

Will get the following upper bound for the numerator in the Peierls weight:

$$\begin{aligned} & Z_{c(\Gamma);\bar{\sigma}}(\eta = \eta_\Gamma \text{ on } \mathrm{sp}(\Gamma); \Theta = \pm 1 \text{ on each } \partial^{\pm}_{\mathrm{out},k}(\Gamma)) \\ \leq \quad & e^{-\Phi_{\Delta_0} + c|\Lambda|\gamma^{1/2}\log\gamma^{-1}} \\ \times \quad & e^{-\Phi_{\Delta_{\mathrm{in}}}(\bar{m}\sigma_{\mathrm{ext}})} \{\prod Z^+(I_k^+)\}\{\prod Z^+(I_k^-)\}. \end{aligned}$$

- spin flip symmetry was used here!

Key point: lower bound on Φ_{Δ_0} (follows from Proposition 2).

$$\Phi_{\Delta_0} \geq \hat{f}_{\epsilon,\mathrm{eq}} \frac{|\Delta_0|}{2} + c \frac{|\Delta_0|}{\gamma^{-(1+\alpha)}\gamma^{-\alpha}} \gamma^{-(1-\alpha)} \min\{\gamma^{\alpha}; \gamma^{2a}\}.$$

(two basic situations contribute here in each Q in Δ_0 (or a neighbor): at least one vertical pair, or a change of sign in the same layer - in η)

• For the lower bound on the denominator of the Peierls weight:

By computing the free energy functional on a suitable test function m on $\mathrm{sp}(\Gamma)$ we get:

(need to take care about a term as the last one on the r.h.s. of (I) but with $(x,i) \in \Delta_0$, $(y,i) \notin \Delta_0$)

$$\begin{aligned} & Z_{c(\Gamma);\bar{\sigma}}(\eta = 1 \text{ on } \mathrm{sp}(\Gamma); \Theta = \pm 1 \text{ on each } \partial_k^{\pm}(\Gamma)) \\ \geq \quad & e^{-\hat{f}_{\epsilon,\mathrm{eq}}\frac{|\Delta_0|}{2} - c(|\mathrm{sp}(\Gamma)|\gamma^{1/2}} \\ \times \quad & e^{-\Phi_{\Delta_{\mathrm{in}}}(\bar{m}\sigma_{\mathrm{ext}})} \{\prod Z^+(I_k^+)\}\{\prod Z^+(I_k^-)\}. \end{aligned}$$

The comparison of upper and lower bounds gives Theorem 2.

Final comments

- A "Lebowitz-Penrose theorem" for the original system.

  (Cassandro, Colangeli, Presutti - preprint - few days ago - in arXiv)

- Can get a better approximation for the spontaneous magnetization?

- phase diagram ?

- Can extend to the system of hard rods?

References

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THANKS