Ising model on networks with an arbitrary distribution of connections

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We find the exact critical temperature T_c of the nearest-neighbor ferromagnetic Ising model on an "equilibrium" random graph with an arbitrary degree distribution P(k). We observe an anomalous behavior of the magnetization, magnetic susceptibility and specific heat, when P(k) is fat tailed, or, loosely speaking, when the fourth moment of the distribution diverges in infinite networks. When the second moment becomes divergent, T_c approaches infinity, the phase transition is of infinite order, and size effect is anomalously strong.

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The Ising model is one of the immortal themes in physics. It is a traditional starting point for the study of the effects of cooperative behavior. Networks with complex architecture display a spectrum of unique effects [1-6], and so they are an intriguing substrate. The simulation of the Ising model on a growing scale-free network [7] has demonstrated that it is extremely far from that on regular lattices and on "planar graphs" [8].

In this paper, we report our exact results and results, which, we believe, are asymptotically exact, for the thermodynamic properties of the Ising model on the basic construction for "equilibrium" random networks. These networks are the undirected graphs, maximally random under the constraint that their degree distribution is a given one, P(k). Here, degree is the number of connections of a vertex. Correlations between degrees of vertices in such graphs are absent. In graph theory, these networks are called "labeled random graphs with a given degree sequence" or "the configuration model" [9]. The earlier interest was mainly in the percolation properties of complex networks and the spread of diseases on them [10-17], and most of the analytical results were obtained just for this basic construction (however, see Refs. [18-20], where the Berezinskii-Kosterlitz-Thouless percolation phase transition was studied in growing networks).

Our results demonstrate the strong effect of the fat tail of the degree distribution on the phase transition in the Ising model. The most connected vertices induce strong ferromagnetic correlations in their close neighborhoods at very large temperatures, and so their role is very important. Surprisingly, we observe very strong effects of these vertices, even when they, at first sight, must be insignificant, namely, when the first and the second moments of the degree distribution are still finite but the fourth moment already diverges ($\langle k^4 \rangle$ $\rightarrow \infty$).

It is convenient to use the power-law degree distribution $P(k) \propto k^{-\gamma}$ for parametrization. Then, $\langle k^4 \rangle$ diverges for $\gamma \leq 5$, $\langle k^3 \rangle$ diverges for $\gamma \leq 4$, and $\langle k^2 \rangle$ is divergent for γ

 \leq 3. When $\langle k^4 \rangle < \infty$, the phase transition is similar to that in the Ising model on high-dimension regular lattices. However, for $\gamma < 5$ its nature is quite different. As γ decreases and the role of the highly connected vertices turns to be more important, T_c grows and the phase transition becomes more "continuous." Below $\gamma = 4$, it is of higher order than the second in Ehrenfest's terminology. Furthermore, at $\gamma = 3$, T_c approaches ∞ , and the order of the phase transition is infinite.

When $\langle k^2 \rangle$ diverges ($\gamma \leq 3$), the effect of the highly connected vertices is crucial. In the infinite network, long-range magnetic order is not destroyed by any temperature, and finite-size effect is very strong. Formally speaking, we develop a theory for infinite networks, but it also allows us to describe the finite-size effect. Our main results are presented in Table I.

INTUITIVE ARGUMENTS

The large networks that are studied in this paper have a treelike "local structure." When we start from a randomly chosen vertex, and add its first nearest neighbors, second, \ldots , *n*th with all their connections, the resulting subgraph is almost surely a tree. Of course, in a finite-size network, there is a boundary for *n*, above which loops appear in such a subgraph.

Cooperative properties, which we study in the present paper, are determined by this "local" environment, where vertices have a quite different structure of connections than in the entire net. Interactions are transmitted through edges, from vertex to vertex. Hence, the following characteristic is crucial: the distribution of the number of connections of the nearest neighbor of a vertex. In the networks under consideration, it is $kP(k)/\langle k \rangle$. Then, the nearest neighbors of a vertex have the average number of connections (the average degree) $\langle k^2 \rangle / \langle k \rangle$, its second nearest neighbors have the same average degree, and so on. Notice that this value is greater than the average number of connections for the entire network $\langle k \rangle$, and it is much greater than $\langle k \rangle$ if $\langle k^2 \rangle$ is large. Therefore, we estimate the critical temperature of the Ising model on the network using the formula $T_c/J = 2/\ln[q/(q)]$ (-2) for the Ising model on a regular Cayley tree [21] with the coordination number $q = \langle k^2 \rangle / \langle k \rangle$. The result is

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TABLE I. Critical behavior of the magnetization M, the specific heat δC , and the susceptibility χ in the Ising model on networks with a degree distribution $P(k) \sim k^{-\gamma}$ for various values of exponent γ . $\tau \equiv 1 - T/T_c$. The right column represents the exact critical temperature in the case $\langle k^2 \rangle < \infty$ and the dependence of T_c on the total number N of vertices in a network.

	М	$\delta C(T < T_c)$	χ	T_{c}
	$\propto au^{1/2} \propto au^{1/2} / (\ln au^{-1})^{1/2}$	jump at T_c decreases as $\langle k^4 \rangle$ grows $\propto 1/\ln \tau^{-1}$	$\propto au^{-1}$	$2/\ln \frac{\langle k^2 \rangle}{\langle k^2 \rangle}$
$3 < \gamma < 5, \langle k^4 \rangle = \infty, \langle k^2 \rangle < \infty$ $\gamma = 3, \langle k^2 \rangle = \infty$ $2 < \gamma < 3, \langle k^2 \rangle = \infty$	$\propto au^{1/(\gamma-3)} \ \propto e^{-2T/\langle k angle} \ \propto T^{-1/(3-\gamma)}$	$ \begin{array}{c} \propto \tau^{(5-\gamma)/(\gamma-3)} \\ \propto T^2 e^{-4T/\langle k \rangle} \\ \propto T^{-(\gamma-1)/(3-\gamma)} \end{array} $	$\propto T^{-1}$ $\propto T^{-1}$	$\frac{2/\ln \frac{\langle k \rangle}{\langle k^2 \rangle - 2\langle k \rangle}}{\langle k \rangle \ln N}$ $\propto \langle k \rangle N^{(3-\gamma)/(\gamma-1)}$

$$\frac{J}{T_c} = \frac{1}{2} \ln \left(\frac{\langle k^2 \rangle}{\langle k^2 \rangle - 2 \langle k \rangle} \right). \tag{1}$$

We will show below that this naive estimate is exact.

GENERAL SOLUTION

Consider the Ising model on a network with the Hamiltonian: $\mathcal{H}=-J\Sigma_{\langle ij\rangle}S_iS_j-H\Sigma_iS_i$, where the first sum is over all edges of the graph, the second one is over all vertices, J>0 and H are the energy of the ferromagnetic interaction and magnetic field, respectively. Hereafter, we set J= 1. It is known that the regular Cayley tree is solved exactly by using recurrence relations [21]. As networks under discussion have a local treelike structure, we apply this method to the Ising model on such nets. Consider spin S_0 on a vertex 0 with k_0 adjacent spins $S_{1,i}$, $i=1,2,\ldots,k_0$. Due to the local treelike structure this spin may be treated as a root of a tree. We introduce

$$g_{1,i}(S_0) = \sum_{S_l = \pm 1} \exp\left[\left(\sum_{\langle lm \rangle} S_l S_m + S_0 S_{1,i} + H \sum_l S_l\right) / T\right],\tag{2}$$

where *T* is temperature. The indices *l* and *m* run only over spins that belong to subtrees with the root spin $S_{1,i}$, including $S_{1,i}$. Let $x_{1,i} \equiv g_{1,i}(-)/g_{1,i}(+)$, then the magnetic moment *M* of the vertex 0 is

$$M = \left(e^{2H/T} - \prod_{i=1}^{k_0} x_{1,i} \right) / \left(e^{2H/T} + \prod_{i=1}^{k_0} x_{1,i} \right).$$
(3)

The parameters $x_{1,i}$ describe the effects of the nearest neighbors on the spin S_0 In turn, $x_{1,i}$ are expressed in terms of parameters $x_{2,l} = g_{2,l}(-)/g_{2,l}(+)$, $l = 1, 2, ..., k_{1,i}$, which describe effects of spins in the second shell on spins in the first shell, and so on. The following recurrence relation between $x_{n,i}$ and $x_{n+1,l}$ holds:

$$x_{n,j} = y \left(\prod_{l=1}^{k_{n,j}-1} x_{n+1,l} \right), \tag{4}$$

 $y(x) = \frac{e^{(-1+H)/T} + e^{(1-H)/T}x}{e^{(1+H)/T} + e^{(-1-H)/T}x}.$ (5)

If a spin $S_{n+1,l}$ is on a dead end, then $x_{n+1,l}=1$. Note that at H>0, $x_{n,l}\leq 1$, while $x_{n,l}\geq 1$ for H<0. For H>0, it is convenient to introduce $x_{n,l}=\exp(-h_{n,l})$. Here, at a given n, $h_{n,l}$ are positive and independent random parameters, which play the role of random effective fields acting on a spin in the nth shell from neighboring spins in the (n+1)th shell. Then, Eqs. (3) and (4) take the form

$$M = \frac{e^{2H/T} - \exp\left(-\sum_{l=1}^{k_0} h_{1,l}\right)}{e^{2H/T} + \exp\left(-\sum_{l=1}^{k_0} h_{1,l}\right)},$$
(6)

$$h_{n,j} = -\ln\left\{ y \left[\exp\left(-\sum_{l=1}^{\kappa_{n,j}-1} h_{n+1,l} \right) \right] \right\}.$$
(7)

At dead ends we have $h_{n+1,l}=0$. At H=0 in the paramagnetic phase $h_{n,l}=0$, while in the ordered phase $h_{n,l}\neq 0$. Equations (6) and (7) determine the magnetization M of a graph as a function of T and H. We emphasize that these equations are valid for any treelike graph.

While deriving the recurrence relations, we started from some spin S_0 and then made the recurrence steps along subtrees. While solving the recurrence relations, we start from distant spins, i.e., from large *n*, and descend along subtrees to the spin S_0 . The recurrence steps Eq. (4) converges exponentially quickly. Therefore, we can set $h \approx 0$ for the starting spins. In the limit $n \rightarrow \infty$ the parameter $h_{1,i}$ is the fixed point of the recurrence steps. The thermodynamic behavior is determined by this fixed point, which is reached from the neighborhood of h = 0.

Let us average the magnetization M over the ensemble of random graphs with a degree distribution P(k). Introducing the distribution function of $h_{n,l}$, $\Psi_n(h) = \langle \delta(h - h_{n,l}) \rangle$, and its Laplace transform $\tilde{\Psi}_n(s) = \int_0^\infty dh e^{-sh} \Psi_n(h)$ we obtain from Eq. (6) the average magnetic moment

$$\langle M \rangle = \sum_{k} P(k) \int_{0}^{\infty} dh \frac{e^{2H/T} - e^{-h}}{e^{2H/T} + e^{-h}} \int_{-i\infty}^{i\infty} \frac{ds}{2\pi i} e^{sh} \tilde{\Psi}_{1}^{k}(s).$$
(8)

where we introduce the function

Here P(k) is the probability that the vertex 0 has k connections. Equation (7) gives the recurrence relation between $\tilde{\Psi}_n(s)$ and $\tilde{\Psi}_{n+1}(s)$:

$$\Psi_n(s) = \sum_k \frac{P(k)k}{\langle k \rangle} \int_0^\infty dh \, y^s(e^{-h}) \int_{-i\infty}^{i\infty} \frac{ds'}{2\pi i} e^{s'h} \Psi_{n+1}^{k-1}(s') \tag{9}$$

with $\tilde{\Psi}_{n+1}(s) = 1$ at a dead end. Here $P(k)k/\langle k \rangle$ is the probability that the neighbor in the (n+1)th shell of a vertex from the *n*th shell has *k* connections. We start from distant spins with $\tilde{\Psi}_{n+1}(s) \approx 1$ and large *n* and make recurrence steps toward smaller *n* until we reach the fixed point. In the limit $n \rightarrow \infty$, the recurrence procedure converges to $\tilde{\Psi}(s)$. The fixed point $\tilde{\Psi}(s)$ is a solution of Eq. (9) in which $\tilde{\Psi}_n(s)$ and $\tilde{\Psi}_{n+1}(s) \approx$ replaced by $\tilde{\Psi}(s)$. Then Eq. (8) with $\tilde{\Psi}_1(s) \rightarrow \tilde{\Psi}(s)$ gives the exact expression for $\langle M \rangle$. At H = 0 in the paramagnetic phase we have $\tilde{\Psi}(s) = 1$.

Let us find the exact critical temperature, T_c . Consider a starting function $\tilde{\Psi}_n(s) = \exp(-s\delta)$, where δ is small: $0 < \delta \le 1$, $s\delta \le 1$. After the first *m* recurrence steps, we obtain $\tilde{\Psi}_{n-m}(s) = \exp(-s\delta f^m)$, where $f = \langle k(k-1) \rangle$ $\langle k \rangle^{-1} \tanh(1/T)$. For f < 1, the recurrence steps lead to the fixed point $\tilde{\Psi}(s) = 1$, which corresponds to the paramagnetic phase. f = 1 at a certain temperature T_c , which satisfies the condition $\langle k(k-1) \rangle \langle k \rangle^{-1} \tanh(1/T_c) = 1$, so that at $T < T_c$ we have f > 1 and the recurrence steps lead away from the point $\tilde{\Psi}(s) = 1$. One sees that T_c is given by Eq. (1). Thus, the estimate (1) is exact. This result is valid for any degree distribution with $\langle k^2 \rangle < \infty$. In this range, the average number of the second nearest neighbors is $z_2 = \langle k^2 \rangle - \langle k \rangle$ [11] $(z_1 \equiv \langle k \rangle)$, so

$$\tanh\frac{1}{T_c} = \frac{z_1}{z_2}.$$
 (10)

At zero temperature we find the solution $\tilde{\Psi}(s) = t_s + (1 - t_s) \delta_{s,0}$, where $\delta_{s,0} = 1$ at s = 0 and $\delta_{s,0} = 0$ at $s \neq 0$, t_s is the smallest root of the equation $t_s = \sum_k P(k)k t_s^{k-1}$. This solution gives $\langle M \rangle = 1 - \sum P(k)t_s^k$, which is exactly the size of the giant connected component of the network. This result is evident. Indeed, only vertices in the giant connected component have a nonzero spontaneous moment, which is equal to 1 at T=0.

ANSATZ

To study the critical behavior of thermodynamic quantities, we develop an ansatz in the spirit of the "effective medium" approach. Notice that the right-hand sides of Eqs. (6) and (7) depend only on the sum of the independent and equivalent random variables $h_{n,j}$. So, let us use the following ansatz:

$$\sum_{l=1}^{k} h_{n,l} \approx kh + O(k^{1/2}), \qquad (11)$$

where $h \equiv \langle h_{n,l} \rangle$ is the average value of the "effective field" acting on a spin. The larger *k* is, the better this approximation will be. Therefore, the most "dangerous" highly connected spins are taken into account in the best way. With this ansatz,

$$\langle M \rangle = \sum_{k} P(k) \frac{e^{2H/T} - e^{-kh}}{e^{2H/T} + e^{-kh}}.$$
 (12)

Applying ansatz (11) to Eq. (7) yields

$$h = -\langle k \rangle^{-1} \sum_{k} P(k)k \ln y [e^{-(k-1)h}] \equiv G(h).$$
(13)

h plays the role of the order parameter. At H=0, h=0 above T_c and is nonzero below T_c .

THERMODYNAMIC QUANTITIES

Let us describe the critical behavior of the thermodynamic quantities of the Ising model on the infinite networks. For this, one must solve the equation of state (13) near T_c at H = 0.

The case $\langle k^4 \rangle < \infty$. The expansion of G(h) over small h has the form $G(h) = g_1 h + g_3 h^3 + \cdots$. For brevity, we do not present exact expressions for the coefficients g_i . Substituting this expansion into Eq. (13) determines T_c and the order parameter $h \approx a \tau^{1/2}$ as a function of the reduced temperature $\tau = 1 - T/T_c$, where $a = [12\langle k(k-1) \rangle^2/(\langle k \rangle \langle k(k-1)^3 \rangle T_c]^{1/2}$. Note that the critical temperature T_c that follows from our ansatz coincides with the exact result (1). At small h and H=0, Eq. (12) gives the spontaneous moment $\langle M \rangle \approx \langle k \rangle a \tau^{1/2}/2$. The magnetic susceptibility can be calculated from Eq. (12), by differentiating over H and then taking into account the dependence of h on H from Eq. (13). We obtain $\chi(H=0) \approx (\langle k \rangle^3 / [2\langle k^2 \rangle \langle k(k-2) \rangle])\tau^{-1}$. At $T > T_c$ the susceptibility has the same behavior $\chi(0) \sim (T/T_c - 1)^{-1}$ but with the double prefactor.

In our ansatz, the average internal energy per spin, $\langle E \rangle = \langle -J \Sigma_{\langle ij \rangle} S_i S_j \rangle_T / N$ (the average is thermodynamic and over the ensemble of graphs), at H=0 is

$$\langle E \rangle = -\frac{1}{2} \langle k \rangle \coth(2/T)$$

+ $\frac{1}{2 \sinh(2/T)} \sum_{k} P(k)k \frac{e^{-h} + e^{-(k-1)h}}{1 + e^{-kh}}.$ (14)

Substituting here $h \approx a \tau^{1/2}$, we find that the specific heat $C = d\langle E \rangle / dT$ has a jump at $T = T_c$,

$$\Delta C = \langle k(k-2) \rangle \langle k^2 \rangle a^2 / (8 \langle k \rangle).$$
(15)

This jump disappears as $\langle k^4 \rangle$ approaches ∞ . When $\langle k^4 \rangle$ diverges, we consider power-law degree distributions, $P(k) \propto k^{-\gamma}$.

The case $\gamma = 5$. The divergence of $\langle k^4 \rangle$ leads to a logarithmic singularity of the function G(h): $G(h) = g_1 h + g_3 h^3 \ln(1/h) + \dots$ Solving Eq. (13) yields

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$$h, M \sim \tau^{1/2} / (\ln \tau^{-1})^{1/2}, \quad \delta C \sim 1 / \ln \tau^{-1}, \quad \chi \sim \tau^{-1}$$
 (16)

[for any γ , we have $\delta C(T > T_c) = 0$]. Note that the critical behavior of χ is not changed.

The case $3 < \gamma < 5$. The function G(h) has two leading terms: $G(h) \approx g_1 h + g_3 h^{\gamma-2}$. Solving the equation of state (13) yields

$$h, M \sim \tau^{1/(\gamma - 3)}, \quad \delta C \sim \tau^{(5 - \gamma)/(\gamma - 3)}, \quad \chi \sim \tau^{-1}.$$
 (17)

Notice that for $\gamma < 5$ the critical exponents of the magnetization and specific heat differ from the standard ones. For $\gamma > 4$, exponent α of the specific heat $(\delta C \sim \tau^{-\alpha})$ is above -1. Hence the second derivative of the free energy over T diverges at T_c . Therefore, the phase transition is of the second order in Ehrenfest's classification. For $\gamma < 4$, we have $\alpha = -(5-\gamma)/(\gamma-3) < -1$ and the transition turns to be of a higher order. The order of the transition tends to infinity as $\gamma \rightarrow 3$. Nevertheless, for $\gamma > 3$, the susceptibility obeys the Curie law.

The case $\gamma=3$. Here, $\langle k^2 \rangle$ diverges. Formally speaking, this leads to the infinite critical temperature for the infinite networks [see Eq. (1)]. In any finite network, $\langle k^2 \rangle < \infty$ and the critical temperature is finite, although it may be very high, $T_c \cong \langle k^2 \rangle / \langle k \rangle$ (see below). We consider temperatures, which are much less than this critical temperature, but where $h \ll 1$, so $T \gg 1$. Using, for brevity, the continuum approximation for the degree distribution, we obtain $G(h) \approx (\langle k \rangle h/2T) \ln[2/(\langle k \rangle h)]$. Then,

$$h \approx (2/\langle k \rangle) e^{-2T/\langle k \rangle}, \quad M \approx e^{-2T/\langle k \rangle},$$
$$\delta C \sim T^2 e^{-4T/\langle k \rangle}, \quad \chi \sim T^{-1}. \tag{18}$$

Without the continuum approximation, we have, instead of $\langle k \rangle$ in the exponentials, a constant that is determined by the complete P(k). Equation (18) describes the behavior of thermodynamic quantities at modest temperatures in the situation, where the phase transition is of infinite order and at "infinite temperature." Notice the paramagnetic dependence $\chi \propto 1/T$. Note that the temperature dependence $M \propto \exp[-2T/\langle k \rangle]$ coincides with the result of the simulation [7] for the Barabási-Albert model (γ =3) [see Fig. 1(a) of Ref. [7]].

The case $2 < \gamma < 3$. Again T_c for large networks is very high. Using the expansion $G(h) \approx g h^{\gamma-2}/T$, we find, in the range $1 \ll T \ll T_c$, the following behavior:

$$h, M \sim T^{-1/(3-\gamma)}, \delta C \sim T^{-(\gamma-1)/(3-\gamma)}, \chi \sim T^{-1}$$
(19)

[compare with Eq. (18)]. Notice that the susceptibility keeps the paramagnetic temperature dependence.

FINITE-SIZE EFFECT

Equation (1) shows that T_c diverges when $\langle k^2 \rangle \rightarrow \infty$. In finite networks, $\langle k^2 \rangle$ is finite because of the finite-size cutoff of the degree distribution. In scale-free networks, it is estimated as $k_{cut} \sim k_0 N^{1/(\gamma-1)}$, where N is the total number of vertices in a network, k_0 is a "minimal degree" or the lower boundary of the power-law dependence, and $\langle k \rangle \approx k_0 (\gamma - 1)/(\gamma - 2)$. Then, actually, repeating estimations from Ref. [4] (see more detailed discussions in Refs. [16,17]), we obtain

$$T_{c} \approx \frac{\langle k \rangle \ln N}{4} \quad \text{at} \quad \gamma = 3,$$

$$T_{c} \approx \frac{(\gamma - 2)^{2}}{(3 - \gamma)(\gamma - 1)} \langle k \rangle N^{(3 - \gamma)/(\gamma - 1)} \quad \text{for} \quad 2 < \gamma < 3.$$
(20)

The first expression can be compared with the simulation [7] of the Ising model on the Barabási-Albert growing network $(\gamma=3)$ with minimal degree $k_0=5$, so $\langle k \rangle = 10$. From Eq. (20) $T_c \approx 2.5 \ln N$ follows. The simulation [7] yields $T_c \approx 2.6 \ln N - 3$. Recall that our results were obtained for the completely uncorrelated network, and correlations in growing networks are extremely strong.

DISCUSSION

Our results may be compared with those for percolation on such networks [16] and the disease spread within them [14]. Of course, the problems are distinct, but one finds a great resemblance (the superstability of long-range order when $\langle k^2 \rangle \rightarrow \infty$, phase transitions of higher order, etc.). All these anomalous features are determined by fat tails in the distributions of connections. Our final results were presented for uncorrelated networks. However, the quantitative agreement with the simulation [7] of correlated nets shows that they are applicable in much more general situations. Furthermore, our analytical results can be easily generalized.

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