Multifractal and critical properties of the Ising model

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(Received 21 November 1997)

Multifractal properties of the two-dimensional Ising model are studied by means of the $f(\alpha)$ spectra of singularities of probability measures supported by energy spectra. These measures are determined through calculations of energy degeneracies for finite-size systems up to 12×12 spins in cases of square and triangular lattices and up to 22×22 spins in the case of the hexagonal lattice. The calculations are performed in an exact manner using the transfer-matrix method. It is argued that, in the thermodynamic limit, the scaling exponent $\alpha_{\max}$ associated with the most probable energy of the system takes at the critical temperature a minimum value and, consequently, it is argued that a given system reveals a phase transition at a finite temperature if $\alpha_{\max}$ possesses a minimum at the finite temperature. It is also shown that, in the thermodynamic limit, the spectrum $f(\alpha)$ shrinks when the critical temperature is approached. [S0163-1829(98)05317-X]

The multifractal formalism, developed for studying complex fractal systems in terms of probability theory,[1,2] bears in some sense resemblance to statistical mechanics. However, contrary to statistical mechanics, which describes systems having an enormously large number of degrees of freedom, the multifractal formalism has been introduced in the context of systems whose complexity does not result from high dimensions of their phase spaces. As a matter of fact, this formalism has originally been applied to characterize multifractal properties of chaotic trajectories generated by one- and two-dimensional nonlinear dynamical systems.[2,3] Nevertheless, this approach can be used in various cases where fractals occur, no matter what their origin and how large the dimensions of spaces in which they are embedded.[4]

In this paper, the multifractal formalism is applied to describe probability measures of energy levels of the two-dimensional Ising model in a zero magnetic field. The measures are obtained at particular temperatures, for finite-size $n\times n$ systems with free and cylindrical boundary conditions. (The term cylindrical boundary conditions is used here for edge constraints of finite-size two-dimensional lattices with periodic boundary conditions in one direction and with free boundary conditions in the second direction.) Properties of the probability measures are investigated using the spectra $f(\alpha)$ of their singularities (with the Hölder exponent α being dependent on the temperature). It is shown that these measures display a multifractal character and that the multifractal spectra $f(\alpha)$ found for them change in a specific way as the temperature varies, enabling one to determine for a given n a pseudocritical temperature. Numerical results obtained for successive n indicate that this pseudocritical temperature tends to the true critical temperature as the thermodynamic limit is approached. Accordingly, it is also shown that the specific behavior of the spectra $f(\alpha)$ near criticality provides a possibility of formulating new criteria for the occurrence of phase transitions on the grounds of multifractal properties of systems of discrete energies.

The zero-field Ising model considered in this Brief Report is defined on $n\times n$ square, triangular, and hexagonal lattices with free and cylindrical boundary conditions. In the case of the free boundary conditions, the square and triangular lattices are assumed to be of the shape of squares and rhombes, respectively. Each system on the hexagonal lattice with free boundary conditions is taken as being obtained from the one on the respective hexagonal lattice with cylindrical boundary conditions by cutting all bonds along a straight line, parallel to the axis of the rotational symmetry of the cylinder. The spin variables $s_i=\pm1$, $i=1,2,\ldots,n\times n$, are assumed to be coupled by nearest-neighbor interactions $K=J/k_BT$ with $J\geqslant0$ being the exchange integral and T denoting the temperature.

Generally, energy levels of the model under study here are highly degenerate. It should be pointed out that, for the $n\times n$ system, there are $2^{n\times n}$ spin configurations, but the number of different energy levels amounts only to $M_n=c_n n\times n$ with $0<c_n<2$ being dependent on the lattice symmetry and boundary conditions (in addition to the n dependence). The degeneracies of energy levels of the considered model are determined here using the transfer-matrix method.[5–7] In the case of the $n\times n$ Ising systems, this approach relies on a construction of larger systems from smaller ones by attaching successive chains of n spins. Consequently, this allows one to determine all possible energy levels at each construction stage and to calculate exactly corresponding degeneracies in a recursive way (for details see, e.g., Ref. 7). The recursion relation for the degeneracies $\mathcal{D}_{k'}^{(m+1)}(\gamma')$ of energies of a subsystem of the size $n\times(m+1)$, $1\leqslant m\leqslant n-1$, (consisting of $m+1$ interacting chains, each of the length n) with k' upsetting bonds, i.e., bonds connecting antiparallel spin (in the ferromagnetic case), and with a spin configuration $1\leqslant\gamma'\leqslant2^n$ of the last added chain of spins is given by[5]

$$\mathcal{D}_{k'}^{(m+1)}(\gamma')=\sum_{\gamma=1}^{2^n}\sum_{k=0}^{N_m}\mathcal{D}_k^{(m)}(\gamma)\,\delta(k'-k-l_{\gamma'}-j_{\gamma,\gamma'}),$$

where δ is the Kronecker δ function, N_m denotes the largest possible number of upset bonds in the $n\times m$ subsystem, $l_{\gamma'}$ is the number of upset couplings in the last added chain in spin configuration γ', while $j_{\gamma,\gamma'}$ stands for the number of upset bonds linking the last [i.e., $(m+1)$th] chain in the configuration γ' to the former (mth) chain in the configuration γ. Obviously, the above formula can be used in the cases of both types of boundary conditions assumed in this paper.

As is well known, an essential limitation of the recursive method of calculating energy degeneracies lies in the finite memory of computers.[7] The largest systems considered below are of size 12×12 in the case of square as well as triangular lattices and of the size 22×22 in the case of the hexagonal lattice. Note that in the case of hexagonal symmetry, energy degeneracies can be computed for much larger systems than in cases of square and triangular symmetries. This follows from the fact that systems on hexagonal lattices of sizes $n\times n$, $n=4,6,\ldots,$ can be considered as chains of n spins, such that any two neighboring chains are coupled by only $n/2$ bonds (the notation $n\times n$ for the size of systems on hexagonal lattices does not reflect their shapes).

The multifractal properties of the studied finite-size Ising model are described here by applying the multifractal formalism to investigate singularities of probability measures of energy spectra of the model. The energy spectrum of a $n\times n$ system is determined by

$$E_i^{(n)}(K)=-K(W_n-m_i) \tag{1}$$

with $i=1,2,\ldots,M_n$ enumerating successive energy levels, W_n denoting the total number of bonds, and m_i being the number of upset bonds associated with the ith energy level ($m_{i+1}>m_i$, $i=1,2,\ldots,M_{n-1}$). Then, the normalized probability that the $n\times n$ system takes on the energy $E_i^{(n)}(K)$ is given by

$$p_i^{(n)}(K)=D_i^{(n)}e^{-E_i^{(n)}(K)}/Z_n(K), \tag{2}$$

where

$$D_i^{(n)}=\sum_{\gamma=1}^{2^n}\mathcal{D}_{m_i}^{(n)}(\gamma) \tag{3}$$

is the degeneracy of the ith energy level and

$$Z_n(K)=\sum_{i=1}^{M_n}e^{-E_i^{(n)}(K)} \tag{4}$$

is the partition function of the system.

According to a general scheme of the multifractal analysis,[2] the probability measure $p_i^{(n)}(K)$ can be expressed as

$$p_i^{(n)}(K)\sim\ell_n^{1/\alpha_i} \tag{5}$$

with ℓ_n standing for the scaling parameter and the scaling exponent α_i being dependent on K and n. Since the energy rescaling factor

$$[E_{i+1}^{(n)}(K)-E_i^{(n)}(K)]/[E_{\max}^{(n)}(K)-E_{\min}^{(n)}(K)]\sim 1/M_n,$$

where $i=1,2,\ldots,M_n-1$, $E_{\max}^{(n)}(K)$ and $E_{\min}^{(n)}(K)$ denote the maximal and minimal energy levels, respectively, the scaling parameter ℓ_n is assumed to be

$$\ell_n=1/M_n. \tag{6}$$

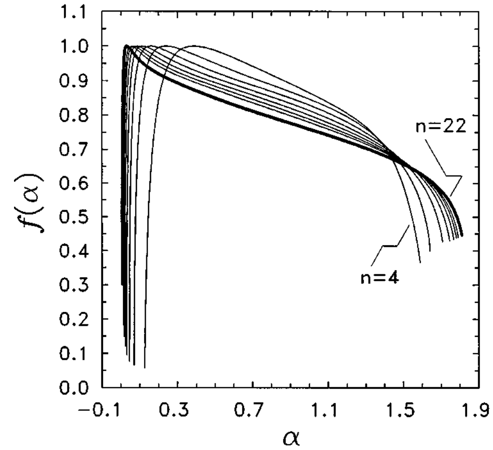

FIG. 1. The spectra $f(\alpha)$ for the $n\times n$ hexagonal Ising system with cylindrical boundary conditions and with the interaction parameter $K=0.5$, for $n=4,6,\ldots,16$ and $n=22$.

It should be pointed out that the scaling exponent α_i is introduced here in a somewhat different way than within the conventional formalism.[2] Due to the special definition adopted in this paper [Eqs. (5) and (6)], the index α_i is determined as a finite quantity for all n (provided that K remains finite). Note that the scaling parameter ℓ_n does not depend on K and thereby the index α_i reflects entirely the dependence of $p_i^{(n)}(K)$ on K. The spectra $f(\alpha)$ characterizing the distribution of exponents α can be found using the relations (cf. Ref. 2)

$$f(\alpha(q,K))=q/\alpha(q,K)-\tau(q,K), \tag{7}$$

$$\alpha(q,K)=[(d/dq)\,\tau(q,K)]^{-1} \tag{8}$$

with the *filtering* parameter $q\in(-\infty,\infty)$ and $\tau(q,K)$ being determined by requiring that the "generalized" partition function

$$\Gamma_n(q,K)=\ell_n^{-\tau(q,K)}\sum_{i=1}^{M_n}[p_i^{(n)}(K)]^q \tag{9}$$

satisfies the condition that $\Gamma_n(q,K)=1$ for all q and K.

The typical shape of the spectra $f(\alpha)$ is illustrated in Fig. 1 by an example of the spectra obtained for hexagonal systems of different sizes, for $K=0.5$. One should notice a rather fast convergence of the curves $f(\alpha)$ when n increases.[8] (It must be stressed that the distribution of energy levels is nonuniform for all $K<\infty$ and for all n.) As shown in Fig. 1, the spectra $f(\alpha)$ found for studied probability measures display a form that is characteristic for multifractal sets (cf. Ref. 2). Note that the maximum value of the spectra $f(\alpha)$ is given by $f(\alpha(0,K))=1$ for each $K<\infty$ and for each n, because the total number of energy levels $M_n=1/\ell_n$.

An interesting question that arises is an examination of the variation of multifractal properties of the studied model as the temperature changes, especially within the critical region. Some characterization of this variation can be obtained by investigating the K dependence of the maximal value of the scaling exponent α, given by $\alpha_{\max}(K)=\alpha(\infty,K)$. It follows from Eqs. (5) and (6) that $\alpha_{\max}(K)$ is associated with the maximum value of the probability of energy levels (i.e., with

TABLE I. Values of the pseudocritical interaction parameter $K_c(n)$ and the scaling exponent $\alpha(\infty,K_c(n))$ for $n\times n$ triangular Ising systems with free edges (columns 2, 3) and with cylindrical boundary conditions (columns 4, 5). The exact value for K_c is also included.

n	$K_c(n)$	$\alpha(\infty,K_c(n))$	$K_c(n)$	$\alpha(\infty,K_c(n))$
3	0.231 049	1.349 077	0.224 990	1.197 228
4	0.287 525	1.308 834	0.261 659	1.282 935
5	0.287 997	1.339 515	0.270 285	1.283 349
6	0.281 961	1.364 884	0.282 889	1.324 890
7	0.280 660	1.385 632	0.279 722	1.352 916
8	0.283 227	1.399 824	0.282 855	1.380 898
9	0.286 814	1.410 811	0.280 947	1.397 473
10	0.286 998	1.419 720	0.280 622	1.414 631
11	0.285 555	1.427 066	0.281 089	1.425 669
12	0.285 607	1.433 395	0.280 685	1.437 415
$K_c=$	0.274 653			

the energy region of the most concentrated probability measure). The dependence of $\alpha_{\max}(K)$ on K proves to be rather nontrivial. Indeed, $\alpha_{\max}(K)$ possesses for each n a unique minimum at a finite value of the interaction parameter $K_c(n)$. Numerical results obtained for $K_c(n)$ suggest that this quantity is convergent to the true critical coupling parameter K_c as n tends to infinity. Therefore, $K_c(n)$ determined for any finite n is called here the pseudocritical interaction parameter, and the corresponding temperature is named the pseudocritical temperature. Obviously, this pseudocritical temperature is, in general, different from those introduced earlier, on the basis of different methods.[9] Values of $K_c(n)$ and $\alpha(\infty,K)$ calculated for systems of various symmetries are listed in Tables I, II, and III. Note that the deviation of $K_c(n)$ from K_c, calculated for the largest of the considered hexagonal systems with cylindrical boundary conditions is less than 0.5%. However, the studied systems turn out to be too small in order to determine the asymptotic behavior of $K_c(n)$ [and $\alpha(\infty,K_c(n))$] for $n\to\infty$.

It is evident that $K_c(n)>K_c$ for systems with free edges and that values of $K_c(n)$ obtained in the case of cylindrical boundary conditions are, in general, closer to the respective exact critical parameter values K_c than in the case of free edges. This follows from the fact that, in systems with cylindrical boundary conditions, the tendency to enlarge the pseudocritical temperature, due to couplings between nearby spins by paths encircling the cylinder, is to some extent balanced by the tendency to diminish the pseudocritical temperature owing to the occurrence of free edges in the direction parallel to the axis of rotation symmetry of the cylinder.

TABLE II. Same as Table I for $n\times n$ square systems.

n	$K_c(n)$	$\alpha(\infty,K_c(n))$	$K_c(n)$	$\alpha(\infty,K_c(n))$
3	0.274 653	1.504 573	0.268 240	1.424 591
4	0.473 063	1.520 452	0.360 389	1.404 840
5	0.476 390	1.526 245	0.398 589	1.408 224
6	0.482 758	1.552 993	0.430 762	1.451 235
7	0.482 233	1.566 928	0.437 128	1.450 387
8	0.482 600	1.576 441	0.440 933	1.493 011
9	0.478 968	1.583 899	0.445 369	1.490 148
10	0.478 229	1.589 707	0.441 138	1.517 369
11	0.475 645	1.594 420	0.444 107	1.514 397
12	0.472 222	1.598 316	0.445 378	1.533 785
$K_c=$	0.440 689			

TABLE III. Same as Table I for $n\times n$ hexagonal systems.

n	$K_c(n)$	$\alpha(\infty,K_c(n))$	$K_c(n)$	$\alpha(\infty,K_c(n))$
4	0.648 952	1.759 205	0.485 448	1.588 654
6	0.681 212	1.763 004	0.608 574	1.604 431
8	0.694 351	1.759 375	0.631 877	1.633 861
10	0.689 488	1.754 697	0.634 475	1.652 013
12	0.696 180	1.751 037	0.643 669	1.656 944
14	0.689 479	1.748 199	0.650 186	1.663 261
16	0.690 026	1.746 037	0.650 200	1.668 020
18	0.687 753	1.744 387	0.653 078	1.671 810
20	0.686 528	1.743 093	0.654 124	1.674 989
22	0.685 846	1.742 079	0.655 369	1.677 692
$K_c=$	0.658 479			

The change of multicritical properties of the finite-size Ising model near the pseudocritical temperature can be described by determining the dependence of $\alpha(\infty,K)$ on K and by investigating the shape of the $f(\alpha)$ spectra for different values of K. The function $\alpha(\infty,K)$ is plotted in Fig. 2 for systems of different symmetries, in the case of cylindrical boundary conditions. The existence of minima of the index $\alpha(\infty,K)$ at some temperature values that converge to a nonzero (and finite) value as $n\to\infty$ appears to be a distinctive feature of systems exhibiting phase transitions at finite temperatures. It is clear that, at zero temperature, one has $\alpha_{\min}(K)=\alpha_{\max}(K)$, where the index $\alpha_{\min}(K)$ is associated with the most rarefied measure of energy levels, and then the system does not reveal multifractal properties.[2] As might be expected, the index $\alpha(\infty,K)$ displays the existence of minima at finite temperatures also in the case of chains of spins coupled by nearest-neighbor interactions. However, it

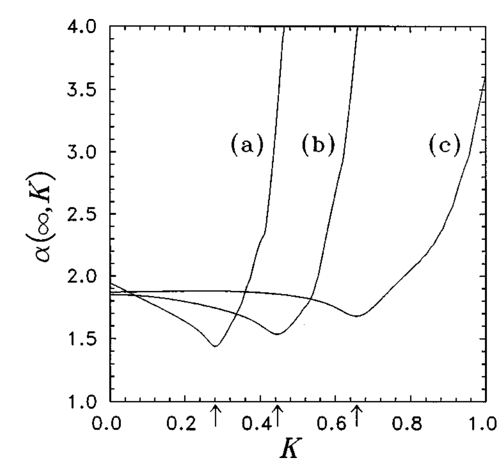

FIG. 2. The scaling exponent $\alpha(\infty,K)$ vs K for systems on lattices with cylindrical boundary conditions: (a) the 12×12 triangular lattice, (b) the 12×12 square lattice, (c) the 22×22 hexagonal lattice. The arrows indicate respective values of the pseudocritical temperature.

proves that, in this case, interaction parameter values at which the minima occur tend to zero as $2/n$ when $n\rightarrow\infty$ [in contradistinction to the case of $n\times n$ spin systems, for which $K_c(n)$ tends to a nonzero limit as $n\rightarrow\infty$].

One can easily show that, for each finite K, the exponent $\alpha_{\min}(K)$ vanishes very fast as n grows. Consequently, the width of $f(\alpha)$, defined for particular values of K as $w(K)=\alpha_{\max}(K)-\alpha_{\min}(K)$, takes a minimum value at some nonzero temperature, dependent on n. As can easily be seen, this temperature value tends to the critical temperature as $n\rightarrow\infty$, and its deviation from the respective pseudocritical temperature decreases very rapidly when n increases. The change of the shape of the $f(\alpha)$ spectra under a variation of K is illustrated in Fig. 3, for the case of the 22×22 system on a hexagonal lattice. This figure exemplifies a shrinking of the $f(\alpha)$ spectra as the temperature varies towards respective pseudocritical temperatures.

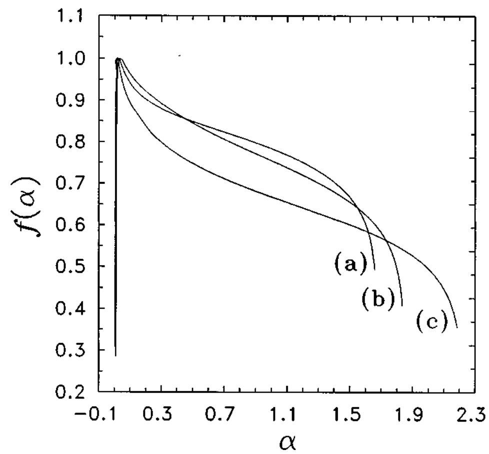

FIG. 3. The spectra $f(\alpha)$ for the 22×22 hexagonal lattice with cylindrical boundary conditions, for different values of the interaction parameter: (a) $K=K_c(22)$, (b) $K=K_c(22)-0.2$, (c) $K=K_c(22)+0.2$, where $K_c(22)$ denotes here the pseudocritical coupling parameter determined for the 22×22 hexagonal system with cylindrical boundary conditions.

Thus, the analysis of multifractal properties of probability measures of energies implies the following new criteria of phase transitions: a system with discrete energies undergoes a phase transition at a finite temperature if the scaling exponent $\alpha(\infty,K)$ and/or the width $w(K)$ of the $f(\alpha)$ spectrum determined for the system displays a minimum at the finite temperature, as the thermodynamic limit is approached. It should be pointed out that these criteria differ essentially from the ones introduced recently on the basis of an analysis of the so-called density of states functions, determined for finite-size systems.[10] The analysis of these functions requires taking into account magnetic energies of considered systems and is then carried out in the dependence on the temperature and the magnetic field.

In summary, investigations of interrelations between multifractal and critical properties of systems considered here have led to formulating new criteria for phase transitions. It should be noted, however, that the criteria have been introduced on the basis of studies of the model which exhibits phase transition of the second order. Therefore, it would be interesting to investigate multifractal properties of systems revealing phase transitions of the first order. Generally, one can conclude that the application of the multifractal formalism to study probability measures of energies of discrete models considered within statistical mechanics can yield new insight into the properties of these systems.

This research was supported by the Polish Committee for Scientific Research under Grant No. 8 T11F 010 08p04.

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