Universal formulas for percolation thresholds

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A power law is postulated for both site and bond percolation thresholds. The formula is $p_c = p_0[(d-1)(q-1)]^{-a}d^b$, where d is the space dimension and q the coordination number. All thresholds up to $d \to \infty$ are found to belong to only three universality classes. For two classes $b = 0$ for site dilution while $b = a$ for bond dilution. The remaining class associated with high dimensions is characterized by $b = 2a - 1$ for both sites and bonds. Classes are defined by a set of value for $\{p_0;\ a\}$. Deviations from available numerical estimates at $d \leq 7$ are within ± 0.008 and ± 0.0004 for high dimensional hypercubic expansions at $d \geq 8$. The formula is found to be also valid for Ising critical temperatures.

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Percolation theory has been known for several decades [1,2]. It deals with the effects of random dilution of either sites or bonds in a lattice. Flory introduced it first in the framework of chemical industry [3]. Upon site or bond dilution a sharp change is found to occur in the connectivity of the system at some threshold p_c in the density of occupied site or bond. Although it is a purely geometrical phenomenon, this change can be described in terms of the usual second-order phase transitions. This mapping to critical phenomena made percolation a full part of the theoretical framework of collective phenomena and statistical physics. It is indeed a very powerful and general tool. Percolation has thus been applied to numerous problems in a large variety of fields, even outside physics (for reviews, see [4–7]).

However, despite both its success and its mathematical ground, percolation theory has resisted exact calculations. Most known data are numerical estimates, from both Monte Carlo simulations and series expansions [6,8]. In particular, analytic calculations of percolation thresholds have proven to be a rather difficult task. For instance, 20 years or so were necessary to prove the numerical estimate of $p_c = \frac{1}{2}$ for the square bond percolation threshold [9]. The bond threshold is also known exactly for the two-dimensional honeycomb and triangular lattices [9]. The situation is even worse in the case of site percolation. Indeed, thresholds are known exactly only in the cases of two-dimensional triangular and Kagomé lattices [9]. At dimension higher than two, no thresholds were determined exactly. From simulations, percolation thresholds are found to depend on both the space dimension d and the coordination number q. Only the pathological Cayley tree has been solved exactly to yield $p_c = 1/(q-1)$ [10]. This expression, which holds for both bonds and sites, yields good results at high dimensions.

Along the general form of the Bethe expression, various empirical formulas have been tried to yield large classes of thresholds without success. For instance, the formula $p_c = d/[(d-1)(q-1)]$ was proposed 12 years ago for site percolation [11]. Another one, $p_c = d/[(d-1)q]$ was suggested for bond dilution [12]. Unfortunately, both formulas are not satisfactory for all lattices, especially at low dimensions. More recently the expression $p_c = 1/\sqrt{q-1}$ was derived for site percolation thresholds [13,14]. Very good results are obtained in two dimensions but not at higher dimensions. Another similar form was also noticed elsewhere [15]. In this paper, for the first time, one unique power law is found to yield within an excellent accuracy both site and bond percolation thresholds for all lattices at all dimensions. The power law is $p_c = p_0\{(d-1)(q-1)\}^{-a}d^b$. From a log-log plot all available data ($d \leq 7$) are found to fit on two straight lines. In both cases $b = 0$ for site dilution and $b = a$ for bond dilution. One line includes two-dimensional triangle, square, and honeycomb lattices, which constitute the first class, characterized by $\{p_0 = 0.8889;\ a = 0.3601\}$ for site dilution and by $\{p_0 = 0.6558;\ a = 0.6897\}$ for bond dilution. Two-dimensional Kagomé and all other regular lattices (for $d \geq 3$) align on the other unique line and constitute the second class, characterized by $\{p_0 = 1.2868;\ a = 0.6160\}$, and $\{p_0 = 0.7541;\ a = 0.9346\}$ for sites and bonds, respectively. Deviations from available numerical estimates are very small and range from 0 to ± 0.008. At high dimensions a third class is found that recovers the infinite Cayley tree limit. It is defined by $\{b = 2a - 1;\ p_0 = 2^{a-1}\}$ for both sites and bonds. Using high-dimensional hypercubic expansions [14,17,18] as data we found $\{a = 0.8800\}$ for sites and $\{a = 0.3685\}$ for bonds. The agreement is excellent with deviations within ± 0.0004. The value of dimension d_c at which the third class holds is between $d = 6$ and $d = 8$. The results and perspectives are discussed.

From an analysis of the Bethe approximation on a regular lattice, we found recently [13,14] an underlying lattice homogeneity breaking. On this basis we obtained a new expression,

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$$x_c = 1/\sqrt{(q-1)}\,, \tag{1}$$

for the percolation threshold, instead of the well-known Bethe expression,

$$x_c^B = 1/(q-1)\,. \tag{2}$$

Equation (1) yields results that are in good agreement with exact and numerical site percolation thresholds at $d = 2$. However, results get poor at higher dimensions. This discrepancy evidences a missing d dependence that could be equal to one at $d = 2$. It thus hints a possible $(d-1)$ dependence. In parallel Eq. (1) did single out a $(q-1)$ dependence. From the hypercube case we could expect dimension and coordinance to play a similar role. Therefore one extension of Eq. (1) is to substitute the product $(d-1)(q-1)$ for $(q-1)$. On this basis, a natural generalization of Eq. (1) is the power law,

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

It is worth noting that Eq. (3) reduces to Eq. (1) for the set $\{p_0 = 1;\ a = 1/2\}$ besides the variable multiplicator factor $(d-1)$, which equals 1 at $d = 2$.

At this stage, we report a log-log plot of known estimates p_c [7,19] as a function of the associated product $(d-1)(q-1)$. The plot is shown in Fig. 1 for the site case. All the points align on only two straight lines, corresponding to the two classes of lattices, mentioned above.

In parallel the log-log plot for bond data [7,19] exhibits constant deviations from a straight line at each dimension. These deviations suggest a dimension rescaling of the variable $(d-1)(q-1)$ resulting in

$$p_c = p_0\left[\frac{(d-1)(q-1)}{d}\right]^{-a}. \tag{4}$$

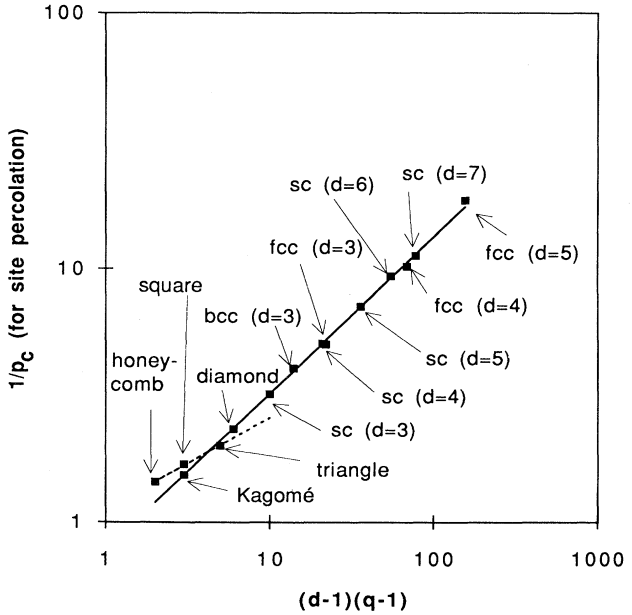

FIG. 1. Inverse of site percolation thresholds as a function of $(q-1)(d-1)$ in logarithmic scales.

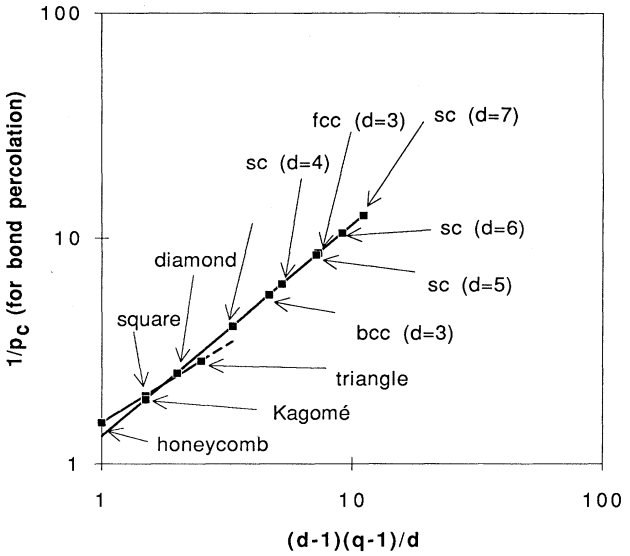

FIG. 2. Inverse of bond percolation thresholds as a function of $(q-1)(d-1)/d$ in logarithmic scales.

The log-log plot using Eq. (4) is shown in Fig. 2. The situation is now identical to the site case, as all points align on two straight lines associated to the two classes of lattices. The percolation thresholds using Eqs. (3) and (4) are shown in Tables I and II together with exact re-

TABLE I. Site percolation thresholds from this work p_c compared to "exact estimates" p_c^e taken from [6,17]. $\Delta \equiv p_c - p_c^e$. $*$ means not included to determine p_0 and a. The first universality class is defined by $p_0 = 0.8889$ and $a = 0.3601$. The second universality class is defined by $p_0 = 1.2868$ and $a = 0.6160$.

Dimension	Lattice	q	p_c^e	p_c	Δ
$d = 2$	Square	4	0.5928	0.5984	+0.0056
	Honeycomb	3	0.6962	0.6925	-0.0037
	Triangular	6	0.5000	0.4979	-0.0021
$d = 2$	Kagomé*	4	0.6527	0.6540	+0.0013
$d = 3$	Diamond	4	0.43	0.43	0
	sc	6	0.3116	0.3115	-0.0001
	bcc	8	0.246	0.253	+0.007
	fcc	12	0.198	0.192	-0.006
$d = 4$	sc	8	0.197	0.197	0
	fcc*	24	0.098	0.095	-0.003
$d = 5$	sc	10	0.141	0.141	0
	fcc*	40	0.054	0.057	+0.003
$d = 6$	sc	12	0.107	0.109	+0.002
	fcc*	60		0.039	
$d = 7$	sc	14	0.089	0.088	-0.001
	fcc*	84		0.028	

TABLE II. Bond percolation thresholds from this work p_c compared to "exact estimates" p_c^e taken from [6,17]. $\Delta \equiv p_c - p_c^e$. * means not included to determine p_0 and a. The first universality class is defined by $p_0 = 0.6558$ and $a = 0.6897$. The second universality class is defined by $p_0 = 0.7541$ and $a = 0.9346$.

Dimension	Lattice	q	p_c^e	p_c	Δ
$d = 2$	Square	4	0.50000	0.49581	-0.00419
	Honeycomb	3	0.6527	0.6558	+0.0031
	Triangular	6	0.34729	0.34859	+0.00130
$d = 2$	Kagomé*	4	0.5244	0.5162	-0.0082
$d = 3$	Diamond	4	0.388	0.394	+0.006
	sc	6	0.2488	0.2448	-0.0040
	bcc	8	0.1803	0.1787	-0.0016
	fcc	12	0.119	0.117	-0.002
$d = 4$	sc	8	0.1601	0.1601	0
	fcc*	24		0.0527	
$d = 5$	sc	10	0.1182	0.1192	+0.0010
	fcc*	40		0.0303	
$d = 6$	sc	12	0.0942	0.0951	+0.0009
	fcc*	60		0.0198	
$d = 7$	sc	14	0.07879	0.07923	+0.00044
	fcc*	84		0.0140	

sults and numerical estimates for site and bond dilution, respectively.

At this stage we have a one-exponent power law for sites [Eq. (3)] and bonds [Eq. (4)]. However, the site variable $(d-1)(q-1)$ has to be rescaled by dimension in the case of bonds. The two expressions can thus be unified under the form

$$p_c = p_0[(d-1)(q-1)]^{-a} d^{\,b}\,. \tag{5}$$

From Eqs. (3) and (4) we have $b = 0$ for sites and $b = a$ for bonds. The agreement is remarkable and holds true from $d = 2$ up to $d = 7$, where threshold estimates are available.

To complete the discussion we compare our results to d-dimensional simple hypercubic lattice percolation thresholds derived as $1/(q-1)$ expansions. For site percolation it is [16]

$$p_c^S = (q-1)^{-1} + \tfrac{3}{2}(q-1)^{-2} + \tfrac{15}{4}(q-1)^{-3} + \tfrac{83}{4}(q-1)^{-4} + \cdots\,, \tag{6}$$

which becomes for bond percolation [17],

$$p_c^B = (q-1)^{-1} + \tfrac{5}{2}(q-1)^{-3} + \tfrac{15}{2}(q-1)^{-4} + 57(q-1)^{-5} + \cdots\,. \tag{7}$$

In parallel from Eq. (5) we get the expansion

$$p_c = p_0 2^{a-b}(q-1)^{b-2a}\left\{1 + (a+b)(q-1)^{-1} + \frac{a^2+a+2ab+b^2-b}{2}(q-1)^{-2} + \cdots\right\}. \tag{8}$$

Equations (6) and (7) have the same first leading term $1/(q-1)$, which is the Bethe result. In our case we have

$$p_0 2^{a-b}(q-1)^{b-2a}\,, \tag{9}$$

which becomes $p_c = p_0 2^a (q-1)^{-2a}$ for sites with the exponent $2a = 1.23$ and $p_c = p_0(q-1)^{-a}$ for bonds with $a = 0.94$. Both cases are clearly different from the Bethe result $1/(q-1)$. The respective $1/(q-1)$ exponent is close to, but definitively different from, one. Therefore we do not recover the Bethe asymptotic limit. Moreover, the site p_c becomes smaller that the bond p_c at $d = 11$, which is clearly nonphysical.

On this basis, although our formula agrees perfectly with available numerical data up to $d = 7$ (see Tables I and II), a third class must exist at high dimensions. To determine its characteristics we first note that the Cayley tree result $x_c^B = 1/(q-1)$ is believed to be the exact $d \to \infty$ asymptotic limit for both bonds and sites. It then indicates that two different constraints $b = 0$ and

$b = a$ for, respectively, sites and bonds cannot hold at high dimensions. The $1/(q-1)$ limit is recovered from Eq. (9) if and only if $b = 2a-1$ together with $p_0 = 2^{a-1}$. Equation (5) becomes

$$p_c = 2^{a-1}[(d-1)(q-1)]^{-a} d^{2a-1}\,, \tag{10}$$

which gives a straight line in a log-log plot of $2dp_c$ versus $2d^2/[(d-1)(q-1)]$.

We then determine the value of exponent a using numerical estimates from the $1/(q-1)$ expansions in Eqs. (6) and (7), which are supposed to be exact in the $d \to \infty$ limit. From Fig. 3 we find $a = 0.8800$ for sites and $a = 0.3685$ for bonds. It is worth noting that while Eqs. (6) and (7) are derived for hypercubes only, Eq. (10) holds for any lattice at $d \geq d_c$.

From Fig. 3 the best estimate for the crossover dimension is $d_c = 8$. However, we cannot preclude that d_c is as small as $d_c = 6$, which is the upper critical dimension for percolation. Differences between numerical estimates and associated values of p_c deduced, on the one hand from Eq. (3) or (4), and on the other hand from Eq. (10), are comparable to numerical errors (see Table III and Fig. 3). From current data we have $6 \leq d_c \leq 8$. Exact determination of d_c requires more accurate numerical estimates of percolation thresholds at these dimensions.

Moreover, the crossover at d_c seems to be driven by a dimensional phenomena. This conjecture is based on the following observation. At $d = 5$, fcc lattice, which has

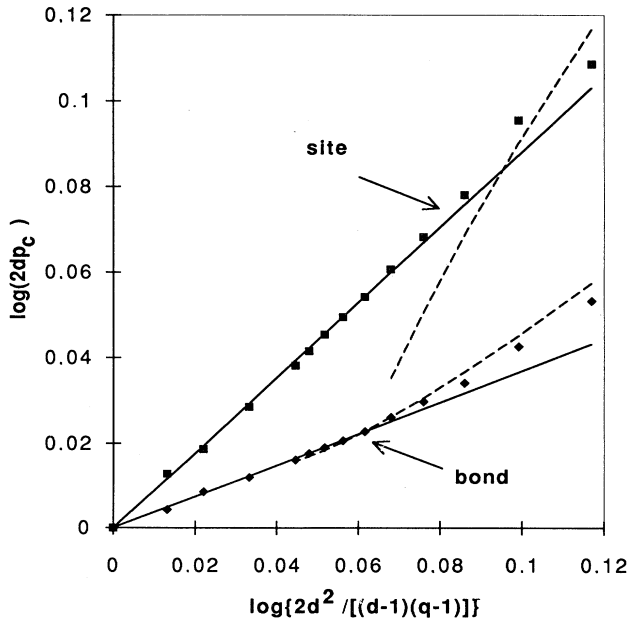

FIG. 3. Percolation thresholds in high-d hypercubes using both numerical estimates for $d = 6$ and $d = 7$ and hypercubic expansions from Refs. [14] and [15] at $d = 8, 9, \ldots 15$, $d = 20, 30, 50$. The origin corresponds to the Cayley tree limit at infinite d. Straight lines are according to Eq. (10). Broken curves correspond to Eqs. (3) and (4), for the second universality class.

TABLE III. High-d hypercube thresholds: p_c site, and p_c bond from Eq. (10) and the "hypercube" expansions p_c^s and p_c^b from [14] and [15], respectively. At $d > 10$ the difference is smaller than 10^{-4}; even relative errors are negligible, as it can be seen in Fig. 3.

Dimension	p_c site	p_c^s	$1/(q-1)$	p_c^b	p_c bond
$d = 6$	0.1056	0.1075	0.0909	0.0936	0.0920
$d = 7$	0.0873	0.0882	0.0769	0.0785	0.0777
$d = 8$	0.0744	0.0748	0.0667	0.0676	0.0672
$d = 9$	0.0648	0.0650	0.0588	0.0595	0.0593
$d = 10$	0.0574	0.0575	0.0526	0.0531	0.0530

$(d-1)(q-1) = 156$ belongs to the second class (see Fig. 1). In parallel hypercube at $d = 9$ belongs to the third class (see Fig. 3) though it has $(d-1)(q-1) = 136$.

The various universality classes for site and bond dilution were found to be identical. One class is restricted to two dimensions and contains triangle, square, and honeycomb lattices. The second universality class embodies Kagomé and all lattices at $3 \leq d \leq d_c$. It is interesting to stress that square and Kagomé, which both have $d = 2$ and $q = 4$ turn out to be in different classes. The third class embodies all lattices at $d \geq d_c$. At $d = 1$ ($q = 2$) exact value $p_c = 1$ for both sites and bonds implies $a = 0$.

At this stage it is worth emphasising that numerical values of p_0 and a have been determined using as input data what is denoted in Tables I and II as "exact" thresholds. Obviously these values will be different using a different set of input or a restricted one. We chose arbitrarily to use and report values from Refs. [6,17]. We are here advocating the power-law form of Eq. (5) rather than the third decimal associated to the determination of p_0 and a.

Error bars for numerical estimates are believed to be on the last given figure. It should thus not exceed ± 0.001 in case p_c is given with four decimals and ± 0.01 in case it is given with three decimals. Therefore deviations $\Delta = p_c - p_c^e$ are significant at $d = 2$ though they are small. For all lattices at this low dimension, $|\Delta|$ exceeds 0.001 (Δ is only 0.0013 in the triangular lattice case, but there, p_c is known exactly).

To further investigate this anomaly at $d = 2$, we have explored percolation thresholds when the connection range includes next-nearest (nnn) and next-next-nearest (nnnn) neighbors. Numerical estimates p_c^e are scarce and restricted to site percolation [20]. They strongly suggest all $d = 2$ lattices enter the second universality class as soon as the connection range exceeds nearest neighbors. Associated site percolation thresholds are then calculated using for q the sum of sites within the connection range. We get, respectively, $p_c = 0.388$ for the nnn square, 0.294 for nnn triangular, nnnn square and honeycomb, and 0.225 for nnnn triangular. It means $10^3\Delta = -1, +1, +2, -6, 0$, respectively, which is always smaller than the numerical estimate error bar ± 0.01. However, available square lattice site percolation

thresholds for longer ranges [21] do not belongs to this class. It shows that an additional class should be added to account for long-range interaction percolation (over nnnn).

At $d \geq 3$, errors Δ may not have a statistical significance. Only the value of the bond percolation threshold for the simple cubic lattice exceeds significantly 0.001. Moreover, the random distribution of deviations opposes the existence of a missing systematic correction to Eq. (5).

Last but not least we found that our power law is also valid to predict Ising critical temperatures T_c. Indeed the phase transition nature of percolation makes critical thresholds similar to critical temperatures. Dealing with pair exchanges, it is natural to use the bond percolation formula [Eq. (4)] for the reduced temperature $K_c = J/k_B T_c$, with J the exchange coupling. Numerical estimates for K_c at $d = 3$ are $K_c^e = 0.2217$, 0.1575, and 0.1021 for sc, bcc, and fcc lattices, respectively [22]. The set $\{p_0 = 0.6525;\ a = 0.9251\}$ in Eq. (4) leads to critical temperatures K_c, which depart from these values by the amount $K_c - K_c^e = +0.0012$, $+0.0008$, and -0.0006, respectively. It is again comparable to the numerical estimate errors.

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