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DETECTING PHASE TRANSITION FOR GIBBS MEASURES

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We propose a new empirical procedure for detecting phase transition from a single sample of a Gibbs–Markov random field. The method is based on frequencies for large deviations when the whole sample is divided in smaller blocks and estimates for the rate function. We relate our approach to an almost sure large deviation principle.

1. Introduction. Phase transition and phase multiplicity in Markov random fields—or equivalently, Gibbs measures—are long-range dependence phenomena. Detecting such a phenomenon from a single sample is a natural question, both on physical grounds and on mathematical and statistical ones.

In the probabilistic theory of Markov fields there exist sufficient conditions for uniqueness, as Dobrushin's and Simon's conditions, but conditions for existence of multiple phases are much harder to obtain [Georgii (1988), Prum (1986)]. The Pigorov–Sinaï theory is a rather qualitative approach, viewing the low temperature case as a smooth perturbation of the zero temperature case and of the set of ground states. So it is natural to look for an empirical criterion rather than an analytical one.

In the statistical analysis of Markov fields, such a criterion would be most useful to justify the use of Gaussian asymptotics for estimates, confidence intervals and hypothesis testing (Guyon, 1992); indeed, phase transition reflects on the validity of the central limit theorem and on the limit behavior of the maximum likelihood estimator. This paper presents such empirical criteria.

Let $X = (X_i)_{i\in\mathbb{Z}^d}$ be a Markov random field with finite range, translation invariant interaction and distribution P. Assume that we observe a single realization of X in the cubic box $\Lambda_n = [-n, n]^d$. In the spirit of Erdős–Rényi laws and large deviation inequalities, we proved recently that one can estimate (consistently if $n \to \infty$) the set $\mathscr{G}_s$ of all stationary Gibbs measures with the same potential as P [Comets (1994)]; more precisely, the estimate is the set of empirical distributions based on smaller boxes with specified size moving inside the box Λ_n of observation. This is a statistical way to detect multiplicity of phases based on multiscale analysis, the different resolution scales being here the different sizes for the moving boxes.

This idea was used later by Dai Pra (1994) to detect nonergodicity in spin-flip processes, using space-time empirical distributions. For practical purposes, we also considered in our previous paper the question of estimating the in-

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terval $A_f = \{\int f\,dQ; Q \in \mathcal{G}_s\}$ with a suitable real function f defined on the configuration space, chosen so as to spread out the different Gibbs measures when many exist. The set A_f reduces to a single point when uniqueness of the Gibbs measure holds; otherwise, it is a nontrivial interval for suitable functions f. In this previous work we noted from simulation experiments that estimates for A_f converge very slowly. However, we note also that it is much more informative to estimate the rate function $I_f(\cdot)$ for large deviations itself and then to use the fact that A_f is the set of zeros of I_f. In such a way we can use some a priori information like convexity on I_f. The estimation procedure there requires inverting some functional estimator, which causes f to fix; this is a serious drawback in a number of examples when it is not clear what are the suitable functions f are. Another drawback is that the maximum of moving averages used in the estimation is highly sensitive to outliers; it may indeed happen in applications that in some subwindow of Λ_n the data are pervaded with systematic error.

In the present paper we propose a new method for estimating $\mathcal{G}_s$, A_f and I_f based on the natural idea of using frequencies, avoiding thus the inversion procedure. Hence this time it is compatible with a parallel search for suitable f's (in the sense of maximal spreading of the data) and gives in addition much smoother estimates. Another application of our results is in comparing statistical estimators on the basis of their inacuracy rates in the asymptotic approach of Bahadur. Csőrgö (1979) developed similar ideas for independent variables. In our case this rate can be expressed in terms of values of such I_f for a large set of functions f [see (5.3) in Comets (1992)]. This rate cannot be computed analytically, but it can be estimated with the method we develop below. Note that in general the f functions under consideration in this case are vector valued.

The paper is organized as follows. For simplicity, we will consider the case of finite state space, finite range interaction Gibbs measures. Nevertheless it is straightforward to extend all results to general Gibbs measures as in Comets (1994); some remarks are set forth in this direction. In the next two sections we give the basic definitions and state our main result. Section 4 recalls the necessary tools, entropy and large deviation estimates. In Section 5 we study the asymptotics of frequency estimates and we prove the main result. Next we show a large deviation principle which is hidden behind our result as well as the Erdős–Rényi laws. In Section 7, we present simulation experiments to illustrate the method.

2. Markov random fields. Let $\mathcal{X}_0$ be a finite set, d some positive integer and $\mathcal{X}$ the product space $\mathcal{X} = \mathcal{X}_0^{\mathbb{Z}^d}$. Let $\mathcal{P}(\mathcal{X})$ be the set of random fields on $\mathcal{X}_0$, that is, of probability measures on $\mathcal{X}$ with its natural product σ-field. Viewing $\mathcal{X}_0$ as a discrete topological space, the space $\mathcal{P}(\mathcal{X})$, endowed with the topology of weak convergence, is itself a compact metrizable space. For $i \in \mathbb{Z}^d$ we denote by θ_i the shift operator on $\mathcal{X}$ defined by $(\theta_i x)_j = x_{i+j}$ with $x = (x_i)_{i\in\mathbb{Z}^d} \in \mathcal{X}$ and $j \in \mathbb{Z}^d$. Let $\mathcal{P}_s(\mathcal{X})$ be the set of stationary random fields (i.e., invariant under the shift operators) and let $\mathcal{P}_e(\mathcal{X})$ be the set of stationary ergodic ones (i.e., those achieving only values 0 on 1 or the events which are shift invariant).

A general translation invariant, finite range interaction potential may be described with a single function as follows. Let V be a finite subset of $\mathbb{Z}^d$ containing the origin 0 and let ϕ: $\mathscr{X}_0^V \longrightarrow \mathbb{R}$ be a real function; V will be called the *support of* ϕ and ϕ the *interaction function*. For any finite subset Λ of the lattice, define the energy inside Λ of the configuration $x \in \mathscr{X}$ as the sum of the self-interaction inside Λ and of the interaction across the boundary of Λ; that is,

$$U_\Lambda(x) = \sum_{i:\ (i+V)\cap\Lambda\neq\varnothing} \phi(\theta_i x), \qquad x \in \mathscr{X}. \tag{2.1}$$

For $x, z \in \mathscr{X}$ we write

$$(x_i)_{i\in\Lambda} = x_\Lambda, \qquad (x_i)_{i\notin\Lambda} = {}_\Lambda x$$

and by $x_\Lambda \vee z$ the element of $\mathscr{X}$ equal to x on Λ and to z on Λ^c. For simplicity we will also use the same symbol x_Λ for a local configuration $(x_i)_{i\in\Lambda}$ (even when x_i is not defined for $i \notin \Lambda$).

Corresponding to the interaction function ϕ the *specification* π is the family of transition probability kernels Π_Λ indexed by the finite subsets Λ of $\mathbb{Z}^d$, $\Pi_\Lambda : \mathscr{X}_0^{\Lambda^c} \mapsto \mathscr{P}(\mathscr{X}_0^\Lambda)$,

$$\Pi_\Lambda(x_\Lambda / {}_\Lambda x) = [Z_\Lambda({}_\Lambda x)]^{-1} \exp\{U_\Lambda(x)\}, \tag{2.2}$$

$$Z_\Lambda({}_\Lambda x) = \sum_{z_\Lambda \in \mathscr{X}_0^\Lambda} \exp\{U_\Lambda(z_\Lambda \vee x)\}. \tag{2.3}$$

A random field $P \in \mathscr{P}(\mathscr{X})$ is called a *Gibbs measure* (or a *Markov random field*) with interaction ϕ if, for all finite subsets Λ of $\mathbb{Z}^d$, Π_Λ is a regular version of the conditional distribution P_Λ of P given ${}_\Lambda x$; that is,

$$P_\Lambda(x_\Lambda | {}_\Lambda z) = \Pi_\Lambda(x_\Lambda | {}_\Lambda z) \quad \text{for } P\text{-a.e. } z. \tag{2.4}$$

Equations (2.4) are called the Dobrushin–Lanford–Ruelle equations. The set $\mathscr{G}$ of all Gibbs measures is a convex, compact, nonempty subset of $\mathscr{P}(\mathscr{X})$; $\mathscr{G}$ coincides with the closed convex hull of all limit points of $\Pi_\Lambda(\cdot|{}_\Lambda z)$ as $\Lambda \nearrow \mathbb{Z}^d$ for all possible boundary conditions z. The set $\mathscr{G}_s = \mathscr{G} \cap \mathscr{P}_s(\mathscr{X})$ is also convex and compact and we have $\varnothing \neq \mathscr{G}_e := \mathscr{G} \cap \mathscr{P}_e(\mathscr{X}) \subset \mathscr{G}_s \subset \mathscr{G}$. *First order phase transition* (or *multiplicity of phases*) occurs when $\mathscr{G}$ contains more than one element. Then $\mathscr{G}_e$ and $\mathscr{G}_s$ themselves contain more than one element, some Gibbs measures are not ergodic and furthermore it may occur that some are not even stationary. For a rather complete study of Gibbs measures, see Georgii (1988). Note that phase uniqueness is equivalent to $\mathscr{G}_s$ reducing to a single point.

EXAMPLE. The nearest neighbor Ising model with inverse temperature β and external field h is given by $\mathscr{X}_0 = \{-1, +1\}$, $\phi(x) = \beta x_0 \sum_{k=1}^d x_{e_k} + h x_0$, where $(e_1, \dots, e_d)$ is the canonical basis of $\mathbb{Z}^d$. Then uniqueness holds iff $h \neq 0$

or $\beta \leq \beta_c(d)$. In dimension $d = 2$, $\beta_c(2) = \frac{1}{2}\ln(1+\sqrt{2}) \simeq 0.441$. In dimension $d \geq 3$, $\mathscr{G}_s \neq \mathscr{G}$ for large enough β.

3. Estimating the rate function. Let f be a numerical function on $\mathscr{X}$ that is local. That is, $f(x)$ depends only on the restriction x_W of x to some finite subset W of $\mathbb{Z}^d$. With the notations $\Lambda_n = [-n, n]^d$ and $|\Lambda|$ for the cardinality of a set Λ, define for $y \in \mathbb{R}$ the *rate function*

$$(3.1)\quad I_f(y) = -\lim_{\varepsilon\to 0}\limsup_{n\to\infty}\frac{1}{|\Lambda_n|}\ln P\left\{\frac{1}{|\Lambda_n|}\sum_{i\in\Lambda_n} f\circ\theta_i(x) \in [y-\varepsilon,\ y+\varepsilon]\right\}$$

By monotonicity in ε, the above limit is well defined in $[0, +\infty]$. In formula (5.7) in Section 5, we will obtain a different expression for I_f and check from it that I_f does not depend on $P \in \mathscr{G}$, that I_f is a lower semicontinuous convex function and that

$$(3.2)\qquad I_f(y) = 0 \quad\Leftrightarrow\quad \exists\ Q \in \mathscr{G}_s\colon \int f\,dQ = y.$$

This statement has the following important meaning. Multiplicity of phases occurs if and only if the convex function I_f achieves its minimum value 0 in more than one point, for some function f. Hence *detecting phase transition* amounts to *detecting a flat bottom* for I_f.

Let us state our main result, which we will prove in Section 5. Recall that the domain of the convex function I_f is defined as $\operatorname{Dom} I_f = \{y \in \mathbb{R};\ I_f(y) < +\infty\}$; here $\operatorname{Dom} I_f$ is a compact interval, and $\operatorname{Dom} I_f = \{\int f\,dQ;\ Q \in \mathscr{P}_s(\mathscr{X})\}$. We will denote by $\partial \operatorname{Dom} I_f$ its boundary.

THEOREM 3.1. *Let $t > 0$ and let $l(n)$ be a nondecreasing sequence of integers such that $l(n) \sim \frac{1}{2}((d/t)\ln n)^{1/d}$ as $n \to \infty$. Define*

$$m_n = \left|\{i \in \mathbb{Z}^d;\ i + \Lambda_{l(n)} + W \subset \Lambda_n\}\right|$$

and the random functions

$$M'_n(y) = \left|\left\{i \in \mathbb{Z}^d;\ i + \Lambda_{l(n)} + W \subset \Lambda_n,\ |\Lambda_{l(n)}|^{-1}\sum_{j\in i+\Lambda_{l(n)}} f\circ\theta_j \geq y\right\}\right|,$$

$$\begin{aligned} &M_n(y) = M'_n(y) \quad \textit{if } 1 \leq M'_n(y) \leq m_n - 1,\\ &M_n(y) = 1 \quad \textit{if } M'_n(y) = 0,\\ &M_n(y) = m_n - 1 \quad \textit{if } M'_n(y) = m_n.\end{aligned}$$

Then, for all $P \in \mathscr{G}$ and $y \notin \partial \operatorname{Dom} I_f$,

$$(3.3)\quad \lim_{n\to\infty}(\ln m_n)^{-1}\ln\left\{\frac{M_n(y)}{m_n}\left[1-\frac{M_n(y)}{m_n}\right]\right\} = -\min\{t^{-1}I_f(y), 1\},\quad P\text{-a.s.}$$

The convergence is P-a.s. uniform on closed subsets not intersecting the boundary of the domain of I_f. In particular, if $t \leq \min\{I_f(y);\ y \in \partial \operatorname{Dom} I_f\}$, the convergence is uniform on $\mathbb{R}$.

In this result we introduce a consistent estimator for $[t^{-1}I_f] \wedge 1$ based on the truncated frequency M_n/m_n of the averages of f on small (but increasing) boxes contained in the observation region Λ_n. This yields an estimate for I_f itself up to the level t, and according to (3.2) this is enough for estimating the interval $A_f = \{\int f\, dQ;\ Q \in \mathscr{G}_s\}$ and deciding whether it reduces to a single point or not.

We emphasize that the theorem holds for any $P \in \mathscr{G}$, hence it applies to samples from any distribution in $\mathscr{G}$. One could also be interested in a slightly different situation, where the available data x_{Λ_n} change with n and are from the specification $\Pi_{\Lambda_n}(\cdot|_{\Lambda_n} z(n))$ with boundary conditions $z(n)$ changing with n; in this case, the method still works with minor changes and the convergence stated in Theorem 3.1 holds in probability.

As mentioned in the introduction, choosing a suitable f for maximal spreading of the set $\mathscr{G}_s$ when this set does not reduce to a single point is an important problem. Some hints may be grasped from the inspection of the ground states, which are, loosely speaking, the configurations minimizing the "infinite volume energy $U_{\mathbb{Z}^d}$" [see Prum (1986) for a more precise definition]. But a more refined choice should also use the data themselves; the estimator proposed in the theorem lends itself to such a procedure, as opposed to the one proposed in Comets (1994) which requires some inversion step for each f.

Also, this estimator is more robust than the previous one. Let us simply remark that its minimum 0 is achieved at the median y of the moving averages of f, though it is achieved for the previous estimator at the mean of f on the whole domain Λ_n. This indicates the robustness property, at least close to the minimum.

We end this section with a remark on the precise behavior of $M'_n(y)$ when f depends on only one coordinate. The Erdős–Rényi law governs the largest moving average, that is, the largest y such that $M'_n(y) \neq 0$. In the case of independent variables, Deheuvels, Devroye and Lynch (1986) give the exact rate of convergence for it; this reflects on sharp asymptotics for $M'_n(y)$ itself for y such that $I_f(y) = t$. In this case similar considerations would also yield a finer approximation for $M'_n(y)$ than the logarithmic equivalent, but of course this seems out of reach in the Gibbsian case as well as when f depends on many coordinates.

4. Entropy and large deviations. The *entropy rate* of a stationary random field $Q \in \mathscr{P}_s(\mathscr{X})$,

$$H(Q) = \lim_{n\to\infty} |\Lambda_n|^{-1} \int [-\ln Q(x_{\Lambda_n})]\, dQ(x) \in [0, \ln|\mathscr{X}_0|], \tag{4.1}$$

exists, as well as the *relative entropy rate* (information gain) of $Q \in \mathscr{P}_s(\mathscr{X})$ with respect to the Markov field $P \in \mathscr{G}$:

$$I(Q) = \lim_{n\to\infty} |\Lambda_n|^{-1} \int \ln \frac{Q(x_{\Lambda_n})}{P(x_{\Lambda_n})}\, dQ(x),$$

which also depends on the interaction function ϕ but not on the particular element $P \in \mathscr{G}$. They are related to one another via

$$(4.2)\qquad \begin{aligned} I(Q) &= -H(Q) - \int \phi \, dQ + p(\phi), \\ p(\phi) &:= \lim_{n\to\infty} |\Lambda_n|^{-1} \ln Z_{\Lambda_n}(z) = \max_{R\in\mathscr{P}_s(\mathscr{X})} \left\{ \int \phi \, dR + H(R) \right\}, \end{aligned}$$

where in the last formula—called the Gibbs variational formula—the limit is uniform in $z \in \mathscr{X}$. The Gibbs variational principle, due to Ruelle, states that

$$(4.3)\qquad I(Q) = 0 \quad \Leftrightarrow \quad Q \in \mathscr{G}_s.$$

The functional I is nonnegative, bounded, affine and lower semicontinuous on $\mathscr{P}_s(\mathscr{X})$; in particular the level sets

$$\Gamma_t = \{R \in \mathscr{P}_s(\mathscr{X});\ I(R) \leq t\}, \qquad t \geq 0,$$

are convex and compact. Note in addition that (4.3) can be rephrased as $\Gamma_0 = \mathscr{G}_s$. These facts are developed in Georgii (1988).

Let us fix from now on an arbitrary $\bar{z} \in \mathscr{X}$. We define the *empirical field* based on a configuration $x \in \mathscr{X}$ observed in a shifted window $i + \Lambda_n$ ($i \in \mathbb{Z}^d,\ n \geq 1$) as the random field

$$(4.4)\qquad R_{i,n,x} = \frac{1}{|\Lambda_n|} \sum_{j\in i+\Lambda_n} \delta_{\theta_j(x_{i+\Lambda_n} \vee \bar{z})}.$$

As $n \to \infty$, $R_{i,n,x} \in \mathscr{P}(\mathscr{X})$ gets closer and closer to the set $\mathscr{P}_s(\mathscr{X})$ and the dependence on $\bar{z}$ gets smaller; heuristically $R_{i,n;x}$ is an "almost stationary" empirical distribution from the observation $x_{i+\Lambda_n}$, completing the missing data with $\bar{z}$. If $Q \in \mathscr{P}_e(\mathscr{X})$, the pointwise ergodic theorem states that $\lim_{n\to\infty} R_{i,n,x} = Q$ for Q-a.e. x, and for every $i \in \mathbb{Z}^d$.

The basic tool in this paper is a uniform *large deviation* principle for empirical fields of Gibbs measures, which turns out to be related to the relative entropy rate; for all sets A in $\mathscr{P}(\mathscr{X})$,

$$(4.5)\qquad \begin{aligned} -I(\mathring{A}) &\leq \liminf_{n\to\infty} \inf_{z,\bar{z}\in\mathscr{X}} \frac{1}{|\Lambda_n|} \ln \Pi_{\Lambda_n}(R_{n,x} \in A|_{\Lambda_n} z) \\ &\leq \limsup_{n\to\infty} \sup_{z,\bar{z}\in\mathscr{X}} \frac{1}{|\Lambda_n|} \ln \Pi_{\Lambda_n}(R_{n,x} \in A|_{\Lambda_n} z) \\ &\leq -I(\bar{A}) \end{aligned}$$

with the notation $I(A) = \inf\{I(Q);\ Q \in A \cap \mathscr{P}_s(\mathscr{X})\}$ and $R_{n,x} = R_{0,n,x}$. Recall that z denotes the boundary condition for Π and that $\bar{z}$ is used to define the empirical field and complete the data. A more general framework for these estimates is given in Theorem 2.2 of Comets (1994) with references therein. Our particular choice (4.4) of the empirical fields clearly does not change the asymptotics [as in Föllmer and Orey (1988) who use nonperiodic versions]. The estimates (4.5) are uniform with respect to the boundary conditions z;

then they also hold if we replace the specification Π with any $P \in \mathcal{G}$. A recent and general account for the large deviation principle for Gibbs measures is given in Georgii (1993). The problem of large deviations inside the set of Gibbs measures is more difficult, and was solved by Dobrushin, Kotecký and Shlosman (1992).

5. Estimates based on frequencies. For $1 \leq l \leq n$ let us define the set of empirical fields based on the translates of Λ_l which are included in Λ_n:

$$\Delta_{n,l}(x) = \{R_{i,l,x}; i + \Lambda_l \subset \Lambda_n\}$$

and, for $A \subset \mathcal{P}(\mathcal{X})$, define the random variable $N(n, l, A)$—depending on x—equal to the number of such fields belonging to A:

$$N(n, l, A)(x) = | \Delta_{n,l}(x) \cap A | .$$

We will describe the asymptotics of this variable as n and l tend to infinity.

THEOREM 5.1. *Let $t > 0$ and let $l(n)$ be an increasing sequence of integers such that $| \Lambda_{l(n)} | \sim t^{-1} \ln | \Lambda_n |$. Then, for all $P \in \mathcal{G}$ and all $A \subset \mathcal{P}(\mathcal{X})$ we have P-a.s.,*

$$\begin{aligned}(1 - t^{-1} I(\mathring{A}))^+ &\leq \liminf_{n\to\infty} (\ln | \Lambda_n |)^{-1} \ln\{N(n, l(n), A) + 1\} \\ &\leq \limsup_{n\to\infty} (\ln | \Lambda_n |)^{-1} \ln\{N(n, l(n), A) + 1\} \\ &\leq (1 - t^{-1} I(\bar{A}))^+\end{aligned}$$

with the notation $y^+ = y \vee 0$ for $y \in \mathbb{R}$.

REMARK 5.1. (i) This result is related to Theorem 3.1 in Comets (1994). We consider $N(n, l, A) + 1$ instead of $N(n, l, A)$ in the statement to avoid the case $N(n, l, A) = 0$. Note that when $1 - t^{-1} I(\bar{A}) < 0$, we already know from our previous paper that $N(n, l, A) = 0$ for large enough n with probability 1.

(ii) The sets A with $I(\mathring{A}) = I(\bar{A})$ are of particular interest, for instance closed half-spaces of the form $A = \{R \in \mathcal{P}(\mathcal{X}); \int f\, dR \geq c\}$ for some bounded continuous function f, with nonempty interior. Indeed, letting then Q_0 be arbitrary in $\mathring{A} = \{R \in \mathcal{P}(\mathcal{X}); \int f\, dR > c\}$, for any $R \in \bar{A}$ the segment $[Q_0, R[$ is included in $\mathring{A}$ and the limit of $I(Q)$ as Q tends to R along this segment is $I(R)$ since I is affine and bounded; hence $I(\bar{A}) \geq I(\mathring{A})$, which implies the equality. This example is all that we need below. More general classes of (convex) sets A with $I(\mathring{A}) = I(\bar{A})$ can be given [Seppäläinen (1996)]; they involve conditions in the vector space of all signed measures on $\mathcal{X}$. See Seppäläinen (1995), page 556, for a flavor of these conditions at the level of the empirical measure.

As in our previous paper, we start with two lemmas.

LEMMA 5.1. *Let $l(n)$ be an sequence of nondecreasing integers tending to infinity, such that $\ln|\Lambda_{l(n)}| = o(\ln|\Lambda_n|)$ and such that $t := \lim_{n\to\infty} |\Lambda_{l(n)}|^{-1} \ln|\Lambda_n|$ exists. Then for all $P \in \mathscr{G}$ and all closed sets A in $\mathscr{P}(\mathscr{X})$ we have*

$$\limsup_{n\to\infty} (\ln|\Lambda_n|)^{-1} \ln N(n, l(n), A) \le (1 - t^{-1}I(A))^+, \quad P\text{-a.s.}$$

with the convention $t^{-1}I(A) = 0$ if $t = I(A) = 0$.

PROOF. We will write N_n instead of $N(n, l(n), A)$ to keep the notation simple. Since $N_n \le |\Lambda_n|$, we only need to consider the case when $I(A) > 0$ and $t < \infty$. We start with the case $t > 0$. It is then enough to consider $I(A) \le t$ since N_n is increasing with A. Let $\alpha := 1 - t^{-1}I(A) \in [0, 1)$ and $\varepsilon > 0$ with $t\varepsilon/2 < I(A)$, $\varepsilon < 1 - \alpha$.

We look first for a maximal subset of $\Delta_{n,\,l(n)}(x) \cap A$ corresponding to small windows mutually separated by corridors of width V (recall that V is the support of the interaction function ϕ). We proceed as follows. We will say that a collection $s = \{i_1 + \Lambda_{l(n)}, \dots, i_{|s|} + \Lambda_{l(n)}\}$ is well separated if $\| i_k - i_{k'} \|_\infty > 2l(n)+1+\mathrm{diam}(V)$ for $k, k' \le |s|$, $k \ne k'$ and of course if $i_k + \Lambda_{l(n)} \subset \Lambda_n (k \le |s|)$. Let $\mathscr{S}_n$ be the set of all well separated s; using the lexicographic order and viewing also s as $(|s|, i_1, \dots, i_{|s|})$, $\mathscr{S}_n$ is totally ordered in a natural way. Given a configuration x we consider now the set $\mathscr{S}_n(A, x)$ of all $s \in \mathscr{S}_n$ such that $R_{i,\,l(n),x} \in A$ for $i = i_1, \dots, i_{|s|}$, and we denote by $S(x)$ its maximal element for the order on $\mathscr{S}_n$. In particular $S(x)$ has maximal cardinality in $\mathscr{S}_n(A, x)$, and corresponds to the desired subset of $\Delta_{n,\,l(n)}(x) \cap A$.

The maximal cardinality property of $S = S(x)$ implies that any window contributing to N_n is within a distance $\mathrm{diam}(V)$ from S and therefore,

$$N_n \le |\, S \,|\, 2^d[2l(n) + 1 + \mathrm{diam}(V)]^d. \tag{5.1}$$

Let $s \in \mathscr{S}_n$ and $\Lambda = \bigcup_{k\le|s|}\{i_k + \Lambda_{l(n)}\}$; we have

$$\begin{aligned} P\{S = s\} &\le P\biggl(\bigcap_{k=1}^{|s|}\{R_{i_k,\,l(n),\,x} \in A\}\biggr) \\ &= \int \Pi_\Lambda\biggl(\bigcap_{k=1}^{|s|}\{R_{i_k,\,l(n),\,x} \in A\}|_\Lambda x\biggr)\, dP(x) \\ &= \int \prod_{k=1}^{|s|} \Pi_\Lambda(R_{i_k,\,l(n),\,x} \in A|_\Lambda x)\, dP(x) \\ &\le \Bigl[\sup_{z\in\mathscr{X}} \Pi_{\Lambda_{l(n)}}(R_{i_k,\,l(n),\,x} \in A|_{\Lambda_{l(n)}} z)\Bigr]^{|s|} \end{aligned} \tag{5.2}$$

using (2.4), the well separate property and conditional independence. Then the large deviation upper bound (4.5) implies that the inequality

$$P\{S = s\} \le \exp\{-\,|\, s \,|\,|\, \Lambda_{l(n)} \,|\,(I(A) - t\varepsilon/2)\} \tag{5.3}$$

holds for large enough n.

Denoting by k_n ($k_n \le |\Lambda_n|$) the integer part of $|\Lambda_n|^{\alpha+\varepsilon}2^{-d}(2l(n)+1+\mathrm{diam}(V))^{-d}$, it follows from (5.1) that

$$\{(\ln|\Lambda_n|)^{-1}\ln N_n > \alpha+\varepsilon\} \subset \bigcup_{k\ge k_n}\ \bigcup_{s\in\mathscr{S}_n,\,|s|=k}\{S=s\}$$

and from (5.3) that for large n

$$\begin{aligned} P\{(\ln|\Lambda_n|)^{-1}\ln N_n > \alpha+\varepsilon\} &\le \sum_{k\ge k_n}\sum_{|s|=k}P\{S=s\}\\ &\le \sum_{k=k_n}^{|\Lambda_n|}\binom{|\Lambda_n|}{k}\exp\{-k\,|\Lambda_{l(n)}|\,(I(A)-t\varepsilon/2)\} \qquad (5.4)\\ &= (1-p_n)^{-|\Lambda_n|}\mathrm{Prob}.\{\mathscr{B}(|\Lambda_n|,\,p_n)\ge k_n\} \end{aligned}$$

where $\mathscr{B}(m,p)$ is a binomial variable with parameters m and p, and $p_n = \exp\{-|\Lambda_{l(n)}|\,(I(A)-t\varepsilon/2)\}$. One easily checks that $\ln(|\Lambda_n|\,p_n) \sim t(\alpha+\varepsilon/2)|\Lambda_{l(n)}|$, $\ln k_n \sim t(\alpha+\varepsilon)|\Lambda_{l(n)}|$; hence Cramér's inequality for the binomial distribution [e.g., Dembo and Zeitouni (1993), Example 2.2.23] yields, for *every* n,

$$\begin{aligned} \ln\mathrm{Prob}.\{\mathscr{B}(|\Lambda_n|,\,p_n)\ge k_n\} &\le -k_n\ln\frac{k_n}{|\Lambda_n|p_n} - (|\Lambda_n|-k_n)\ln\frac{1-k_n/|\Lambda_n|}{1-p_n}\\ &\sim -k_n\ln\frac{k_n}{|\Lambda_n|p_n}\\ &\sim -k_n|\Lambda_{l(n)}|t\varepsilon/2. \end{aligned}$$

Coming back to (5.4), one also checks that $|\Lambda_n|\ln(1-p_n) = o(k_n)$ and since $|\Lambda_n|^\gamma = o(k_n)$ for $0<\gamma<\alpha+\varepsilon$, we have finally $P\{\ln|\Lambda_n|^{-1}\ln N_n > \alpha+\varepsilon\} \le \exp-|\Lambda_n|^\gamma$ for large n.

So the Borel–Cantelli lemma implies Lemma 5.1 when $t>0$.

In the case $t=0$ and $I(A)>0$, we first choose an open set A' containing $\Gamma_0 = \mathscr{G}_s$ with $A\cap A' = \varnothing$, from a compactness argument. Then Lemma 3.2 in Comets (1994) states that $N(n, l(n), A') = 0$ for large enough n, P-a.s.; hence $N_n = 0$ also holds, and implies our statement. □

LEMMA 5.2. *Let a_n be a positive sequence such that*

$$\liminf_{n\to\infty}\,(\ln|\Lambda_n|)^{-1}\ln a_n > 0,$$

let $A\subset\mathscr{P}(\mathscr{X})$ and let

$$b = -\liminf_{n\to\infty} a_n^{-1}\ln\inf_{z,\,\bar z\in\mathscr{X}}\Pi_{\Lambda_n}\{R_{n,\,x}\in A|_{\Lambda_n}z\} \ge 0.$$

Then for any nondecreasing sequence of integers $l(n)$ with $a_{l(n)}\sim\ln|\Lambda_n|$, we have

$$\liminf_{n\to\infty}(\ln|\Lambda_n|)^{-1}\ln\{N(n,l(n),A)+1\} \ge (1-b)^+, \quad P\text{-a.s.}$$

PROOF. We assume $b < 1$ without loss of generality and we let $\alpha = (1 - b)^+ = 1 - b$ and $0 < \varepsilon < \alpha$. We fix an element s_n of maximal cardinality in the set $\mathscr{S}_n$ previously defined and we denote by $\Delta'_{n,\,l(n)}(x)$ the subset of $\Delta_{n,\,l(n)}(x)$ composed of the corresponding empirical fields. In particular we have

$$|s_n| = |\Delta'_{n,\,l(n)}(x)| \sim |\Lambda_n|/|\Lambda_{l(n)}| \quad \text{as } n \to \infty$$

$$\begin{aligned} B_n &:= \{x;\ (\ln|\Lambda_n|)^{-1}\ln(N_n + 1) < \alpha - \varepsilon\} \\ &\subset \{(\ln|\Lambda_n|)^{-1}\ln(N'_n + 1) < \alpha - \varepsilon\} \end{aligned} \tag{5.5}$$

with the notations $N_n = N(n, l(n), A)$ and $N'_n = |\Delta'_{n,\,l(n)}(x) \cap A|$.

Since s_n is well separated, these empirical fields are conditionally independent under P given Λ^c [defined below (5.1) with $s = s_n$]; hence N'_n is the sum of $|s_n|$ conditionally independent Bernoulli variables, with different parameters but nevertheless bounded from below by $p_n = \inf_{z\in\mathscr{X}} \Pi_{\Lambda_{l(n)}}(R_{l(n),x} \in A/_{\Lambda_{l(n)}} z)$. Denoting again by $\mathscr{B}(m, p)$ a binomial variable, it follows that N'_n is stochastically larger than $\mathscr{B}(|s_n|, p_n)$ and then

$$P(B_n) \le \text{Prob.}\{\mathscr{B}(|s_n|, p_n) < |\Lambda_n|^{\alpha-\varepsilon}\} \tag{5.6}$$

by the assumption $p_n \ge |\Lambda_n|^{-b-\varepsilon/2}$ for large n. Then $|s_n| p_n > |\Lambda_n|^{\alpha-\varepsilon}$, which entitles us to use Cramér's inequality: for *every* such n it holds that

$$P(B_n) \le \exp\left[-|s_n|\left\{\frac{|\Lambda_n|^{\alpha-\varepsilon}}{|s_n|}\ln\frac{|\Lambda_n|^{\alpha-\varepsilon}}{|s_n| p_n} + \left(1 - \frac{|\Lambda_n|^{\alpha-\varepsilon}}{|s_n|}\right)\ln\frac{1 - |\Lambda_n|^{\alpha-\varepsilon}/|s_n|}{1 - p_n}\right\}\right].$$

When p_n ranges over $[|\Lambda_n|^{-b-\varepsilon/2}, 1]$, the previous bound is maximized at the leftmost point; next, the previous bound is certainly less than the one replacing the ratio $|\Lambda_n|^{\alpha-\varepsilon}/|s_n|$ by $|\Lambda_n|^{\alpha-\varepsilon}/|\Lambda_n|^{1-\varepsilon/3} = |\Lambda_n|^{-b-2\varepsilon/3}$ and therefore we have, for large n,

$$\begin{aligned} P(B_n) &\le \exp\left[-|s_n|\left\{-\frac{\varepsilon}{6}|\Lambda_n|^{-b-2\varepsilon/3}\ln|\Lambda_n| + (1 - |\Lambda_n|^{-b-2\varepsilon/3})\ln\frac{1 - |\Lambda_n|^{-b-2\varepsilon/3}}{1 - |\Lambda_n|^{-b-\varepsilon/2}}\right\}\right] \\ &= \exp\left[-|s_n|\left\{(1 - |\Lambda_n|^{-b-2\varepsilon/3})\ln\frac{1}{1 - |\Lambda_n|^{-b-\varepsilon/2}} + O(|\Lambda_n|^{-b-2\varepsilon/3}\ln|\Lambda_n|)\right\}\right] \\ &\le \exp[-|\Lambda_n|^{\alpha-\varepsilon}]. \end{aligned}$$

Then the lemma follows from the Borel–Cantelli lemma. □

PROOF OF THEOREM 5.1. The upper bound is a direct application of Lemma 5.1, and the lower bound of Lemma 5.2 with $a_n = t|\Lambda_n|$ together with (4.5). □

REMARK 5.2. The finite range property of the interaction allows here the use of the Markov property (conditional independence). In the infinite range case the strategy developed in Lemma 3.3 of Comets (1994) can be used instead.

We now focus on the framework of Section 3. The contraction principle applied with the continuous functional $Q \mapsto \int f\, dQ$ on $\mathscr{P}(\mathscr{X})$ transforms the large deviation principle with rate function I for the empirical field stated in Section 3 into a large deviation principle for the space averages of f, and the new rate function is $y \mapsto \inf\{I(Q);\ \int f\,dQ = y\}$. Since I has compact level sets, the right-hand side of (3.1) has to coincide with this rate function,

$$I_f(y) = \inf\left\{I(Q);\ Q \in \mathscr{P}_s(\mathscr{X}),\ \int f\,dQ = y\right\}, \tag{5.7}$$

with the convention that the infimum is $+\infty$ if the set is empty. Since I_f is the minimum of a lower semicontinous (l.s.c.) affine function under a linear continuous constraint, I_f is a l.s.c. and convex function of the constraint value. Note finally that (3.2) follows from lower semicontinuity of I_f, from compactness and from (4.3).

PROOF OF THEOREM 3.1. Note that the condition on $l(n)$ in the statement of the theorem is equivalent to $|\Lambda_{l(n)}| \sim t^{-1}|\Lambda_n|$. Let $A = \{R \in \mathscr{P}(\mathscr{X}); \int f\,dR \geq y\}$. If n_0 denotes the diameter of W, then of course $|\Lambda_n|$, $|\Lambda_{n-n_0}|$, m_n are equivalent as $n \to \infty$, and $N(n-n_0, l(n), A) \leq M_n(y) \leq N(n, l(n), A)$. Then, using Theorem 5.1 twice [once with $n, l(n)$ and once with $n - n_0, l(n)$], we obtain

$$\lim_{n\to\infty} (\ln m_n)^{-1} \ln M_n(y) = (1 - t^{-1} I(A))^+, \quad P\text{-a.s.}, \tag{5.8}$$

provided that $I(\mathring{A}) = I(\bar{A})$. Here A is a half-space, and from Remark 5.2(ii), the equality may fail only when $\mathring{A} = \varnothing$, and of course $A \neq \varnothing$, or equivalently only when y is on the boundary of $\operatorname{Dom} I_f$. We may apply the same arguments to the set A^c instead of A, and we then get

$$\lim_{n\to\infty} (\ln m_n)^{-1} \ln(m_n - M_n(y)) = (1 - t^{-1} I(A^c))^+, \quad P\text{-a.s.}, \tag{5.9}$$

for $y \neq \min f$. Clearly one of the two numbers $I(A)$ and $I(A^c)$ is 0 and the other one is $I_f(y)$, and so we have proved the pointwise convergence statement of the theorem. To obtain uniform convergence, it is enough to notice that in both (5.8) and (5.9) we have P-a.s. convergence on a dense countable subset of $\mathbb{R}$ of a sequence of monotone functions to a bounded continuous limit and to use Dini's theorem. □

REMARK 5.3. In the case when y belongs to the boundary of $\operatorname{Dom} I_f$, we believe that Theorem 3.1 holds true, but we could not prove it. Clearly $\operatorname{Dom} I_f \subset [\min f, \max f]$ but these sets are different in general; for instance we may have, for $l \geq 2$,

$$\max\left\{|\Lambda_l|^{-1} \sum_{j\in\Lambda_l} f\circ\theta_j(x); x \in \mathscr{X}\right\} < \max f. \tag{5.10}$$

On the other hand, we study in the next result a particular but interesting case where the equality holds in (5.10) as well as the convergence in (3.3) with $y \in \partial \operatorname{Dom} I_f = [\min f, \max f]$.

PROPOSITION 5.1. *Let $f\colon \mathscr{X} \to \mathbb{R}$, depending only on a single coordinate. Under the assumptions and notations of Theorem* 3.1 *we have for all $P \in \mathscr{G}$ and all $y \in \mathbb{R}$*:

$$\lim_{n\to\infty} (\ln m_n)^{-1} \ln\left\{\frac{M_n(y)}{m_n}\left[1 - \frac{M_n(y)}{m_n}\right]\right\} = -\min\{t^{-1} I_f(y), 1\}, \quad P\text{-}a.s. \tag{5.11}$$

Moreover the convergence is P-a.s. uniform on closed intervals where the limit is continuous.

This result applies in particular to estimating the large deviation rate function for the magnetization in the Ising model; see the example in Section 2 and the simulations in Section 7.

PROOF. We can assume that $f(x)$ depends only on x_0. Define $\mathscr{X}_0^\flat = \{x_0 \in \mathscr{X}_0; f(x) = \max f\}$. Following the proof of Theorem 5.1, we see that it is enough to prove a.s. convergence when $y = \max f$. Acording to Theorem 5.1 this will follow from

$$\liminf_{n\to\infty} |\Lambda_n|^{-1} \ln \inf_{z\in\mathscr{X}} \Pi_{\Lambda_n}\{x_{\Lambda_n} \in (\mathscr{X}_0^\flat)^{\Lambda_n} |_{\Lambda_n} z\} \geq -I_f(y).$$

From (2.3) we have

$$\begin{aligned}\Pi_{\Lambda_n}(x_{\Lambda_n} \in (\mathscr{X}_0^\flat)^{\Lambda_n} /_{\Lambda_n} z) &= [Z_{\Lambda_n}({}_{\Lambda_n} z)]^{-1} \sum_{x_{\Lambda_n} \in (\mathscr{X}_0^\flat)^{\Lambda_n}} \exp\{U_{\Lambda_n}(x_{\Lambda_n} \vee z)\} \\ &= [Z_{\Lambda_n}({}_{\Lambda_n} z)]^{-1} \quad Z^\flat_{\Lambda_n}({}_{\Lambda_n} z)\end{aligned}$$

with the notations $Z^\flat$, $p^\flat$ when using $\mathscr{X}^\flat = (\mathscr{X}_0^\flat)^{\mathbb{Z}^d}$ as state space instead of $\mathscr{X}$. From (4.2) we have

$$\begin{aligned}&\liminf_{n\to\infty} |\Lambda_n|^{-1} \ln \inf_{z\in\mathscr{X}} \Pi_{\Lambda_n}\{x_{\Lambda_n} \in (\mathscr{X}_0^\flat)^{\Lambda_n} |_{\Lambda_n} z\} \\ &\qquad = -p(\phi) + p^\flat(\phi) \\ &\qquad = -p(\phi) + \max\left\{\int \phi\, dQ + H(Q);\ Q \in \mathscr{P}_s(\mathscr{X}),\ Q(\mathscr{X}^\flat) = 1\right\} \\ &\qquad = -\min\left\{I(Q);\ Q \in \mathscr{P}_s(\mathscr{X}), \int f\, dQ = y\right\} \\ &\qquad = -I_f(y),\end{aligned}$$

using (4.1) and (4.2), which is the desired result. □

We now consider the vector case, which is of interest for applications as emphasized in the introduction. Let f be a local function from $\mathscr{X}$ to $\mathbb{R}^\nu$, $\nu \geq 1$, depending only on the restriction x_W of x to some finite set $W \subset \mathbb{Z}^d$, and we define again

$$I_f(v) = \min\left\{I(Q); Q \in \mathscr{P}_s(\mathscr{X}),\ \int f\, dQ = v\right\}, \qquad v \in \mathbb{R}^\nu.$$

Then $\mathrm{Dom}\, I_f := \{v \in \mathbb{R}^\nu;\ I_f(v) < \infty\}$ coincides with $\{\int f\, dQ;\ Q \in \mathscr{P}_s(\mathscr{X})\}$; it is a convex subset of $\mathbb{R}^\nu$ and

$$I_f(v) = \max\{I_{u\cdot f}(u \cdot v);\ u \in \mathscr{S}\}$$

with $\mathscr{S}$ the unit sphere in $\mathbb{R}^\nu$. Similarly to Theorem 3.1 we will consider the random variables

$$M'_{n,u}(y) = \left| \left\{ i \in \mathbb{Z}^d;\ i + \Lambda_{l(n)} + W \subset \Lambda_n,\ |\Lambda_{l(n)}|^{-1} \sum_{j \in i + \Lambda_{l(n)}} u \cdot f \circ \theta_j \ge y \right\} \right|$$

for y real, and $M_{n,u}(y) = \{M'_{n,u}(y) \vee 1\} \wedge \{m_n - 1\}$ with m_n as before.

THEOREM 5.2. *Let $l(n)$ be a nondecreasing sequence of integers with $|\Lambda_{l(n)}| \sim t^{-1} \ln |\Lambda_n|$, $t > 0$. For all $P \in \mathscr{G}$ and v not belonging to the boundary $\partial\, \mathrm{Dom}\, I_f$ of the domain of I_f we have, P-a.s.,*

$$\lim_{n\to\infty} (\ln m_n)^{-1} \min_{u \in \mathscr{S}} \ln \frac{M_{n,u}(u \cdot v)}{m_n} = -\min\{t^{-1} I_f(v), 1\}. \tag{5.12}$$

Even though it looks somewhat different, (5.12) is exactly the extension of Theorem 3.1. From the elementary facts $(1/2)[p \wedge (1-p)] \le p(1-p) \le p \wedge (1-p)$, $p \in (0,1)$ and $\min_u\{p_u \wedge (1-p_u)\} = \min_u p_u \wedge \min_u (1-p_u)$, $p_u \in (0,1)$, we have indeed

$$\frac{1}{2} \le \min_{u \in \mathscr{S}} \left\{ \frac{M_{n,u}}{m_n} \left[1 - \frac{M_{n,u}}{m_n} \right] \right\} \Big/ \left(\min_{u \in \mathscr{S}} \frac{M_{n,u}}{m_n} \wedge \min_{u \in \mathscr{S}} \left[1 - \frac{M_{n,u}}{m_n} \right] \right) \le 1,$$

where $M_{n,u}$ is a shorthand for $M_{n,u}(u \cdot v)$. On the other hand, we can see from the proof below that (5.12) still holds with $1 - M_{n,u}/m_n$ instead of $M_{n,u}/m_n$ (in fact they yield very close values for $\min_{u \in \mathscr{S}}$ in (5.12) since $\mathscr{S}$ is symmetric with respect to 0). Hence (5.12) also holds when replacing $M_{n,u}$ with $M_{n,u}[1 - M_{n,u}/m_n]$, which is our claim.

PROOF. Define $A(u, y) = \{Q \in \mathscr{P}(\mathscr{X});\ u \cdot \int f\, dQ \ge y\}$, $u \in \mathscr{S}$, $y \in \mathbb{R}$. From Lemma 5.1 with $A = A(u, u \cdot v)$ it follows immediately that $\limsup_{n\to\infty} (\ln m_n)^{-1} \min_{u \in \mathscr{S}} \ln(M_{n,u}(u \cdot v)/m_n)$ is not larger than the right-hand side of (5.12). For the reverse inequality, we may assume that v belongs to the interior of Dom I_f. We start by proving that $\forall\ \delta > 0, \exists\ k_0 \ge 1$ and $u_1, \ldots, u_{k_0} \in \mathscr{S}$ such that $\forall\ u \in \mathscr{S}, \exists\ k \le k_0$:

$$\{w \in \mathrm{Dom}\, I_f;\ u_k w \ge u_k v + \delta\} \subset \{w \in \mathrm{Dom}\, I_f;\ uw \ge uv\}. \tag{5.13}$$

Since f is bounded, we can find $r < \infty$ such that $\mathrm{Dom}\, I_f$ is contained in the ball with center v and radius r. Let $u_1, \ldots, u_{k_0} \in \mathscr{S}$ such that the balls with radius δ/r and center u_k, $k \le k_0$ cover the sphere $\mathscr{S}$. Then for $u \in \mathscr{S}$ and u_k with $|u - u_k| < \delta/r$, the inequality $u_k(w - v) \ge +\delta$ implies $u(w - v) \ge 0$ for any $w \in \mathrm{Dom}\, I_f$. This proves (5.13). □

Recall that $M_{n,u}(y) \geq N(n - n_0, l(n), A(u, y))$ with $n_0 = \operatorname{diam} V$ and note that $\int f\,dQ \in \operatorname{Dom} I_f$ for all Q. The relation (5.13) implies that

$$\min_{u \in \mathscr{S}} M_{n,u}(uv) \geq \min_{k \leq k_0} N(n - n_0, l(n), A(u_k, u_k v + \delta)). \tag{5.14}$$

According to Theorem 5.1 we have, P-a.s. for large n,

$$\liminf_{n\to\infty} (\ln m_n)^{-1} \ln\{N(n, l(n), A) + 1\} \geq (1 - t^{-1} I(\mathring{A}))^+ \tag{5.15}$$

for $A = A(u_k, u_k \cdot v + \delta)$, $k \leq k_0$. Since v belongs to the interior of $\operatorname{Dom} I_f$, we have

$$\lim_{\delta\to 0} I(\mathring{A}(u_k, u_k \cdot v + \delta)) = I(A(u_k, u_k \cdot v)) \leq I_f(v).$$

This together with (5.14) and (5.15) implies that P-a.s.,

$$\lim_{n\to\infty} (\ln m_n)^{-1} \min_{u \in \mathscr{S}} \ln[M_{n,u}(u \cdot v)/m_n] = -t^{-1} I_f(v). \qquad \square$$

We investigate now the critical case $l(n) \sim (\ln n)^{\alpha}$ with $\alpha \in]1/d, 1/(d-1)[$.

THEOREM 5.3. *Assume $d \geq 2$. Let $l(n)$ be a nondecreasing sequence of integers such that $|\Lambda_{l(n)}|/\ln|\Lambda_n| \to \infty$ and $|\Lambda_{l(n)}|/(\ln|\Lambda_n|)^{d/(d-1)} \to 0$. Then, for all $P \in \mathscr{G}$ and $A \subset \mathscr{P}(\mathscr{X})$, we have P-a.s.,*

$$\begin{aligned} \mathbb{1}_{\mathring{A}\cap\mathscr{G}_s \neq \varnothing} &\leq \liminf_{n\to\infty} (\ln|\Lambda_n|)^{-1} \ln\{N(n, l(n), A) + 1\} \\ &\leq \limsup_{n\to\infty} (\ln|\Lambda_n|)^{-1} \ln\{N(n, l(n), A) + 1\} \\ &\leq \mathbb{1}_{\bar{A}\cap\mathscr{G}_s \neq \varnothing} \end{aligned}$$

with the notation $\mathbb{1}_{A\neq\varnothing} = 1$ if $A \neq \varnothing$, $\mathbb{1}_{A\neq\varnothing} = 0$ if $A = \varnothing$, $(A \subset \mathscr{P}(\mathscr{X}))$.

PROOF. The upper bound follows directly from Lemma 5.1 with $t = 0$. In order to prove the lower bound, we can restrict ourselves to the case when $\mathring{A} \cap \mathscr{G}_s$ contains at least one element Q. By assumption on $l(n)$, we can find a sequence $(a_l)_{l\geq 1}$ which coincides with $\ln|\Lambda_n|$ when $l = l(n)$, $n \geq 1$, and such that $a_n = o(|\Lambda_n|)$ and $|\Lambda_n| = o(a_n^{d/(d-1)})$. Then

$$b = -\liminf_{n\to\infty} a_n^{-1} \ln \inf_{z, \bar{z} \in \mathscr{X}} \Pi_{\Lambda_n}\{R_{n,x} \in A/_{\Lambda_n} z\}$$

is equal to zero, from Lemma 4.2(b) in Comets (1994), for large deviation inside the set of Gibbs measures. Then our Lemma 5.2 applies and implies the lower bound. $\square$

6. Large deviation principle for an empirical measure. We want to stress the large deviation principle which is behind our results as well as the Erdős–Rényi law (1970). Let

$$\hat{\mu}_n = \hat{\mu}_n(x)$$

be the uniform measure of the set of "moving" empirical fields $\Delta_{n,\,l(n)}(x)$:

$$\hat{\mu}_n = |\{i;\ i + \Lambda_{l(n)} \subset \Lambda_n\}|^{-1} \sum_{i:\ i+\Lambda_{l(n)}\subset\Lambda_n} \delta_{R_{i,\,l(n),\,x}}. \tag{6.1}$$

Then $\hat{\mu}_n$ is a probability measure on $\mathscr{P}(\mathscr{X})$ and we have

$$\hat{\mu}_n(A) = |\{i;\ i + \Lambda_{l(n)} \subset \Lambda_n\}|^{-1} N(n, l(n), A). \tag{6.2}$$

We consider again a nondecreasing sequence of integers $l(n)$ with $|\Lambda_{l(n)}| \sim t^{-1} \ln |\Lambda_n|$ for some $t > 0$. Note that the functional

$$J(Q) = I(Q) \quad \text{if } I(Q) \le t,$$
$$J(Q) = +\infty \quad \text{if } I(Q) > t$$

is lower semicontinuous from the compact space $\mathscr{P}_s(\mathscr{X})$ to $[0, +\infty]$. We set as above $J(A) = \inf\{J(Q);\ Q \in A \bigcap \mathscr{P}_s(\mathscr{X})\}$.

THEOREM 6.1. *For any $P \in \mathscr{G}$, the sequence $\hat{\mu}_n$ obeys an almost sure large deviation principle in the scale $|\Lambda_{l(n)}|$ with rate function J. More precisely, for P-a.e. x, we have, for all $A \subset \mathscr{P}(\mathscr{X})$,*

$$\begin{aligned} -J(\mathring{A}) &\le \liminf_{n\to\infty} \mid \Lambda_{l(n)} \mid^{-1} \ln \hat{\mu}_n(A) \\ &\le \limsup_{n\to\infty} \mid \Lambda_{l(n)} \mid^{-1} \ln \hat{\mu}_n(A) \\ &\le -J(\bar{A}). \end{aligned} \tag{6.3}$$

See also Torrent (1996) for related results and a more systematic study. This theorem complements Theorem 3.1 in Comets (1994), which states that the support $\Delta_{n,\,l(n)}(x)$ of $\hat{\mu}_n$ converges in the Hausdorff distance to the level set $\Gamma_t = \{Q \in \mathscr{P}_s(\mathscr{X});\ I(Q) \le t\} = \{Q \in \mathscr{P}_s(\mathscr{X});\ J(Q) < \infty\}$.

PROOF. We first prove that (6.3) holds P-a.s. for any given A.

Since $\ln x \le \ln(x+1),\ x \ge 0$, the upper bound in (6.3) follows from Theorem 3.1 when $I(\bar{A}) \le t$, and from Remark 5.1(i) when $I(\bar{A}) > t$.

It is enough to prove the lower bound when $J(\mathring{A}) < +\infty$, that is, when $I(Q) \le t$ for some $Q \in \mathring{A}$. Then there exists also some $R \in \mathring{A}$ with $I(R) < t$ since I is affine, and so $I(\mathring{A}) = J(\mathring{A}) < t$. We have $1 - t^{-1}I(\mathring{A}) > 0$, and with the elementary bound $\ln(1 + x) \le \ln 2 + \ln x,\ x \ge 1$ we see that the lower bound in (6.3) follows from Theorem 3.1.

To complete the proof, we now check that we can interchange "$\forall A$" and "P-a.s." Since $\mathscr{P}(\mathscr{X})$ is a separable metric space, we can perform the interchange for the lower bound. As for the upper bound, we define the level set $\Gamma_s = \{Q \in \mathscr{P}_s(\mathscr{X});\ J(Q) \le s\},\ s \ge 0$, and its ε-neighborhood $\Gamma_{s,\,\varepsilon}$ in the Prohorov metrics on $\mathscr{P}(\mathscr{X})$. Then $J(\Gamma^c_{s,\,\varepsilon}) < s$, and the set

$$\mathscr{X}' = \left\{x \in \mathscr{X};\ \forall\ \varepsilon \in \mathbb{Q}^*_+\ \forall\ s \in \mathbb{Q}_+,\ \limsup_{n\to\infty} \mid \Lambda_{l(n)} \mid^{-1} \ln \hat{\mu}_n(\Gamma^c_{s,\,\varepsilon}) \le -s\right\}$$

has P-probability 1. Let A with $J(\bar{A}) > 0$; for all $s \in [0, J(\bar{A})[$ we can choose $\varepsilon \in \mathbb{Q}^*_+$ with $A \bigcap \Gamma_{s,\,\varepsilon} = \varnothing$, and therefore we have

$$\limsup_{n\to\infty} \mid \Lambda_{l(n)} \mid^{-1} \ln \hat{\mu}_n(A) \le \limsup_{n\to\infty} \mid \Lambda_{l(n)} \mid^{-1} \ln \hat{\mu}_n(A)$$
$$\le -s$$

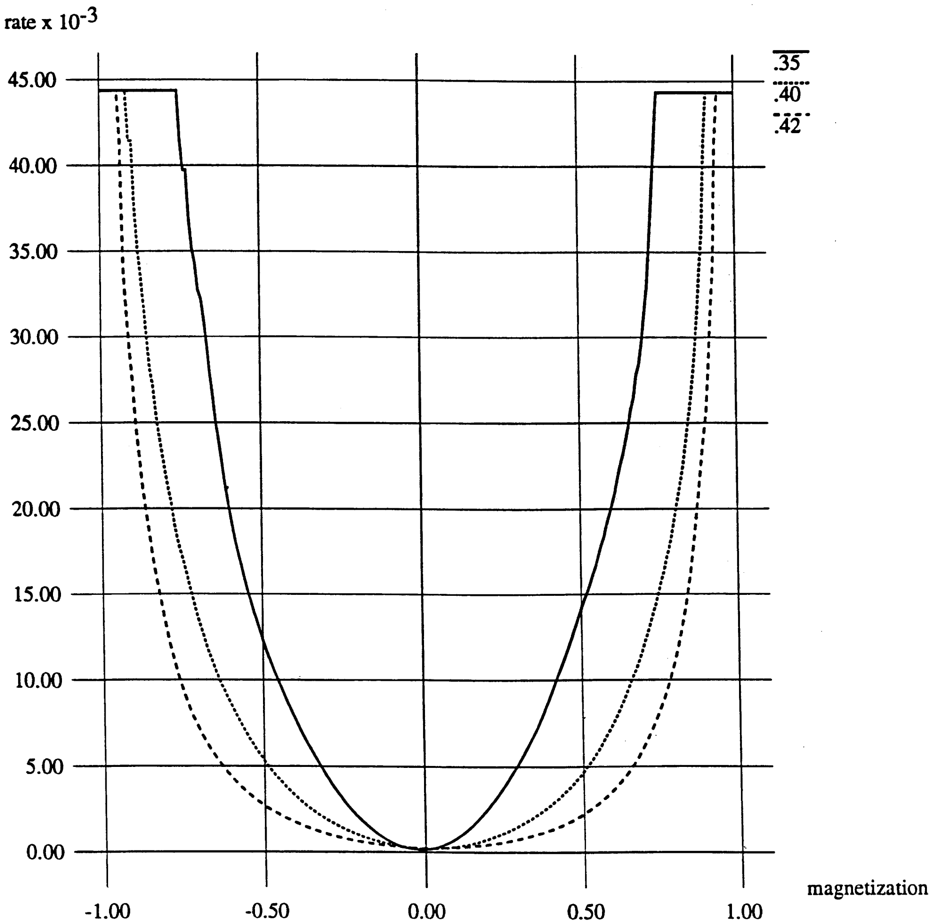

FIG. 1. *$h = 0$ and high temperature: $\beta = 0.35$ (solid line), $\beta = 0.40$ (dotted line), $\beta = 0.42$ (dashed line).*

for all $x \in \mathscr{X}'$. Hence the upper bound is valid on the set $\mathscr{X}'$ which has full measure. □

7. Simulation experiments. We illustrate now the practical interest of the method. Samples from the two-dimensional nearest neighbor Ising model [see the example in Section 2] were simulated via the Gibbs sampler algorithm with precomputed transition probabilities. We have used periodic boundary conditions on square boxes $\Lambda_n = [-n, n]^2$ with $n = 200$ in general. The well-known finite-size effects lead to an "experimental critical inverse temperature" lower than the real value $\beta_c(2) = 0.4406868\ldots$. For the function of interest we have taken the magnetization $f(x) = x_0$.

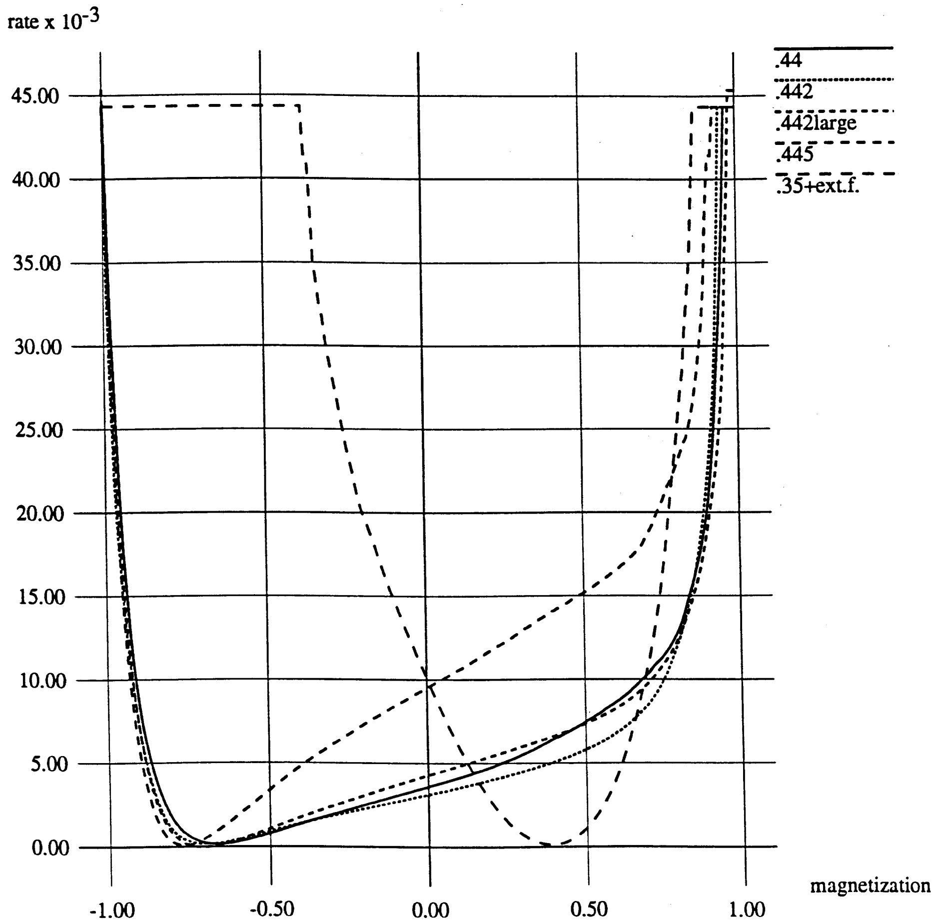

FIG. 2. *Low temperature*: $h = 0$ *and* $\beta = 0.44$ (*solid line*), $\beta = 0.442$ *with* $n = 200$ (*dotted line*), $\beta = 0.442$ *with* $n = 800$ (*short dashes*), $\beta = 0.445$ (*medium dashes*); *high temperature and external field*; $h = 0.03$ *and* $\beta = 0.35$ (*large dashes*).

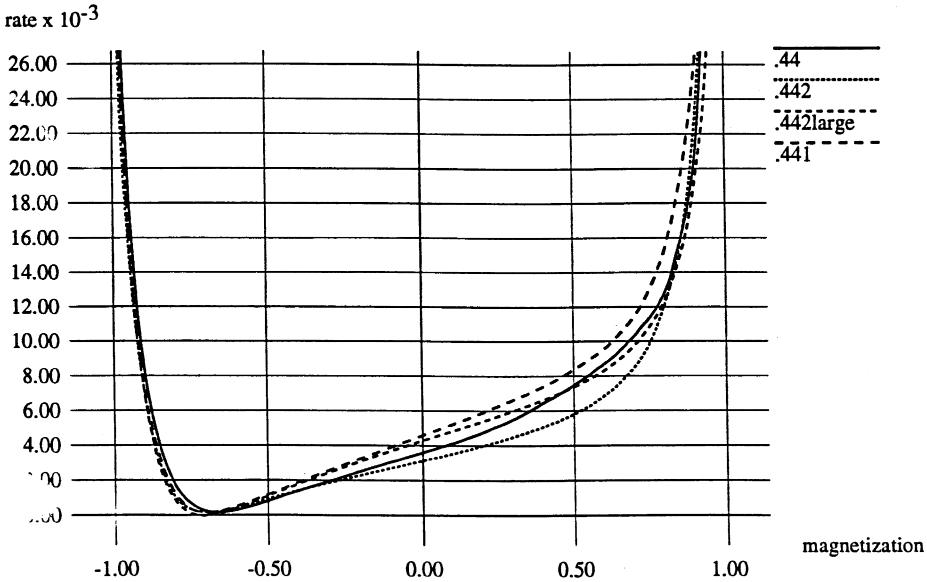

FIG. 3. *Zoom on the critical region at low temperature, zero external field*: $\beta = 0.44$ (*solid line*), $\beta = 0.441$ (*large dashes*), $\beta = 0.442$ *and* $n = 200$ (*dotted line*), $\beta = 0.442$ *and* $n = 800$ (*small dashes*). *This indicates the amplitude of fluctuations.*

In Figures 1–3 we show estimates of I_f from simulations with various values of the parameters. More precisely, we plot the function of y:

$$-(\ln m_n)^{-1} t \left\{ \ln \left\{ \frac{M_n(y)}{m_n} \left[1 - \frac{M_n(y)}{m_n} \right] \right\} + 2\ln(2) \right\},$$

which is the estimator from Section 3, with the slight modification of adding $2\ln 2$ to reduce the bias at the bottom of the curve. This does not change the asymptotics of Theorem 3.1, and it converges to $\min\{t^{-1} I_f(y), 1\}$. The parameter t was taken as 0.05. In general our estimates "look like" a convex function. For small values of β and $h = 0$ the curvature is large close to the bottom. As β increases the bottom part becomes flatter and flatter. At criticality and after, the spontaneous magnetization appears and reflects in the minimum of the estimate. A flat part seems to extend from this value to its opposite. At the critical point, a drastic change occurs in the curvature of the estimate close to its minimum.

The present figures should be compared with those in Comets (1994). The ones here are much smoother and closer to convexity; they are obtained via a single sample, though an average of over ten samples was performed in our previous paper. They show a significant improvement compared to the previous results, and they could be suitable for hypothesis testing of phase transition, based on the curvature of the estimate for I_f. Note that our choice of t here is arbitrary.

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