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Magnetization fluctuations in a ferromagnet with mean-field interactions on a slab

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Abstract. The spin probability distribution at equilibrium in a multicomponent mean-field model of a ferromagnetic slab made of N rows is considered. Everywhere, but at the critical point, the spin fluctuations converge, as the number of spins per row tends to ∞, to Gaussians with covariance equal to the thermodynamic susceptibility matrix. At criticality, abnormal coherent fluctuations along the positive eigenvector of the interaction matrix are found, whose limit distribution is an $\exp(-x^4)$ law.

1. Introduction

An important problem in equilibrium statistical mechanics is to determine how macroscopic observables are distributed around their mean values. This is especially interesting when the equilibrium state is non-homogeneous, e.g. due to a free surface, in which case a local study is necessary. Unfortunately, the control of non-trivial (interacting) systems is quite difficult, in that it requires limit theorems for sums of (strongly) dependent random variables, and rigorous results in this area are scarce. Notable exceptions are mean-field type models. The Curie–Weiss model of a homogeneous ferromagnet has been studied by Ellis and Newman (1978a, b) using large-deviation techniques. The same method worked for a similar model, which had large-scale non-homogeneities: the circle model (Ellis and Rosen 1982). The monograph by Ellis (1985) contains a fair description of the subject.

In this paper we consider the spin probability distribution in a mean-field-type model with sharp non-homogeneities: the ferromagnetic slab. The model is defined as follows.

Consider a rectangular array of N rows, labelled by $i=1,\ldots,N$, and M columns, $\mu=1,\ldots,M$, of 'spins' $S_{i\mu}$, i.e. real random variables, *a priori* independent and identically distributed (i.i.d.) with an even probability measure concentrated on $[-1, 1]$. The interaction energy is taken as

$$H_{M,N}(S^M)=-\frac{M}{2}\sum_{i,j=1}^{N} J_{i,j}S_i^M S_j^M - M\sum_{i=1}^{N} h_i S_i^M \qquad (1.1)$$

where $S^M=\{S_i^M\}_{i=1,\ldots,N}\in\mathbb{R}^N$ is the vector of average row magnetizations

$$S_i^M=M^{-1}\sum_{\mu=1}^{M} S_{i\mu} \qquad i=1,\ldots,N. \qquad (1.2)$$

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The couplings J_{ij} and external fields h_i are assumed to satisfy

$$J_{i,j} \geqslant 0 \quad h_i \geqslant 0 \quad \forall i, j = 1, \ldots, N \qquad J = (J_{i,j}) > 0 \tag{1.3}$$

i.e. J is strictly positive-definite). Moreover, the *a priori* measure ρ is assumed to be a 'GHS measure' (Ellis and Newman 1978c), i.e. its moment generating function

$$F(t) := \log \int e^{tx} \, d\rho(x) \tag{1.4}$$

has strictly concave derivative on $[0, \infty)$.

We are interested here in the (joint) probability distribution of the random vector S^M in the equilibrium state at inverse temperature β,

$$d\mu_M^\beta(S^M) = Z^{-1} \exp[-\beta H_{M,N}(S^M)] d\mu_M^0(S^M) \tag{1.5}$$

in the asymptotic regime $M \to \infty$ (mean-field limit); in equation (1.5) $\mu_M^0 = \rho^{MN} \circ (S^M)^{-1}$ is the distribution of S^M in the non-interacting case (i.e. under the product measure ρ^{MN}), and Z is the normalizing factor (partition function).

The thermodynamics of the model and of its $N \to \infty$ limit have been studied in detail by Angelescu *et al* (1972a, b, 1981); it is, as expected, a non-homogeneous mean-field model, i.e. the expectations of S^M in the Gibbs measure (1.5) converge as $M \to \infty$ to the solution $m \in \mathbb{R}^N$ of a system of self-consistency equations, and m is correctly related to the derivatives of the free energy:

$$f = \lim_{M \to \infty} -(\beta M)^{-1} \log Z. \tag{1.6}$$

Assumption (1.4) ensures a normal ferromagnetic behaviour: the phase diagram consists of a first-order transition line $h = 0, \beta > \beta_c^N$, terminating at a Curie point.

Physically, there are two different situations which can be described with the Hamiltonian (1.1): (i) a ferromagnetic thin film, where M is large, but N is kept fixed at a finite value; (ii) a semi-infinite ferromagnet, where both M and N are large, but consideration is restricted to rows near the surface, $i \ll N$. (We have chosen here to view the M spins in a row as part of a 'two-dimensional layer', therefore to view equation (1.1) as a model of a three-dimensional sample; of course, this is purely conventional, because equation (1.1) is invariant under permutations within each row.)

Here we shall concern ourselves only with case (i). We show that, under assumptions (1.3) and (1.4), the random vectors S^M converge in distribution to a Dirac measure concentrated at the thermodynamic magnetization vector m, and the fluctuations

$$Y^M = M^{1/2}(S^M - m) \tag{1.7}$$

also converge in distribution (after a suitable conditioning in the two-phase region). The limit distribution of Y^M is a Gaussian on $\mathbb{R}^N$ with covariance equal to the susceptibility matrix $\chi = \partial m / \partial h$ everywhere, but at the critical point $h = 0$, $\beta = \beta_c^N$, where abnormal fluctuations along the positive eigenvector of J are found, $M^{-1/4} Y^M$ converge in distribution to an $\exp(-x^4)$ law along that direction. The result and the method are generalizations to N dimensions of those in Ellis and Newman (1978a, b). The same approach applies to other *a priori* measures; however, the limit distributions will depend on ρ, more precisely on the nature of the different transition points on the phase diagram.

In the semi-infinite case (ii), one has to study the large-M asymptotic distribution of the infinite sequence S_i^M, $i \in \mathbb{N}$. But in this case it is well known that the behaviour is different even at the level of thermodynamics, e.g. the critical index of m_1 equals 1 in the limit $N \to \infty$, in contradistinction to its value of $\frac{1}{2}$ for finite N (Angelescu *et al* (1981, 1987); for previous results, mainly in the continuum approximation, see references in Binder (1983)). Under these circumstances the asymptotic control of the sequence of Markov chains $\{S_i^M, i \in \mathbb{N}\}$ is far from trivial and the corresponding analysis will be published elsewhere.

2. The large deviations of S^M

In the non-interacting case, i.e. under μ_M^0, the law of large numbers ensures that $S^M \to 0$ in distribution.

Let F^* be the Legendre transform of F (equation (1.4)):

$$F^*(x) = \sup_{t \in \mathbb{R}} (tx - F(t)). \tag{2.1}$$

By the classical Cramér theorem (Deuschel and Stroock 1988, theorem 2.1.6), μ_M^0 obeys the large-deviation principle with the rate function

$$I_0(x) = \sum_{i=1}^{N} F^*(x_i) \qquad x = (x_i)_{i=1,\ldots,N} \in \mathbb{R}^N \tag{2.2}$$

i.e. for every Borel subset $A \subset \mathbb{R}^N$:

$$-\inf_{x \in \operatorname{Int} A} I_0(x) \leqslant \liminf_{M \to \infty} M^{-1} \log \mu_M^0(A) \leqslant \limsup_{M \to \infty} M^{-1} \log \mu_M^0(A) \leqslant -\inf_{x \in \bar{A}} I_0(x). \tag{2.3}$$

This means that, if A is far from the origin of $\mathbb{R}^N$, the probability of $S^M \in A$ is exponentially small.

In the interacting case, by the transfer principle of the large-deviation theory (Deuschel and Stroock 1988, theorem 2.1.10 and exercise 2.1.24), μ_M^β satisfies the large-deviation principle too, with the rate function

$$I_\beta(x) = -\frac{\beta}{2}(x, Jx) - \beta(x, h) + I_0(x) - \beta f \tag{2.4}$$

where

$$-\beta f = \sup \left[\frac{\beta}{2}(x, Jx) + \beta(x, h) - I_0(x) \right]. \tag{2.5}$$

Notation (2.5) is legitimate: by taking $A = \mathbb{R}^N$ in the analogue of expression (2.3) for $Z\mu_M^\beta$, one obtains the existence of the thermodynamic limit of the free energy, equation (1.6), with f given by equation (2.5).

By the analysis in Angelescu *et al* (1972a), under assumptions (1.3) and (1.4), $\inf I_\beta = 0$ is attained, for $h \neq 0$ or $\beta \leqslant \beta_c^N$, at a unique point $m \in \mathbb{R}^N$, while for $h = 0$ and $\beta > \beta_c^N$ it is attained at two points $\pm m \in \mathbb{R}^N$. Here β_c^N is the largest β for which $I_0''(0) - \beta J > 0$, i.e.

$$\beta_c^N \lambda_{\max}(J) = F^{*\prime\prime}(0) = 1/F''(0) \tag{2.6}$$

and, in all cases, m is the unique positive solution of the system:

$$m_i = F'(\beta(Jm + h)_i) \qquad i = 1, \ldots, N. \tag{2.7}$$

As a consequence, we have the following proposition.

Proposition 1. Under assumptions (1.3) and (1.4), the distributions μ_M^β of S^M converge weakly as $M \to \infty$ to δ_m, if $h \neq 0$ or $\beta \leqslant \beta_c^N$, and to $\frac{1}{2}(\delta_m + \delta_{-m})$, if $h=0$ and $\beta > \beta_c^N$.

3. The central limit theorem in the non-critical case

Once the convergence in distribution of S^M to the magnetizations m predicted by the mean-field theory has been established in proposition 1, one can ask about the distributions of their (suitably scaled) deviations Y^M defined in equation (1.7). In this section we consider the non-critical case, for which we prove a central limit theorem.

Non-criticality is defined in terms of the behaviour of $I_\beta(x)$ around its minimum at m as strict positive-definiteness of its second differential: $\lambda_{\min}(I''_\beta(m)) > 0$, where

$$I_\beta(x) = \tfrac{1}{2}(x-m, I''_\beta(m)(x-m)) + o(\|x-m\|^2) \tag{3.1}$$

with

$$I''_\beta(m) = I''_0(m) - \beta J \tag{3.2}$$

$$I''_0(m)_{ij} = F^{\star\prime\prime}(m_i)\delta_{ij} = \delta_{ij}/F''(\beta(Jm+h)_i) \qquad i,j=1,\ldots,N. \tag{3.3}$$

The minimum is non-critical for all $(\beta, h) \neq (\beta_c^N, 0)$ (Angelescu *et al* 1972a). Indeed, if $m=0$, then $h=0$ and $\beta < \beta_c^N$, hence $I_\beta(0) = F^{*\prime\prime}(0)I - \beta J > 0$, by definition of β_c^N; otherwise, defining $\Gamma_{ij} = \delta_{ij} F^{*\prime}(m_i)/m_i$, one has $I''_\beta(m) > \Gamma - \beta J$ by assumption (1.4), and $\Gamma - \beta J \geqslant 0$, because it has non-positive off-diagonal entries and $(\Gamma - \beta J)m = h$ with $m_i > 0$, $h_i \geqslant 0$, by the self-consistency equation (2.7).

One has to distinguish between the cases of uniqueness and non-uniqueness of the mean-field prediction. In the latter case, which arises for $\beta > \beta_c^N$, $h=0$, one can expect convergence in distribution of Y^M only after conditioning S^M to stay far from one of the two solutions. We therefore define

$$\nu_M^\beta(\cdot) = \mu_M^\beta(\cdot \mid S^M \in A) \circ (Y^M)^{-1} \tag{3.4}$$

the distribution of Y^M in the conditional μ_M^β measure, where A is an open set containing m, such that $\bar{A}$ contains no other minimum point of $I_\beta(x)$.

Proposition 2. Under assumptions (1.3) and (1.4), and if $(\beta, h) \neq (\beta_c^N, 0)$, ν_M^β converges weakly to the Gaussian measure of mean 0 and covariance $\chi = I''_\beta(m)^{-1}$.

Proof. Let us first remark that, by the large-deviation principle for μ_M^β, the conditioning set A in equation (3.4) can be replaced by a ball $\{\|x-m\| < \delta\}$ of arbitrarily small radius δ. Denote by $\chi_M(y)$ the characteristic function of $\{\|y\| < M^{1/2}\delta\}$.

Next, we change to another free measure $\tilde{\mu}_M^0$, defined by

$$\frac{\mathrm{d}\tilde{\mu}_M^0}{\mathrm{d}\mu_M^0}(x) = \exp M \sum_{i=1}^N [F'^{-1}(m_i)x_i - F(F'^{-1}(m_i))]. \tag{3.5}$$

Clearly, $\tilde{\mu}_M^0$ is a product probability measure on $\mathbb{R}^N$ and $\int x\,\mathrm{d}\tilde{\mu}_M^0(x) = m$. If $\tilde{\nu}_M^0 = \tilde{\mu}_M^0 \circ (Y^M)^{-1}$ is the distribution of Y^M in the new measure, we know by the classical central limit theorem that $\tilde{\nu}_M^0$ converges weakly to the Gaussian measure of mean 0 and covariance $I''_0(m)^{-1}$.

A straightforward calculation shows that, for every bounded continuous function f: $\mathbb{R}^N \to \mathbb{R}$,

$$\nu_M^\beta(f) = \frac{\int f(y)\chi_M(y)\exp[\frac{1}{2}\beta(y, Jy)]\,\mathrm{d}\tilde{\nu}_M^0(y)}{\int \chi_M(y)\exp[\frac{1}{2}\beta(y, Jy)]\,\mathrm{d}\tilde{\nu}_M^0(y)} \tag{3.6}$$

Hence, the proof will be complete if we show that the functions $\chi_M(y)\exp[\frac{1}{2}\beta(y, Jy)]$ are uniformly integrable. This will follow in turn from the boundedness of the sequence

$$\int \chi_M(y)\exp\left[\frac{\beta_1}{2}(y, Jy)\right]\mathrm{d}\tilde{\nu}_M^0(y)$$

for some $\beta_1 > \beta$. To see this, it is suffucient to choose $\beta_1 > \beta$, $\alpha < 1$ and $\delta > 0$ in such a way that (*a*) $\alpha I_0''(m) - \beta_1 J > 0$ and (*b*) the sequence $\int \chi_M(y)\exp[\frac{1}{2}\alpha(y, I_0''(m)y)]\,\mathrm{d}\tilde{\nu}_M^0(y)$ is bounded. (The latter is the uniform integrability bound 'in one dimension', e.g., see Ellis 1985.)

4. The abnormal fluctuations at the critical point

The critical point has been defined by $\lambda_{\min}(I_\beta''(m)) = 0$. As already discussed, this happens only for $(\beta, h) = (\beta_c^N, 0)$. Thereby, $m = 0$ and hence the eigenvector of $I_\beta''(m) = I_{\beta_c^N}''(0)$ corresponding to the zero eigenvalue is the positive eigenvector of J, which we denote e:

$$\left(\frac{1}{F''(0)}I - \beta_c^N J\right)e = 0 \qquad \|e\| = 1. \tag{4.1}$$

Let $P = (e, \cdot)e$ be the one-dimensional orthogonal projection onto e, $P^\perp = I - P$, and decompose:

$$Y^M = M^{1/4}Z^M e + P^\perp Y^M \tag{4.2}$$

i.e. the random variable Z^M is the rescaled fluctuation along e.

Proposition 3. With the above notation at $(\beta, h) = (\beta_c^N, 0)$ and under assumptions (1.3) and (1.4) supplemented with

$$F^{(4)}(0) < 0 \tag{4.3}$$

the random vector $(Z^M, P^\perp Y^M)$ converges in the μ_M^β distribution as $M \to \infty$ to $(Z, Y_\perp)$, where Z and $Y_\perp$ are independent; the distribution of Z has density

$$C\exp\left[\frac{F^{(4)}(0)}{F''(0)^4}\sum_{i=1}^N \frac{e_i^4}{24}z^4\right] \tag{4.4}$$

while $Y_\perp \in P^\perp\mathbb{R}^N$ is Gaussian of mean zero and covariance $\chi^\perp$ equal to the inverse of the restriction of $I_\beta''(0)$ to $P^\perp\mathbb{R}^N$.

Proof. We shall prove the convergence as $M \to \infty$ of the moment-generating function of $(Z^M, P^\perp Y^M)$, g_M: $\mathbb{R} \times P^\perp \mathbb{R}^N \to \mathbb{R}$:

$$g_M(\zeta, \eta) = \mu_M^\beta \exp(Z^M \zeta + (P^\perp Y^M, \eta)) = \int \exp(M^{1/4}(e, PS^M)\zeta + M^{1/2}(P^\perp S^M, \eta))\, d\mu_M^\beta(S^M). \tag{4.5}$$

Using the Gaussian identity for expressing $\exp[(1/2M)(S^M, \beta J S^M)]$, one obtains

$$g_M(\zeta, \eta) = h_M(\zeta, \eta)/h_M(0, 0) \tag{4.6}$$

where

$$h_M(\zeta, \eta) = \exp[-\tfrac{1}{2}M^{-1/2}(e, (\beta J)^{-1}e)\zeta^2 - \tfrac{1}{2}(\eta, (\beta J)^{-1}\eta)] \times \int_{\mathbb{R}^N} \exp[(Pt, e)\zeta + (P^\perp t, \eta)] \exp\Big\{-\tfrac{1}{2}M^{1/2}(Pt, \beta J P t) - \tfrac{1}{2}(P^\perp t, \beta J P^\perp t) + M \sum_{i=1}^{N} F([\beta J(M^{-1/4}Pt + M^{-1/2}P^\perp t)]_i)\Big\}\, dt. \tag{4.7}$$

The convergence of h_M will follow from the dominated convergence theorem. Pointwise convergence of the integrand in equation (4.7) is immediate from the Taylor expansion of F up to fourth order: for fixed $t \in \mathbb{R}^N$, the only terms inside the braces which survive for $M \to \infty$ are

$$-\tfrac{1}{2}(P^\perp t, \beta J P^\perp t) + \tfrac{1}{2}F''(0)\|\beta J P^\perp t\|^2 + \tfrac{1}{24}F^{(4)}(0) \sum_{i=1}^{N} (\beta J P t)_i^4. \tag{4.8}$$

So, were we allowed to take $\lim_{M\to\infty}$ under the integral sign, the assertions in proposition 3 would follow by performing the Gaussian integration over $P^\perp t$ and combining the result with the exponential in front of equation (4.7); to recognize the density (4.4) in the remaining integral over $z = (Pt, e)$ use is made of equation (4.1).

In order to obtain an integrable bound, we use the following consequence of assumption (1.4) and of $\operatorname{supp}\rho \subset [-1, 1]$: for $\varepsilon > 0$ sufficiently small, there exists $T > 0$ such that

$$F(t) \leqslant \tfrac{1}{2}F''(0)t^2 - \varepsilon t^4 \qquad \text{if } |t| \leqslant T \tag{4.9}$$

$$F(t) \leqslant \tfrac{1}{2}(F''(0) - \varepsilon)t^2 \qquad \text{if } |t| \geqslant T. \tag{4.10}$$

Indeed, inequality (4.9) is true, because $F^{(4)}(0) < 0$ and $F(t) - \frac{1}{2}F''(0)t^2 < 0$ for $t \neq 0$ by equation (1.4); on the other hand, expression (4.10) holds for T sufficiently large, because $F(t) \leqslant |t|$.

Splitting the integration domain into

$$S_{T,M} = \{t \in \mathbb{R}^N : \|\beta J(M^{-1/4}Pt + M^{-1/2}P^\perp t\| < T\}$$

and its complement $S_{T,M}^c$, using the equivalence of different norms on $\mathbb{R}^N$ and the orthogonality of Pt and $P^\perp t$, one can bound the exponent in equation (4.7) by $-\delta(\|Pt\|^4 + \|P^\perp t\|^2)$ on $S_{T,M}$, and by $-\delta(M^{1/2}\|Pt\|^2) + \|P^\perp t\|^2)$ on $S_{T,M}^c$, for some $\delta > 0$. The integral over $S_{T,M}^c$ converges to zero, and the bound on $S_{T,M}$ is uniform in M. This completes the proof.

The physical picture that emerges from proposition 3 is that, at the critical point, the row magnetizations experience simultaneously giant fluctuations, the amplitudes of which are proportional to the components of the spontaneous magnetization vector at nearly $\beta > \beta_c^N$. Indeed, they are proportional to e_i, and for $\beta \searrow \beta_c^N$ the linearized form of equation (2.7) shows that $m/\|m\| \to e$. The fluctuations of Y^M from the direction of e (i.e. of $Y^M/\|Y^M\| - e$) are of the order of $M^{-1/4}$, i.e. negligible for large M.

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