Critical behavior of Ising spins in a tridimensional percolating nano system with noninteger fractal dimension.

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Abstract

In an artificial 3D percolation nano medium, the clusters filled by the Ising magnets give rise to a topologically nontrivial magnetic structure, leading to new features of the ferromagnetic phase transition without an external magnetic field. In such an inhomogeneous system, the standard Ising model is strongly modified by the spatial percolation cluster distribution. We found numerically that at percolation occupation probability $p < 1$ far from the percolation threshold $p_{c3D}$, the magnetization shows ferromagnetic-paramagnetic phase transition with the transition temperature $T_c$ depending considerably on the probability $p$. We provide numerical evidence that in vicinity $p_{c3D}$ the dependence $T_c(p)$ is affected by the noninteger fractal dimension $D_H(p)$ of the incipient percolation spanning cluster.
I. INTRODUCTION

The Ising model with no external magnetic field possesses by the critical behavior, when below the critical temperature the phase transition from paramagnetic state to ferromagnetic state occurs. However, do the critical properties of the three dimensional (3D) Ising model still exist for a noninteger dimension case with a fractal (Hausdorff) dimension of $D_H < 3$? (Let us remind that the fractal dimension, $D_H$, is a statistical quantity that gives an indication of how completely a fractal appears to fill space, as one zooms down to finer and finer spatial scales\cite{1}) To answer this question, we study the nano structure of a spanning cluster in 3D embedded percolation environment for the creation an object with a fractional dimension. The spanning cluster in such a situation provides the connection between the input and output (opposite sides) of the sample. As a result, the opportunity to incorporate the spins into such an opened nano structure becomes possible. Forcing the spin ensemble through such a percolation medium allows creating a network of spins, leaving other parts of the system unchanged. Since for 3D geometry the fractal dimension of the incipient spanning cluster is $D_H \approx 2.54$ (see e.g. \cite{2}, \cite{3}), in principle, this allows studying experimentally the properties of phase transition in the Ising model in geometry with noninteger dimension.

The original idea to study critical behavior for non-integer space by use of a fractal lattice is due to Gefen, Mandelbrot and Aharony\cite{4}. The spin model chosen is the Ising model, where spins are classical variables taking the values ±1. The idea suggested by Gefen et. al. was to construct a space domain with noninteger dimension via a fractal lattice (the Sierpinski carpets), and then study its critical behavior as a function of the noninteger dimension. However, in which way could such a critical behavior be studied experimentally in spin- and optoelectronics?

The Ising model near criticality in 2D and 3D dimensions has been studied numerically via Monte Carlo methods by Cambier and Nauenberg\cite{5}. They considered the system closely below the critical temperature $T_c$ and studied the cluster size distribution. Using such definition of critical clusters, Coniglio\cite{6} was able to compute the fractal dimension of these clusters, by mapping the Potts model to the Coulomb gas. The Coniglio-Klein clusters of the Ising model in 3 dimensions have been investigated by Wang and Stauffer\cite{7} using Monte Carlo simulations.

Let us recall that for fractals involving a random element, one speaks about a statistical
self-similarity, meaning equivalent, after the proper rescaling, statistical distributions characterizing the geometry of a part and of the whole fractal. It’s worth to note that such a compound system (clusters with spins) can be created in the experiment if to fill the voids of percolating clusters by nano-particles of a ferromagnetic (magnetorheological) fluids that recently were synthesized\[8]-\[14]. The registration of incipient percolation cluster by optical methods was recently considered in Ref.\[15\], while the specific dynamical field properties of radiated nanoemitteres incorporated in a percolating cluster are studied in Ref.\[16\].

In a percolation medium filled by the spins, there are two distinct physically important order parameters that are defined by a geometrical configuration of the nearest neighbors in such a compound system. The first (percolating $P_{3D}$) order parameter is defined by the occupation probability of the lattice cells $p$. The percolation structure normally creates a hollow fractal network of channels that can be filled by a liquid, gas, conductivity electrons, etc.

In this paper we consider the properties of a 3D percolation medium where the percolation channels are filled by the spins. The second order parameter (average magnetization $M$) depends on the temperature $T$. We numerically show that the critical properties of such an extended Ising model (EIM) depend on the percolation occupation probability $p$ and the temperatures $T$ as well. If the probability $p$ is close to 1 (far from the percolation criticality), then the percolation clusters expand throughout the system. In such a situation, the critical properties of the EIM mainly coincide with well-known unbounded case\[2\], \[3\]. However, for a smaller $p$ (closer to the percolation phase transition), the system becomes quite inhomogeneous, and does not yet possess a translation symmetry. As our simulations have shown, even in such a situation, the ferromagnetic phase transition in EIM still exists; however, the critical temperature $T_c$ acquires considerable dependence on the occupation probability $p$. In this case, the dependence $T_c(p)$ is affected by the noninteger fractal dimension of the incipient percolation spanning cluster.

The properties of spins system in $3D$ disordered mediums are an area of active research\[17]-\[19\]. Nevertheless, the critical properties of the Ising system in a network of percolation $3D$ clusters are still studied insufficiently. However, the phase transition of spontaneous magnetization driven by concentration $p$ of the pores and spins (incorporated into such voids) is very attractive for various applications of quantum spin- and optoelectronics.
percolation medium has poorly been considered thus far, though it is a logical extension of previous work in this area.

This paper is organized as follows. In Sec. II, the basic equations and our numerical scheme for studying the structure of 3D percolation clusters is discussed. In Sec. III, we study the ferromagnetic phase transition of Ising magnets incorporated into the spanning cluster, which is considered in Sec. II. Discussion and conclusions from our results are found in the last Section.

II. BASIC EQUATIONS AND NUMERICAL ALGORITHM.

First, we study the geometrical properties of percolation clusters in a cubic lattice embedded in a 3-dimensional (3D) medium. It is assumed that the probability $p$ for each site of the lattice to be "occupied" is given, and we investigate the spatial distribution of the resulting clusters over sizes and other geometrical parameters. We recall that a cluster here means a conglomerate of occupied sites, which communicate via the nearest-neighbor rule.

In our algorithm, the connectivity of cluster voids (pores) is initially examined locally, so that two pores produce a cluster if they have at least one edge in common. In such an approach, the spanning occurs when the size of the largest (spanning) cluster reaches the size of the system. The rest of the cluster is referred to as a collection of "dead" or "dangling" ends. In a large enough sample, the internal topology is changed substantially at the critical concentration of the percolation voids $p_{c3D}$. We have found that such an intrinsic topological structure affects the dimensionality of the percolation transition; as a result, the connectivity of a percolating network acquires the form of a fractal, see Fig.1. It is worth noting that in the three-dimensional case, no percolation threshold is known exactly; only numerical data are available [2]. Fig.1 shows the incipient spanning cluster for the supercritical probability $p \gtrsim p_{3D} = 0.311$ when the spanning 3D cluster emerges for the first time forming a fractal network of voids.

In general, the analysis of such a compound system requires quite long computations. The first step deals with the identification of the spanning cluster $P_{3D}$ as a function of occupations probability $p$. In this step, the percolation system on a lattice is simulated by a random variable $s$ that accepts only values 1 or 0 (with probability $p$) that defines whether or not a cell is a percolating one. The percolation order parameter $P_{3D}$ is defined as the
FIG. 1: (Color online). Spatial distribution of the spanning cluster. Supercritical concentration of defects \((p = 0.317)\) is taken slightly above threshold \(p_{3D}\). Only clusters are shown, contacting with the input side of a material opened for the spin flow. We observe that a spanning cluster which spans the sample completely from input up to output sides has arisen. See details in the text.

ratio of the number of cells belonging to the spanning cluster to the general number of cells. Obviously that \(P_{3D}\) is distinct from zero only when exceeding the threshold concentration \(p \gtrsim p_{3D}\). Corresponding dependencies are shown in Fig.[2] In the second step, the properties of spins incorporated into the percolation structure (known from the first step) are evaluated with the use of the Monte Carlo technique (see [20], [25] and references therein). In this step, all values 1 in conducting cells are replaced (with probability 0.5) by +1 or −1 instead; correspondingly parallel or antiparallel spin state in such a cell is generated.

The resulting average magnetization \(M\) will be defined not only by the temperature \(T\) (more details are given below, see Eq.(5)), but also by the occupation probability \(p\). We recall that the nature of a percolation problem as a critical phenomenon is characterized
by the critical exponents $\beta$ and $\nu$. In theory, the exponent $\beta$ is related to the intensity of the order parameter $P_t$ (we supply $P_t$ by index $t$ to separate this one from the numerically evaluated quantity $P_{3D}$) as

$$P_t = (p - p_{3D})^\beta, \quad p > p_{3D}, \quad \text{and} \quad P_t = 0 \quad \text{for} \quad p \leq p_{3D},$$

(1)

and the exponent $\nu$ is related to the correlation length $\xi$ as

$$\xi \approx |p - p_{3D}|^{-\nu}, \quad \text{where} \quad p \simeq p_{3D}.$$ 

(2)

The latter is a measure of the range over which fluctuations in one region of space are correlated with those in another region. Two points which are separated by a distance larger than the correlation length $\xi$ will each have fluctuations which are independent, that is, uncorrelated. Thus the divergence of the correlation length $\xi$ at the critical point means that points being very far from each other become correlated. The exponents $\beta$ and $\nu$ are ones of the standard set of critical exponents\textsuperscript{[21]} that govern the singular behavior of different quantities near the critical point. These exponents depend only on the dimension of the space and not on the type of lattice or the kind of percolation problem.

In two dimensions ($d = 2$), these $\beta$ and $\nu$ are known analytically\textsuperscript{[26], [27]}, namely, $\nu = 4/3$ and $\beta = 5/36$. For $d = 3$, only numerical estimates are available: $\nu \simeq 0.90$ and $\beta \simeq 0.40$ (see Table III in Ref.\textsuperscript{[2]}). It has been established that critical exponents $\nu$ and $\beta$, as well as all others, do not depend on the kind of lattice (e.g., square, triangular, etc.) or the kind of percolation problem (site or bond). The corresponding power exponents are structurally stable; that is, they are unchanged by a small perturbation of the lattice model or the mapping, respectively, see\textsuperscript{[2]} and references therein. From the finite size scaling theory\textsuperscript{[2], [20]} various values of $P_t$ at given values of $p$ and $L$ can be fitted by a single scaling function $F(x)$ (that depends only on a single variable, but is not otherwise given explicitly by the theory\textsuperscript{[22], [23]}) that leads to strong dependence of order parameter on the values of $\beta$ and $\nu$. The dependence $p_{3D}$ on the value $L$ is rather weak.

III. NUMERICAL SIMULATIONS OF THE 3D CLUSTER STRUCTURE

Motivated by the essential fractal form of the incipient spanning cluster shown in Fig.\textsuperscript{1} we study the dependence of the fractal dimension of a percolation cluster $D_H(p)$ on probability
FIG. 2: (Color online). The order parameter $P_{3D}(p)$, fractal dimension $D_{H3D}/d_3$ of the spanning percolation cluster, and critical temperature $T/T_{c0}$ for Ising spins (placed in such a cluster), as function of the occupation probability $p$. To compare different dependencies, the following normalizations are used: $d_3 = 3$, $T_{c0} = 4.54$. The size of the system is $L^3 = 140^3$; $dt(p)$ is the time interval required to calculate corresponding value $P_{3D}(p)$. The percolation arises close to the critical value $p_{3D} \approx 0.311$, where the fractal dimension becomes noninteger $D_{H3D} = 2.54$, and the value $dt(p)$ has a high peak. See details in text.

$p$, see Fig 2. (At calculation $D_H$ it was used the approach [24] that we have adapted for evaluation of the fractal dimension for 3D spanning cluster.) From Fig 2 we observe that the behavior of $D_H(p)$ is separated into two well defined parts: $I$ and $II$. In part $I$ for $p > 0.5$ (when the spanning clusters expand throughout the system), the fractal dimension $D_H$ increases very slowly from 2.96 to 3 (the dimension of the embedded 3D space), see Fig 2. However, in the part $II$ (critical zone) the value $D_H$ increases rapidly from 2.54 to 2.96 when $p$ increases from the critical probability $p_{c3D} = 0.311$ to 0.5. For our simulation
we have used a 3D lattice with $L^3 = N^3$ where $N = 80, 90, 120, 140$, but since corresponding curves were very closely placed only case $N = 140$ in Fig.2 is shown.

From our numerical data in Fig.2 we found quite simple analytical formula (similar the shifted Boltzmann distribution (with respect to $p$)) that fits the fractal dimension of the spanning cluster:

$$D_H(p) = a \exp(-b/(p - c)), p > c,$$

where $a = 2.99, b = 0.00194$, and $c = 0.303$. The behavior of the percolation order parameter $P_{3D}(p)$ is fitted with great accuracy (with $\chi^2 = 2 \cdot 10^{-5}$) by the expression: $P_{3D}(p) \approx \Psi(p) = [(p - p_{c3D})^C + A]^B$, with $0.315 < p < 1$, and $A = 0.024, B = 0.294, C = 3.21$. This differs from the well-known percolation critical dependence $|p - p_{c3D}|^{-0.15}$ that is valid only in vicinity $|p - p_{c3D}| \to 0$.

Furthermore, we suppose that magnetic "liquid" (spins) fills up the percolation structure (from input to output), and as a result the network of 3D Ising magnets is generated. Since the fractal dimension $D_H$ of spanning cluster is noninteger, it is interesting to study the ferromagnetic-paramagnetic phase transition in such a compound system (spins in the percolation cluster) at the change of temperature $T$ (see Eq.(5)) where the energy Hamiltonian has well-known form[7], [3]:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j,$$

where $J > 0$ (throughout this paper we set $J = 1$) is the coupling constant between nearest-neighbor spins $S_i$ and $S_j$, where $\langle ij \rangle$ denotes that the sum runs over next-neighbor sites. We are interested, if the magnetization $M$ in such a percolation fractal system still has critical property of separation in the ordered and disordered magnetic phases. In general, the spatial non-uniform percolation effects lead to a complicated magnetic energy landscape, so the finding of an optimal energy state becomes a global optimization problem.

The simulations are performed with single spin-flip rates: local changes in the system are accepted with the probability $\pi$ given by the Metropolis rate,

$$\pi = \min(1, \exp(-\Delta \mathcal{H}/T)),$$

where $T$ is the temperature and $\Delta \mathcal{H}$ is the energy difference corresponding to the proposed single spin flip[2], [30].
Fig. 2 shows the dependence of the normalized critical temperature $T_c(p)/T_{c0}$ of the phase transition $T_c(p)$ on the occupation probability $p$, where $T_{c0} = 4.54$ is the critical Ising temperature for the unbounded 3D geometry. (More details are depicted in Fig. 3.) It is worth to note that the Metropolis algorithms shows the critical slowing down that leads to a dramatic increase of temporal scales in vicinity of ferromagnetic phase transition. This is due to a high energy penalty required to flip a single spin (or pair of spins) in a cluster of uniformly oriented neighbors. To overcome this problem, the cluster algorithms with non-local dynamics, the Swendsen-Wang and Wolff approaches commonly used for simulation in the vicinity of the criticality. As we observe from Fig. 2 beyond of the area of phase transition the Metropolis algorithm can be used again for calculation of that average magnetization.

From numerical data shown in Fig. 2 we have found the expression that fits the dependence of the critical temperature as

$$T_c(p)/T_{c0} = p_1 \exp(-p/p_2) + p_3 + p_4 p,$$

with $p_1 = 18.44$, $p_2 = 0.059$, $p_3 = -0.162$, $p_4 = 1.16$. It is noticeable that in the latter all numerical coefficients $p_i$ have a rather slow dependence on the system size $L$.

As already it was mentioned in the above such an extended Ising system has two order parameters: the percolation order parameters $P_{3D}$ and the average magnetization $M$. It is instructive to compare the behavior with respect of $p$ other quantities that are closely connected with both $P$ and $M$, namely the fractal dimension of percolation clusters $D_H(p)$ and critical temperature of the ferromagnetic phase transition $T_c(p)$ correspondingly. From Fig. 2 we observe that in area of part I (where $D_H(p) \simeq 3$) the dependence $T_c(p)$ is practically linear; for such an area ($p \leq p_{c3D}$) in $T_c(p)$, the exponential term $\sim \exp(-p/p_2)$ is negligibly small. However, in zone II, where $D_H$ is noninteger, the term $\exp(-p/p_2)$ sufficiently affects the linear dependence $T_c(p)$: in such a zone $T_c$ slowly depends on $p$, and $T_c(p) \sim 0.3 \cdot T_{c0}$. More details of critical behavior $M(T)$ and specific heat $C_v(T)$ are shown in Fig. 3. From Fig. 3 (a) we observe that the temperature dependencies $M(T)$ have well separated disordered phase (at $T > T_c$) and ordered (ferromagnetic) phase (at $T < T_c$); the magnetization drops off sharply near the critical temperature $T_c$. Fig. 3 (b) shows that the specific heat $C_v(T)$ has well defined peak at the critical temperature $T_c$. Furthermore, the value of the critical temperature $T_c$ strongly depends on the probability $p$: $T_c(p)$ decreases
FIG. 3: (Color online) Plot of spontaneous average magnetization $M$ and specific heat $C_V$ corresponding to disordered phase ($T > T_c$) and broken phase ($T < T_c$) at various probabilities $p$. The continuous curves are a fit to the data points. We observe that for large $p \leq 1$ values, the behavior $M$ and $C_v$ is similar to the unbounded case, but with the shift of the critical temperature $T_c(p)$.

with decreased $p$. We found that the critical behavior $M(T)$ and $C_v(T)$ is similar to the unbounded case, but with the shift of the critical temperature dependent on probability $p$. Fig. 2 shows that for area $I$ fractal dimension $D_F$ the of percolation cluster is nearly equal to the dimension of embedded space $d_3 = 3$, and $T_c(p)/T_{c3D}$ is close to the cluster order parameter $P_{3D}(p)$ up to the critical zone $II$.

Fig. 3 also shows the behavior $M(T)$ and $C_v(T)$ in zone $II$ close to the critical point $p_{c3D} \simeq 0.311$ (area of incipient percolation spanning cluster). We observe from Fig. 3 (a), (b) that separation in the ordered and disordered phases is still seen clearly, and the critical behavior of $M$ and $C_v$ remains well pronounced. However, the peaks of $C_v$ become smoother when compared to zone $I$. Since the percolation spanning cluster still has a significant
number of spins, we can conclude that in this area the topologically nontrivial magnetic structure arises; as a result, the critical behavior of $M$ and $C_v$ is strongly affected by the noninteger fractal dimension of the percolation clusters.

Our numerical simulations provide mainly the numerical evidence that the dependence that the dependence $T_c(p)$ is strongly affected by the noninteger fractal dimension $D_H(p)$ of the incipient percolation spanning cluster in such extended Ising model. More rigorous results relating to the renormalization group theory and the scaling properties of studied extended Ising model require significant mathematical efforts and will be published elsewhere.

IV. CONCLUSION

In conclusion, we studied the critical properties of Ising spins placed in the percolation clusters of 3D percolation medium. We focus on a novel aspect of such a model as an extension of the properties of Ising magnets incorporated in a percolation medium, where the critical phase transitions would be affected by the percolation criticality. We found that in such an inhomogeneous system the standard Ising model is strongly modified by the spatial percolation cluster distribution. This gives rise to a topologically nontrivial magnetic structure leading to a modification of the critical phenomenon without an external magnetic field. We numerically found that at large occupation probability $p$ (far from criticality) the magnetization shows well known critical behavior, however, with the shifted critical temperature $T_c(p)$. At a smaller $p$ such dependence is affected by the noninteger fractal dimension of the incipient percolation spanning cluster. We discuss analytic formulae that fit the dependencies of the percolation order parameter and the fractal dimension of clusters on the occupation probability. Studied features of critical behavior of 3D compound systems (percolation cluster filled by spins) can open new opportunities in advanced spin- and optoelectronics of disordered nanostructures, in particular in quantum spin electronics evolving manipulations of coherent spin states.

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