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Critical exponents and percolation thresholds in two-dimensional systems with a finite interplane coupling

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Classical site percolation was used to study numerically the effect of interplane coupling in the range 10^{-1}–10^{-6} of the in-plane coupling on the static correlation length exponent ν and the critical dimension D. It was found that even for the smallest coupling values the exponents take their three-dimensional (3D) values for sufficiently large system sizes. The percolation threshold p_c, however, varies continuously from the 2D to the 3D value with a power-law exponent $\kappa = 0.41(2)$, which, to within error, is the same for simple cubic, bcc, and fcc lattices. As predicted by renormalization-group theory this exponent equals the inverse of the susceptibility exponent $\gamma = 43/18$.

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The static critical behavior of quasi-two-dimensional magnetic systems has become of theoretical and experimental interest again since the discovery of superconductivity in doped La_2CuO_4 in 1986 [1]. One focus of such investigations was the possibly anomalous critical behavior of diluted magnetic systems, where Cu is replaced with nonmagnetic atoms. Contrary to the classical two-dimensional (2D) magnets, which follow closely the theoretical expectations of 2D Ising models [2], diluted $La_2(Cu_{1-x}Mg_x)O_4$ was reported to have a much smaller critical threshold concentration x_c for a finite Néel temperature (T_N) [3]. While the former are well described by the site percolation on a 2D lattice ($x_c \approx 0.41$) the threshold in $La_2(Cu_{1-x}Mg_x)O_4$ was reported to extrapolate to $x_c \approx 0.2$. This behavior, most recently, lead to the proposal of an effective 2D quantum nonlinear sigma model combined with classical percolation theory which was able to reproduce a lower critical threshold [4]. Essentially, the quantum fluctuations were made responsible for the deviation from the classical percolation value for the threshold. These results, however, were contradicted by quantum Monte Carlo simulations, which showed that for all spin values studied ($S = 1/2$, 1, 3/2, and 2) the threshold remained the classical percolation one [5]. Instead, some of the critical exponents near x_c were found to take on spin-dependent values. Other refinements of the 2D Heisenberg antiferromagnetic model include in-plane next-nearest-neighbor interactions [6] or the study of two interpenetrating Cu systems with different Néel temperatures such as in $Sr_2Cu_3O_4Cl_2$ [7].

The coupling of spins to neighboring planes in the quasi-2D magnetic system is small (on the order of 10^{-3}–10^{-6} of the in-plane coupling) and may be neglected in a zeroth-order approach. However, it serves as the seed for the observed 3D ordering that would else not occur at finite temperatures. The transition to long-range order in the La_2CuO_4 system was discussed, e.g., in Ref. [8]; in spite of the weak coupling a Néel temperature of 325 K marks the importance of 3D coupling. Keimer *et al.* suggested that the effective interplane coupling constants α_{eff} is scaled by the square of the correlation length $\alpha_{eff}\xi^2 \approx 1$ [8]. In more complicated systems, such as $YBa_2Cu_3O_6$, there are two interplane coupling constants, one between the spins in the two CuO_2 planes in each unit cell and one connecting the spins between unit cells [9]. The effect of interplane coupling on the linewidth in electron-spin resonance spectroscopy was compared in the quasi-2D magnetic system K_2MnF_4 (antiferromagnetically ordered) and a system with an appreciable coupling ($NaCrS_2$, in-plane ferromagnet) [10]. A crossover from 1D to 2D has been studied for weak and intermediate couplings in a spin-ladder system $Sr(Cu_{1-x}Zn_x)_2O_3$ [11,12].

Theoretically, the dimensional crossover was studied by renormalization-group methods by Liu and Stanley [13] and Chang and Stanley [14]. They showed rigorously that the crossover exponent should equal the susceptibility exponent of the in-plane dimension. The crossover in quasi-2D systems has not been studied using percolation methods to our knowledge.

We study numerically the effect of an arbitrary interplane coupling on the static correlation length exponent ν (near p_c) and on the threshold p_c in classical site percolation. The critical exponent ν takes its 2D value for small coupling in small systems; for sufficiently large systems, even for the weakest interplane coupling studied (10^{-5} and 10^{-6}), the 3D behavior is approached. Similar results are obtained for the critical dimensionality D at p_c. However, even a weak 3D coupling in quasi-2D lattices has a significant influence on the percolation threshold in the infinite-size limit. Over a range of six orders of magnitude in interplane coupling, p_c and hence the critical concentration $x_c = (1 - p_c)$ vary continuously between the limiting 2D and 3D values with an exponent κ. This exponent agrees well with the renormalization-group predicted value of $\kappa = \gamma^{-1} = 18/43 \approx 0.419$ [14,15].

We determined the percolation threshold p_c, the critical exponents ν and D by studying the cluster properties of randomly generated $L \times L \times L$ lattice sites of simple cubic (sc), body-centered and face-centered-cubic systems. We focused on two types of wrapping probabilities employing periodic boundary conditions similar to the procedure by Newman and Ziff [16]. They are (i) a wrap around two lattice directions and not the third and (ii) a wrap only around one direction and neither of the two others. In the 3D isotropic limit these probabilities are triply degenerate for wrapping

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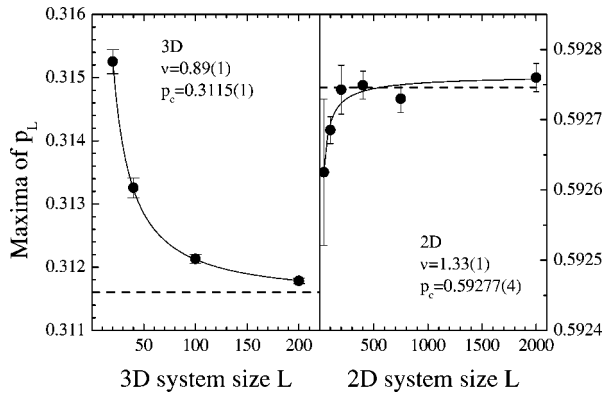

FIG. 1. 2D and 3D site percolation thresholds as determined by the finite-size scaling method. The dashed lines indicate the most accurate literature values from Refs. [16] (2D) and [18] (3D). The critical exponents ν in two and three dimensions were extracted from Fig. 2 and agree with the literature values ($4/3 \approx 1.33$ and 0.88 [15]).

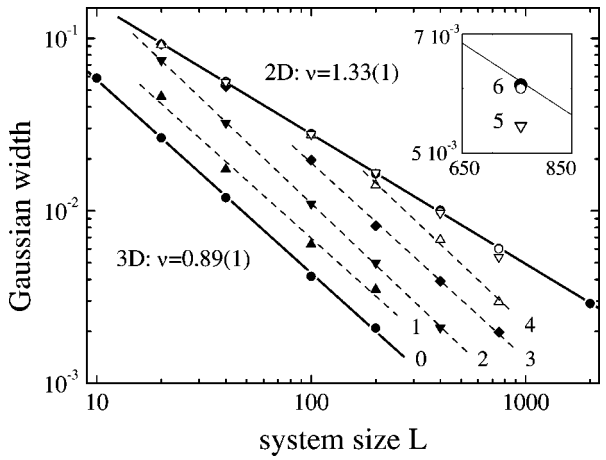

FIG. 2. Gaussian width of the wrapping probability type (ii) (see text) as a function of size L in a simple cubic system for various interplane coupling coefficients. The number given is the negative exponent in the coupling strength, i.e, $1 \rightarrow 10^{-1}$, etc. The critical exponent ν is determined from the slope of these curves. The fits to the 2D and 3D limits are shown as full lines, the dashed lines are least square fits with the 3D exponents $\nu = 0.90$, 0.85, 0.88, and 0.85 (± 0.03) for $c_f = 10^{-1}$, 10^{-2}, 10^{-3}, and 10^{-4}, respectively. The inset shows on an enlarged scale how in the largest system studied the points for $c_f = 10^{-5}$ and 10^{-6} deviate from the 2D limit (black dots) towards 3D behavior.

around x, y, or z and serve as an independent check for the random number generation. In 2D and for a finite interplane coupling the wrapping of type (ii) is doubly degenerate in x and y. Other wrapping probabilities are, in principle, interesting (e.g., the probabilities to wrap around either direction), but those studied here are most suitable for determining the critical threshold due to their local maximum near p_c. We mapped the interplane coupling strength onto the percolation problem by connecting in-plane nearest neighbors in a given cluster with full probability ($=1$) and those in a plane above or below with probability $0 \leqslant c_f \leqslant 1$ (sc and fcc); for the bcc system a similar schema was adapted. For $c_f = 1$ ($c_f = 0$) the 3D (2D) isotropic limits are recovered.

For the cluster analysis we developed an efficient, multispin coded algorithm that, for a particular occupation probability p, determines the sizes of all clusters, one cluster at a time. If one or several of the six wrapping probabilities described occurred, this was noted, the cluster-size distribution then sorted, and zeroth, first, and second moment calculated. This procedure was repeated for each probability p between 10 and 10 000 times to obtain the desired statistical significance and then p incremented through the threshold region. The two types of wrapping probabilities in three dimensions for a given system size L have a different maximum near the percolation threshold. Both maxima, however, converge to the critical threshold for an infinitely large system in the usual way [15], i.e.,

$$p_c^L - p_c \propto L^{-1/\nu}, \tag{1}$$

where ν is the critical exponent of the system under consideration. It is determined by fitting the maxima to a Gaussian with width Δ that is proportional to $\Delta \propto L^{-1/\nu}$ [15]. As was suggested by Watanabe [17] and demonstrated for 2D in Ref. [16], the periodic boundary conditions make for a rapid convergence. In Fig. 1 we show the convergence of our p_c^L towards the best literature values in two [0.592 746 21(13) Ref. [16]] and three dimensions [simple cubic, 0.311 608 0(4) Ref. [18]], as a function of system size. We find p_c^{2D} and p_c^{3D} in agreement with these values and of sufficient accuracy (on the order of 10^{-4}) for the current work. In Fig. 2 we show the dependence of the width on system size, which determines $\nu^{3D} = 1.33(1)$ and $\nu^{2D} = 0.89(1)$ compared to the literature values of $4/3 \approx 1.33$ and 0.88 [15]. The fractional dimensionality D at threshold p_c was also determined. It is derived from the logarithmic slope of the largest cluster at p_c vs system size, and we found $D^{2D}(p_c) = 1.906(6)$ (exact value $91/48 \approx 1.896$) and $D^{3D}(p_c) = 2.51(2)$ (literature value 2.53) [15]. In general, the agreement is excellent and shows that our algorithm performs adequately in these limits [19].

We first show our results of interplane coupling on the critical exponent ν, which describes the divergence of the correlation length ξ in a physical system in the vicinity of p_c [15],

$$\xi \propto |p - p_c|^{-\nu}. \tag{2}$$

It is expected that for large enough anisotropic systems the 3D behavior will be obtained. In Fig. 2 we show the linewidths of our wrapping probabilities as a function of system size for various values of the interplane coupling coefficient c_f. The data points for $c_f = 10^{-1}$ and 10^{-2} apparently all lie on a line parallel to the 3D isotropic limit ($c_f = 1$) but are shifted vertically by some amount. In other words, for a given system size a decreasing coupling strength leads to larger linewidths, and the linewidths continue to scale with the 3D critical exponent $\nu = 0.88$. For smaller interplane coupling values (10^{-3}–10^{-6}) a different behavior is observed. In smaller systems the linewidth falls on the limiting curve for two dimensions and deviates from this limit only as the

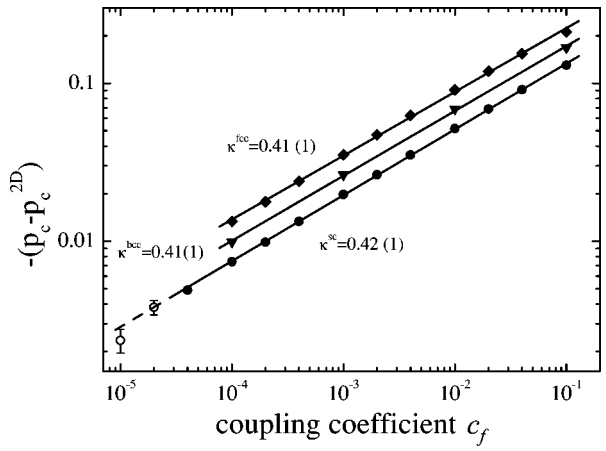

FIG. 3. The percolation threshold p_c as a function of coupling coefficient in three differently coordinated cubic systems [sc (circles), bcc (triangles), and fcc (diamonds)]. The solid symbols correspond to maxima in the wrapping probabilities. The slopes, best fits to the solid symbols, are the same, to within error, for sc, bcc, and fcc lattices: $\kappa = 0.41(2)$ and define a power-law exponent. The open symbols were not size converged and not included in the fit [20].

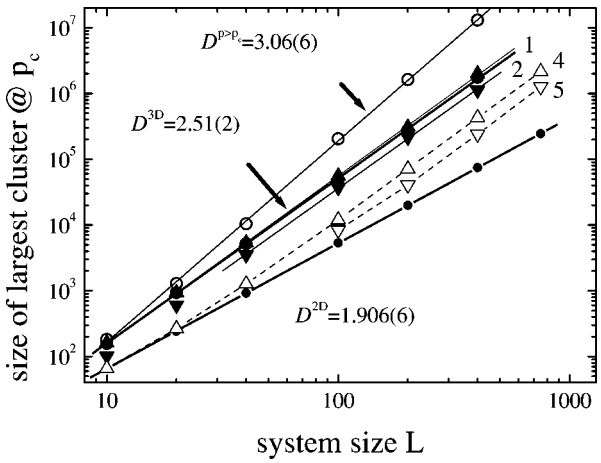

FIG. 4. Maximal cluster size at percolation threshold for different interplane coupling strengths c_f in the sc system. The slopes of these curves yield the critical dimension D. The crossover from 2D to 3D is nicely seen from curve 4 (i.e., $c_f = 10^{-4}$). Also shown for $c_f = 10^{-1}$ are the data for $p > p_c$ where the $D = 3$ classical space dimension is recovered.

system size increases. This is the crossover region where the exponent ν changes from 2D to 3D value. For large c_f this crossover occurs for small system sizes, for small c_f larger and larger systems are needed to feel the interplane coupling. We thus confirm that in the infinite-size limit the critical exponent ν always takes its 3D value, even for an infinitesimal (but finite) interplane coupling strength. Studies of the quantities related to the critical exponent ν, e.g., the correlation length ξ, in quasi-2D physical systems (which usually are in the large-size limit) should thus be performed on the basis of the 3D value of ν.

How does the percolation threshold depend on the strength of the interplane coupling? The observed crossover from 2D to 3D behavior in Fig. 2 as a function of system size makes it impracticable to apply the scaling law Eq. (1) for the determination of p_c. For the smallest interplane coupling the exponent ν is not constant in the crossover region and the usual straight line on a log-log plot is not expected. However, for large enough system sizes p_c has reached its asymptotic value within our statistical error, and we can take the largest system investigated for a specific c_f to have a converged value. In Fig. 3 we plot the so determined thresholds p_c in sc, bcc, and fcc as given by the maxima in the wrapping probabilities. For interplane couplings $< 4 \times 10^{-5}$ (sc) the finite-size effects become noticeable, in that even the largest system studied has not yet reached a constant threshold value (open symbols). We fitted the solid points in Fig. 3 to a power law and find the same exponent $\kappa = 0.41(2)$ for the three differently coordinated cubic systems. The interplane coupling coefficient c_f and the threshold for percolation in the range studied are thus related by

$$-(p_c - p_c^{2D}) = A(c_f)^{\kappa}. \tag{3}$$

We find a power-law relationship between these two quantities for $c_f \ll 1$ with an exponent $\kappa = 0.41(2)$ and coefficients $A^{sc} = 0.348(5)$, $A^{bcc} = 0.44(2)$, and $A^{fcc} = 0.57(1)$. To within error, κ is independent of the coordination number in the three cubic systems. This result is to be compared to the renormalization-group prediction of Chang and Stanley [14]. Indeed we find that the inverse of κ in Eq. (3), to high accuracy, equals the susceptibility exponent in 2D: $\kappa = \gamma^{-1} = 18/43 \approx 0.419$ [15]. From a percolation point of view our result means that an unlikely additional z-direction path in a quasi-2D percolation problem will substantially increase the wrapping chances and hence reduces p_c compared to the 2D value. In physical terms this predicts that even a small coupling as always present in real crystals will sensitively influence the phase transition in a way described by Eq. (3). To give a quantitative example, only for an interplane coupling strength of 10^{-10}—much smaller than typically observed—does the threshold deviate less than 10^{-4} from the exact 2D value. In a real sample the interplane coupling always increases the critical concentration $x_c = 1 - p_c$ for magnetic ordering. Inhomogeneities and thus a spatially fluctuating interplane coupling are a source of broadening or even shifts in quasi-2D phase transitions.

After having determined p_c, it is interesting to take a look at the critical dimension D at p_c which describes how fractal the largest cluster is or, in other words, how the mass s of the largest cluster scales with system size L,

$$s \propto L^D. \tag{4}$$

In Fig. 4 we show our data that determine D for coupling coefficients between 10^0 and 10^{-5} taking for p_c the data points of Fig. 3. There is apparently a 2D-3D crossover in the critical dimension as well (best seen for $c_f = 10^{-4}$), and again we confirm that in the limit of infinite system size even the smallest interplane coupling leads to a three-dimensional behavior of the critical dimension. The size dependence of the largest cluster should sensitively depend on being close to p_c. In Fig. 4 (open circles) we show data for $p > p_c$ (c_f

$=10^{-1}$), where D should be equal to the space dimension [15]; our value of $D_{(p=0.4728)}=3.06(6)$ shows that at $p=0.4728$ we are indeed above the threshold [$p_{c,(c_f=10^{-1})}=0.4628$]. This study of the fractal nature of the largest cluster at p_c shows again the crossover from 2D to 3D.

In conclusion, we studied numerically the consequences of interplane coupling on the phase transition in quasi-2D percolation. In a range of relative coupling strengths from 10^0 to 10^{-6} of the intraplane coupling, both the static correlation length exponent ν and the critical dimension D at threshold show a crossover from 2D to 3D for sufficiently large system sizes as expected from renormalization-group theory. Quasi-2D magnetic systems, in spite of their weak interplane coupling strengths, should thus be regarded as 3D systems with respect to their critical exponents as we explicitly show for ν and D. The threshold has an entirely different behavior: p_c varies continuously with a power-law dependence (for $c_f \ll 1$) on the interplane coupling coefficient from 2D to 3D even in the infinite-size limit, giving rise to an exponent $\kappa=0.41(2)$ which is the same for sc, bcc, and fcc coordination. The exponent confirms accurately the 30-year-old prediction of renormalization-group methods that the crossover exponent equals the susceptibility exponent. One consequence of classical site percolation is that for finite coupling the threshold is always lower than the 2D value and hence the critical concentration in diluted magnetic systems is always larger than the 2D one. Smaller values of x_c in such systems are thus not due to interplane coupling.

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[19] In order to give a feeling of the efficiency of our algorithm we mention some absolute performance times as obtained on a laptop (Pentium III, 1 GHz, 512 Mbytes) operating under a Linux operating system. In 2D, a $10\,000\times10\,000$ system at p_c, on average took 8 sec and 17 sec for the cluster generation and identification, respectively, and used about 120 Mbytes of memory. Our combined random number generation and cluster identification are faster by a factor of 6, the memory requirement, due to the multispin coding, is smaller by a factor of 10 than the code described, e.g., by Newman and Ziff, Phys. Rev. E **64**, 016706 (2001), running on the same computer. In 3D, a $750\times750\times750$ cube at p_c takes 180 sec for generating all random sites and identifying the clusters.

[20] The system sizes in this figure were: sc, $L=200$ ($c_f=0.1$), $L=400$ ($4\times10^{-2}\geqslant c_f\geqslant2\times10^{-3}$), $L=750$ ($10^{-3}\geqslant c_f\geqslant2\times10^{-4}$), and $L=900$ ($c_f\leqslant10^{-4}$); bcc, $L=200$ ($c_f\geqslant10^{-3}$), and $L=400$ ($c_f=10^{-4}$); fcc, $L=200$ ($c_f>10^{-4}$) and $L=400$ ($c_f=10^{-4}$).