# Possible crossover of a nonuniversal quantity at the upper critical dimension

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We report on a possible crossover of a nonuniversal quantity at the upper critical dimensionality in the field of percolation. Plotting recent estimates for site percolation thresholds of hypercubes in dimension $6 \leqslant d \leqslant 13$ against corresponding predictions from the Galam-Mauger (GM) formula $p_c = p_0[(d-1)(q-1)]^{-a} d^b$ for percolation thresholds, a significant departure of $p_c$ is observed for $d \geqslant 6$. This result is reminiscent of the crossover undergone by universal quantities in critical phenomena. For bond percolation, evidence of such a crossover of dimensionality would require an improvement of the GM formula to reach a relative error of typically 0.2%, while it is currently at 0.9% for hypercubes.

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## I. INTRODUCTION

The discovery of renormalization group techniques by Wilson in the early 1970s has allowed the powerful elucidation of the mystery of critical phenomena [1]. It is based on the existence of relevant variables, irrelevant variables, and universality classes. Accordingly all parameters are classified as universal quantities and nonuniversal quantities. For continuous phase transitions the critical exponents are universal while critical temperatures are not.

In this framework dimension plays a key role in categorizing the effects of fluctuations. At very low dimensions, fluctuations are too strong and prevent any long-range order from occurring. The limit from which it does not happen is called the lower critical dimension $d_l$. Only for $d > d_l$ can long-range order sustain fluctuations. On the other extreme, there exists some dimension $d_c$ called the upper critical dimension $d_c$, beyond which fluctuations are averaged out and do not influence the critical properties. For $d > d_c$ there exists only one class of universality: the mean-field one. Therefore it is in the range $d_l < d < d_c$ that fluctuations are instrumental in determining the critical properties.

In parallel, percolation is a geometric phenomena with no temperature. However, it was shown to be indeed identical to usual critical phenomena with $d_c = 6$. Therefore its critical exponents are universal quantities while percolation thresholds $p_c$ are not. Accordingly the value of $p_c$ must be calculated for each system and varies from one geometry to another. However, at odds with this universality principle, a lot of efforts have been devoted to the finding of formulas for the percolation threshold for about half a century. Several formulas have been proposed, which involve only two parameters: the dimension $d$ and coordination number $q$ [2–7]. The limits of such a choice have been discussed by Wierner and Naor *et al.* [8,9], who also considered that the most accurate of such formulas are the Galam-Mauger (GM) laws [6]. Indeed the high degree of accuracy of the GM law predictions hints at the existence of an underlying universality principle for percolation thresholds.

In this work, we report on a possible crossover of a nonuniversal quantity at the upper critical dimensionality in the field of percolation. Using the GM laws and a series of recent numerical estimates for hypercube percolation thresholds ($6 \leqslant d \leqslant 13$), site percolation thresholds are found to undergo a drastic change of behavior at the percolation upper critical dimension $d_c = 6$. This result is reminiscent of the crossover undergone by universal quantities in critical phenomena. At contrast, nothing similar is evidenced at any dimension for the bond percolation.

Considering only the case $d > 2$ of interest in the present work, the GM laws are split in two. One applies to $3 \leqslant d \leqslant d_c$ and can be written

$$p_c = p_0[(d-1)(q-1)]^{-a} d^b, \quad 3 \leqslant d \leqslant d_c. \tag{1}$$

The site percolation $p_c^S$ is approximated by Eq. (1), with $b = 0$, $p_0 = 1.2868$, and $a = 0.6160$. As for the bond percolation threshold, $p_0 = 0.7541$ and $b = a = 0.9346$. This law corresponds to the so-called second class (the first one being related to $d = 2$ only) and will be called for this reason the GM2 law. Equation (1) cannot extend up to $d \to \infty$. Among several reasons outlined in [6], one comes from the fact that, in this limit, the percolation threshold should reduce to that of the Cayley tree for both sites and bonds. In other words, one must recover the Bethe asymptotic limit

$$p_c^S = p_c^B = (q-1)^{-1}, \quad d \to \infty. \tag{2}$$

Equation (2) is violated by the GM2 law. This drawback of the GM2 law was the main motivation for introducing another law associated with a third class, which applies at high dimension and has the proper Bethe asymptotic limit. This is the asymptotic GM3 law

$$p_c = 2^{a-1}[(d-1)(q-1)]^{-a} d^{2a-1}, \quad d \gg d_c, \tag{3}$$

with $a = 0.088\,00$ for sites and $a = 0.3685$ for bonds.

 

TABLE I. Numerical estimates for the percolation thresholds $p_c^S$(num), together with the results of the GM2 and GM3 laws. For sc lattices at $d=5$ and $d=6$, the data of Refs. [11,12] have been substituted by those of Ref. [10], since they are more accurate.

| Lattice | $p_c^S$(GM2) | $p_c^S$(GM3) | $p_c^S$(num) | $p_c^B$(GM2) | $p_c^B$(GM3) | $p_c^B$(num) |
|---|---|---|---|---|---|---|
| Kagomé | 0.65400 | 0.59264 | 0.65270 | 0.51620 | 0.38885 | 0.52440 |
| Diamond | 0.42675 | 0.43824 | 0.43000 | 0.39454 | 0.24984 | 0.38800 |
| sc ($d=3$) | 0.31154 | 0.27957 | 0.31160 | 0.24476 | 0.20697 | 0.24880 |
| bcc ($d=3$) | 0.25322 | 0.20792 | 0.24600 | 0.17872 | 0.18284 | 0.18030 |
| fcc ($d=3$) | 0.19168 | 0.13969 | 0.19800 | 0.11714 | 0.15479 | 0.11900 |
| sc ($d=4$) | 0.19725 | 0.18109 | 0.19700 | 0.16009 | 0.14599 | 0.16010 |
| fcc ($d=4$) | 0.094794 | 0.063570 | 0.098000 | | | |
| sc ($d=5$) | 0.14152 | 0.13352 | 0.14100 | 0.11917 | 0.11287 | 0.11820 |
| fcc ($d=5$) | 0.057352 | 0.036740 | 0.054000 | | | |
| sc ($d=6$) | 0.10901 | 0.10562 | 0.10902 | 0.095092 | 0.092028 | 0.094202 |
| sc ($d=7$) | 0.087898 | 0.087319 | 0.088951 | 0.079233 | 0.077697 | 0.078675 |
| sc ($d=8$) | 0.073191 | 0.074401 | 0.075210 | 0.067991 | 0.067232 | 0.067708 |
| sc ($d=9$) | 0.062410 | 0.064802 | 0.065210 | 0.059602 | 0.059255 | 0.059496 |
| sc ($d=10$) | 0.054198 | 0.057390 | 0.057593 | 0.053097 | 0.052971 | 0.053093 |
| sc ($d=11$) | 0.047756 | 0.051497 | 0.051590 | 0.047904 | 0.047893 | 0.047795 |
| sc ($d=12$) | 0.042578 | 0.046699 | 0.046731 | 0.043659 | 0.043704 | 0.043724 |
| sc ($d=13$) | 0.038336 | 0.042718 | 0.042715 | 0.040124 | 0.040190 | 0.040188 |

Despite the fact that the GM2 law is not exact, its accuracy is sufficient to materialize the dimensional dependence of the percolation threshold for the bcc, fcc, and hypercubic lattices up to $d=6$. Due to the lack of data for the percolation thresholds in larger dimension, however, it has not been possible so far to explore the existence of a critical crossover dimension $d_c$ above which the percolation threshold would follow a formula different from the GM2 law (approximated by the GM3 law). Recent Monte Carlo estimates for site and bond percolation thresholds with negligible standard deviations in simple hypercube lattices from $d=6$ up to $d=13$ [10] now make this investigation possible.

It is the purpose of this work to make a comparison of the data including these Monte Carlo results with the predictions of Eqs. (1) and (3). For the site percolation threshold, the crossover between the two laws is clearly evidenced at dimension $d_c=6$. For bond percolation thresholds, however, no sizable deviations from the GM2 law as defined by Eq. (1) is detected up to the highest dimension $d=13$ investigated. Such a crossover for bonds, if it exists, cannot be detected, since the GM2 and GM3 laws do not depart significantly from each other in the range $7 \leqslant d \leqslant 13$.

## II. ANALYSIS

The numerical estimates $p_c^S$ and $p_c^B$ of the percolation thresholds for sites and bonds, respectively, are reported in Table I, together with the results of the GM2 and GM3 laws. For simple cubic (sc) lattices at $d=5$ and $d=6$, the data of Refs. [11,12] have been substituted by those of Ref. [10], since they are more accurate; we shall return to this point later on.

### A. Site percolation

As $b=0$ for site percolation, the GM2 law is best illustrated in a log-log plot of $p_c^S$ versus $(d-1)(q-1)$, in which case it is a straight line. This is illustrated in Fig. 1. We have reported on the same plot the numerical results of $p_c^S$ taken from [10–12]. For comparison, we have also reported (crosses) the values of $p_c^S$ predicted by the asymptotic GM3 law. Note according the GM3 law, $(d-1)(q-1)$ is not the pertinent variable, hence a randomlike distribution of the crosses which cannot be connected to generate a curve. Indeed, since the $p_c^S$'s depend on both $d$ and $q$, only the crosses corresponding to lattices with the same topology, defined by the relation linking $d$ and $q$, can be connected.

In practice, it means that the crosses corresponding to all the hypercubes (sc) from $d=3$ up to $d=13$ do belong to a single curve, since the same relation $d=2q$ holds true for all these lattices. The crosses corresponding to fcc lattices should also belong to another curve, but the fcc percolation threshold for the site is known for $d=3$, 4, and 5 only, and three data points are not sufficient to materialize a curve. All the $p_c^S$'s up to the $d=6$ line up on the GM2 law (within the uncertainty limit above mentioned) as stated in Ref. [6].

The new data for the sc lattices at higher dimensions, however, give evidence of a deviation of the $p_c^S$'s from the linear GM law which increases with $d$, illustrated in Fig. 1. An equivalent formulation is to note a negative curvature of the "numerical" $p_c^S(d)$ curve for sc hypercube lattices at $d>6$ to match the GM3 law. To quantify this effect, we have plotted in Fig. 2 the relative difference $\Delta p_c^S/p_c^S=[p_c^S(\text{num})-p_c^S(\text{GM2})]/p_c^S(\text{num})$ as a function of $d$ for the hypercubes (since data are available only for these lattices at high dimensions). $p_c^S$(num) is the numerical percolation threshold [10] and $p_c^S$(GM2) the prediction of the GM2 law.

We have reported in [6] that $|\Delta p_c^S|$ can reach 0.008 for some lattices in $d \leqslant 6$. This measures the accuracy of the GM2 law when applied to *any* Bravais lattice sc, bc, or fcc in $3 \leqslant d \leqslant 6$. However, regarding the simple cubic and hyper-

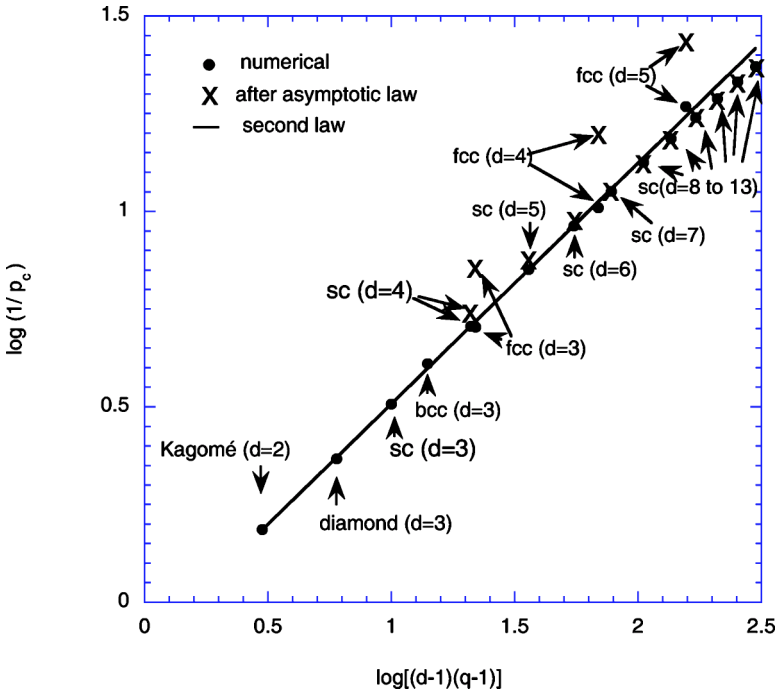


FIG. 1. Site percolation threshold as a function of the variable $(d-1)(q-1)$ pertinent to the GM2 law, in decimal logarithms. The numerical estimates (●) are from Refs. [10–12]. The crosses are predictions of the GM3 asymptotic law; the solid line materializes the GM2 law.

cubes only, the accuracy is much better. In particular, in our prior work (see Table I in Ref. [6]), $|\Delta p_c^S|$ for sc lattices was within $5\times10^{-4}$ at all dimensions $d<7$, except at $d=6$ where an outstanding deviation $|\Delta p_c^S|=0.002$ was pointed out between the numerical estimate 0.107 available at that time and 0.109 predicted by the GM2 law. The new numerical calculations [10] have corrected the estimate of $p_c^S$ at $d=6$, raising $p_c^S$ from 0.107 to 0.109 017, now in agreement with the prediction of the GM2 law. With the new estimates of Ref. [10], which are $\simeq$30 times more precise than the previous ones, we find $|\Delta p_c^S|/p_c^S\leqslant 0.4\%$ in the whole range $3\leqslant d\leqslant 6$ [6]. That is why we consider as significant a departure from the GM2 law with $|\Delta p_c^S|/p_c^S\geqslant 0.4\%$ in Fig. 2.

This plot then provides evidence for a crossover at $d_c=6$: at $d\leqslant 6$, the GM2 law applies; at $d>6$, this is no longer the case. The systematic quasilinear increase of $\Delta p_c^S/p_c^S$ as a function of $d$ which extrapolates to zero at $d=6$ corroborates this value for the crossover dimension. Note that $d_c$ is also known to be the upper marginal dimension where critical exponents for the percolation transition reach mean-field values. However, in phase transition theory, only universal quantities are supposed to undergo a crossover at $d_c$. This

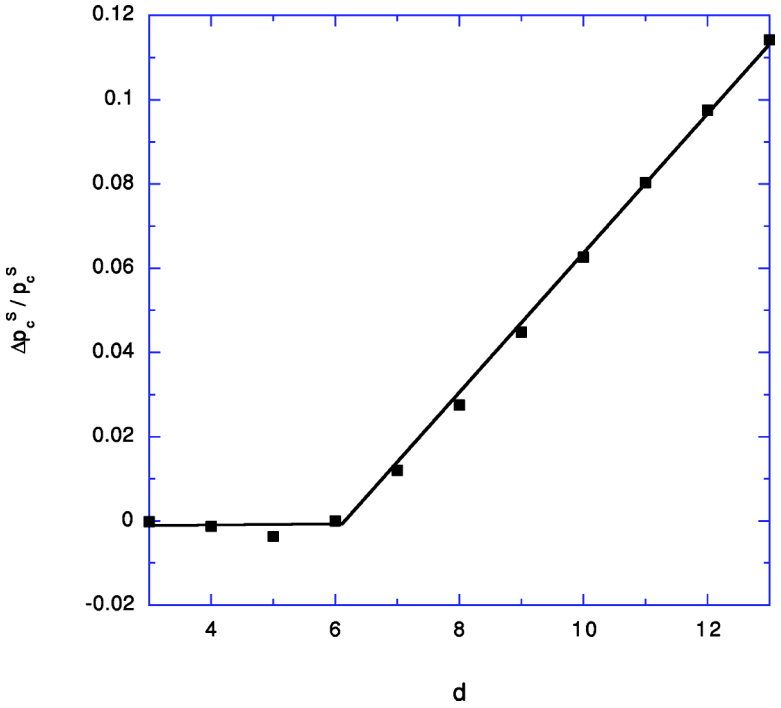


FIG. 2. Relative difference $[p_c^S(\text{num})-p_c^S(\text{GM2})]/p_c^S(\text{num})$ between the numerical data $p_c^S(\text{num})$ and the the GM2 law $p_c^S(\text{GM2})$ (solid squares) as a function of the dimension $d$ of the hypercubes. Lines are guides for the eyes.

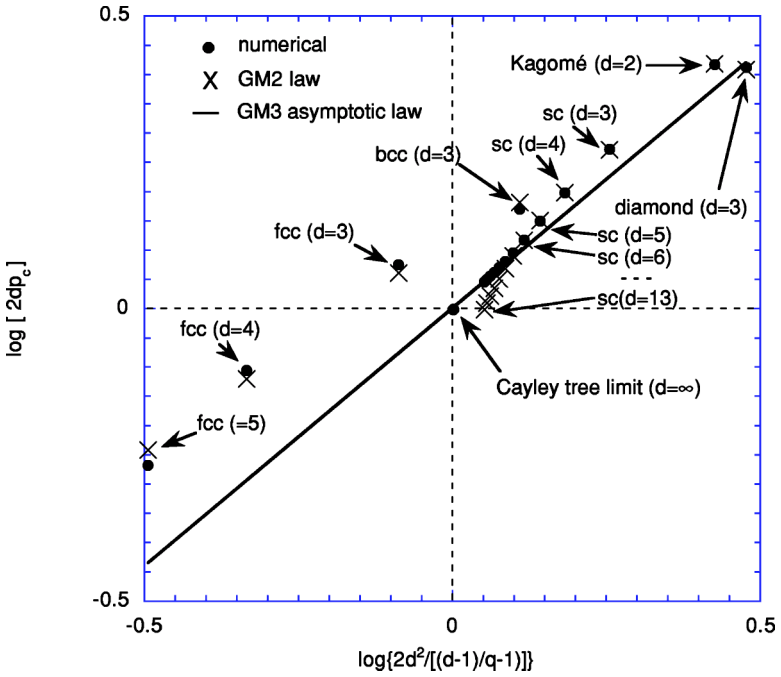


FIG. 3. Site percolation threshold as a function of the variable $2d^2/[(d-1)(q-1)]$ pertinent to the GM3 law, in decimal logarithms. The numerical estimates (●) are from Refs. [10–12]. The crosses are predictions of the GM2 asymptotic law; the solid line materializes the GM3 law.

site percolation transition gives an outstanding example where a nonuniversal quantity like $p_c^S$ also undergoes a crossover at $d_c$.

Instead of choosing the GM2 law as the reference, we can also choose the GM3 law and investigate how the the percolation thresholds approach this asymptotic law. The GM3 law is best illustrated in the log-log plot of $2dp_c^S$ versus $x=2d^2/[(d-1)(q-1)]$ in Fig. 3 since it reduces to a straight line. For comparison, the data have been also reported, and the crosses now correspond to the values of $p_c^S$ as predicted by the GM2 law. As $x$ is not the pertinent variable according to the GM2 law, once again, only the crosses corresponding to all the hypercubes (sc) from $d=3$ up to $d=13$ do belong to a single curve. As we can see in Fig. 2, this curve has a negative curvature and crosses the straight line corresponding to the GM3 law. $p_c^S$(num) as a function of $d$ then shifts from the GM2 law at $d_c=6$, to approach the GM3(law) assumed to be its asymptote in the GM model.

To illustrate this behavior, we have reported, in Fig. 4, $\Delta p_c^S/p_c^S=[p_c^S(\text{num})-p_c^S(\text{GM3})]/p_c^S$ as a function of $d$ for hypercubes in high dimensions. From this figure, it can be seen that this asymptotic limit is indeed reached at $d=13$. It is then important to note that the crossover at $d_c=6$ does not mean an abrupt shift from the GM2 law to the GM3 law.

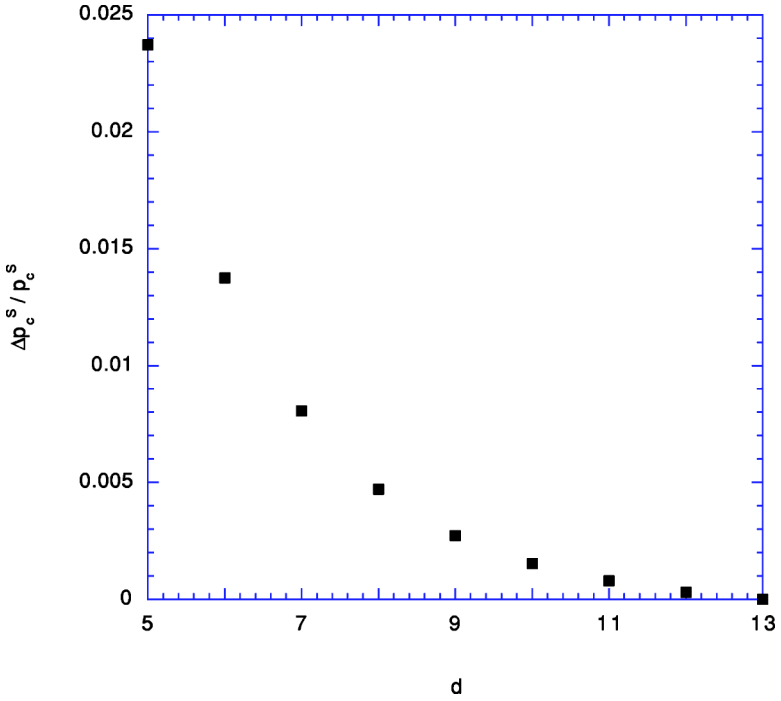


FIG. 4. Relative difference $[p_c^S(\text{num})-p_c^S(\text{GM3})]/p_c^S(\text{num})$ between the numerical data $p_c^S(\text{num})$ and the the GM3 law $p_c^S(\text{GM3})$ as a function of the dimension $d$ of the hypercubes.

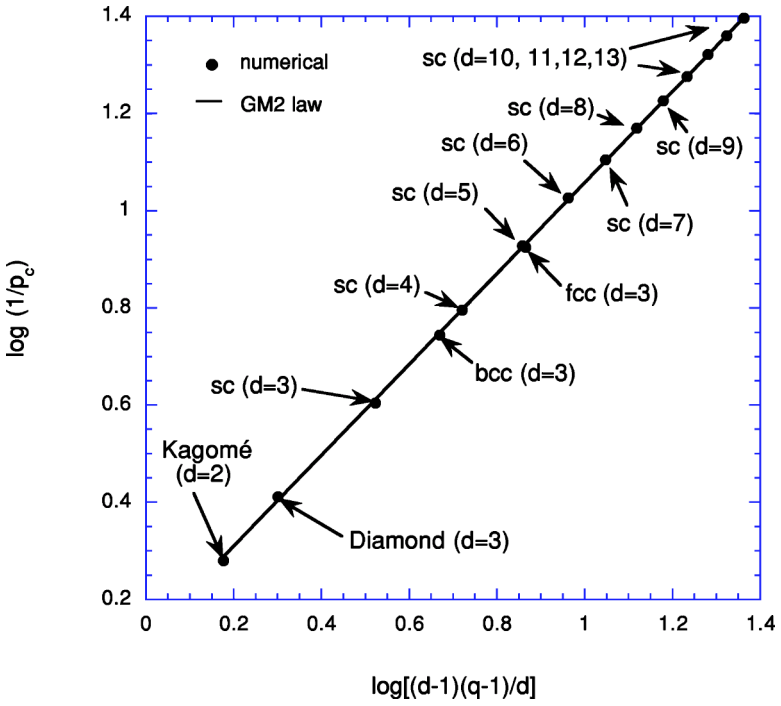


FIG. 5. Bond percolation threshold as a function of the variable $(d-1)(q-1)/d$ pertinent to the GM2 law, in decimal logarithms. The numerical estimates (●) are from Refs. [10–12]. The solid line materializes the GM2 law.

Instead, it is a crossover to another law which is missing here. More important, it indicates this law $p_c^S(\mathrm{num})$ as a function of $d$ is not embedded in the GM formula and accepts the GM3 law only as an asymptote in the large-$d$ limit, eventually reached (within the error bars) at $d \geqslant 13$. Actually, the systematic and increasing deviation of $p_c^S$ from the GM3 law as $d$ decreases from $d=13$ can be viewed as a pretransitional effect upon approaching the upper critical dimension from below, beyond the scope of the GM3 law.

### B. Bond percolation

Let us now investigate the situation for bonds. The GM2 law in this case is illustrated in a log-log plot of $p_c^B$ as a function of $(d-1)(q-1)/d$ (Fig. 5). No deviation from the GM2 law can be evidenced for any lattice up to the highest dimension $d=13$ investigated. To be more specific, we have reported in Fig. 6 the differences $\Delta p_c^B/p_c^B$ with $\Delta p_c^B = p_c^B(\mathrm{GM2}) - p_c^B(\mathrm{num})$ and $\Delta p_c^B = p_c^B(\mathrm{num}) - p_c^B(\mathrm{GM3})$. Note the sign inversion in the definition of $\Delta p_c^B$ to have this quan-

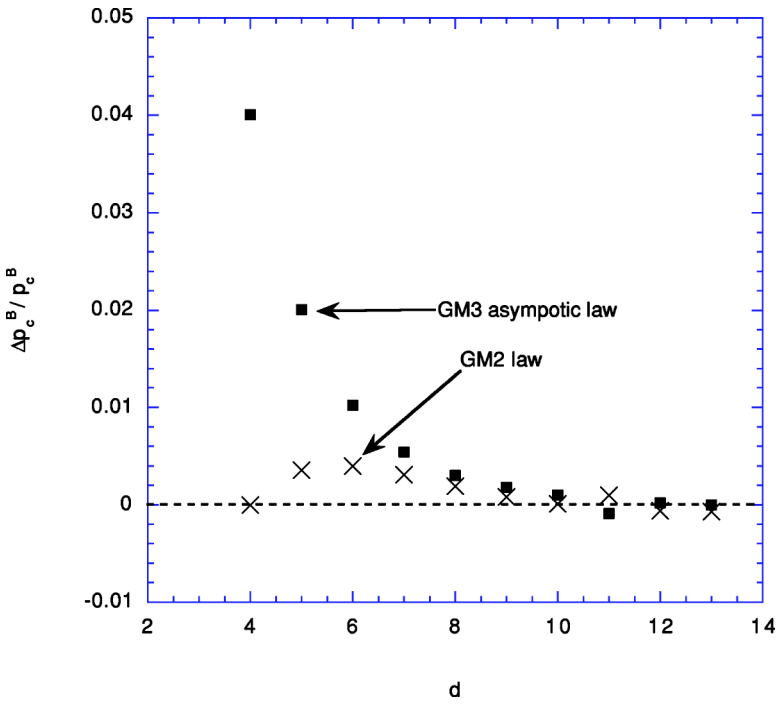


FIG. 6. Relative difference $\Delta p_c^B/p_c^B(\mathrm{num})$ with $\Delta p_c^B = p_c^B(\mathrm{GM2}) - p_c^B(\mathrm{num})$ (crosses) and $\Delta p_c^B = p_c^B(\mathrm{num}) - p_c^B(\mathrm{GM3})$ (solid squares) as a function of the dimension $d$ of the hypercubes.

tity positive, which means that the numerical estimates are in between the estimates of the GM2 and GM3 laws. Clearly, the exact (numerical) results match the GM2 law at $d \leqslant 6$, as expected. The relative deviation of the GM2 law with respect to the numerical result at $d \leqslant 6$ is in the range $\Delta p_c^B / p_c^B \leqslant 0.9\%$, so that we can take as significant a departure from the GM2 law $\Delta p_c^B / p_c^B \geqslant 0.9\%$.

However, the relative deviation between numerical estimates and the GM2 law is smaller in all dimensions $7 \leqslant d \leqslant 13$. Actually, the relative deviation of the numerical estimates does not exceed 0.4% in the whole range $9 \leqslant d \leqslant 13$, not only with respect to the GM2 law, but also with respect to the GM3 law, so that no significant difference between the two laws can be detected. Therefore, in contrast with the situation met in the site percolation problem, the GM3 law is not accurate enough to detect a crossover at $d=6$.

To explain why it is not possible to distinguish between the GM2 and GM3 laws in the range $7 \leqslant d \leqslant 13$, we note that the leading term in a $q-1$ expansion of the GM2 law at large $q$ is in $(q-1)^{b-2a}$. For bonds, $b-2a=-0.94$, very close to the exponent $-1$ of the leading term in the GM3 law. For sites, however, $b-2a=-1.23$, which is markedly different from $-1$, so that a clear distinction between the GM2 and GM3 laws can be made even at the scale of a short dimension interval for sites, while this is impossible for bonds.

To be more specific, we note that the deviation of both the GM2 and GM3 laws with respect to the numerical results—i.e., $|p_c^B(\mathrm{GM2}) - p_c^B(\mathrm{num})|$ and $|p_c^B(\mathrm{GM3}) - p_c^B(\mathrm{num})|$—is only on the fourth digit in dimension $d>7$, which amounts to a relative error within 0.4%, while, as we have stated above, a deviation with respect to the GM laws can be regarded as significant only if it exceeds 0.9% for bonds. Therefore, evidence of a crossover of dimensionality at $d_c=6$ for bonds requires an improvement of the GM law and its substitution by a new formula which would improve the accuracy typically a factor 3.

## III. DISCUSSION

Van der Marck [13] has shown that, if there is to be an exact universal formula for percolation thresholds, it must be based on more information than $d$ and $q$ only. In particular, the body-centered-cubic lattice and the stacked triangular lattice both realize $d=3$ and $q=8$, but they have different $p_c$'s. This simple consideration is sufficient to show that Eqs. (1) and (3) cannot be exact. Nevertheless, the deviation with respect to the exact or the almost exact (deduced from the best numerical estimates) thresholds of sc, bcc, and fcc lattices is so small that the GM laws have the operational power to address the problem of the crossover dimensionality.

On this basis, the present analysis of the percolation thresholds for sc (hypercubes) hints at the possible existence of a crossover at $d_c=6$ for the site percolation threshold, although it is a nonuniversal parameter. At higher dimensions, $p_c^S$ departs from the GM2 law to approach the GM3 asymptotic law which is reached at $d=13$. For bonds no similar behavior at $d_c=6$ is detected.

Because of the relation $d=2q$ for hypercubes, study of hypercubes alone does not allow us to distinguish between the variables $d$ and $q$ to know which one is pertinent for the possible crossover. However, some indication can be extracted from the data in Fig. 1. Let us consider in particular the fcc lattice, which has a coordinance $q$ much larger than the hypercube at the same dimension. For instance, $q=24$ and 40 for fcc lattices in dimensions $d=4$ and $d=5$, respectively. Those are the coordination numbers of hypercubes in dimensions 12 and 20, respectively. The fcc percolation thresholds at $d=4,5$ have been reported in Fig. 1, along with the values predicted by the GM2 and GM3 laws. This figure shows unambiguously that these two fcc lattices do satisfy the GM2 law and not the GM3 law, despite the fact that their coordinance numbers are those of the hypercubes in dimensions $d=12$ and $d=14$.

It corroborates that the pertinent variable responsible for the possible crossover behavior in the percolation thresholds is indeed the dimension $d$, while the coordination $q$ does not play any significant role. It also justifies the term crossover of dimensionality used in this work. For universal variables, such as the critical exponents, the renormalization group technique provides us with an elaborate theory to understand the crossover of dimensionality at the associated identification of universality classes. However, such a behavior is not expected for nonuniversal quantities like percolation thresholds. The explanation for this unexpected result is thus a new challenge in the field of phase transition theory.

We note that $d_c$ is the upper critical limit for percolation transition phenomena in general, not for the hypercubes only. The question then arises whether the possible crossover of dimensionality we have observed for hypercubes also applies to other lattices with a different topology. So far, accurate numerical estimates of percolation thresholds beyond $d=6$ could be achieved on the hypercubes only. The lack of data prevents us for the moment from addressing this question. Nevertheless, we believe that progress in methods to compute percolation thresholds will make possible the simulation of percolation of other systems more complex with a larger coordinate number $q$ in the near future.

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