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COMMENT

Empirical phase boundaries for site–bond percolation

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Abstract. The expression $bs^x = \text{constant}$ is proposed as a suitable and possibly correct description of site-bond percolation phase boundaries. Bond thresholds, b, as a function of site thresholds, s, for this model agree with published numerical results to better than $\pm 2\%$. The exponent x and the constant are determined solely by the site-only and bond-only thresholds, s_c and b_c, so that the model may be applied to any percolation problem for which these are known.

Site-bond percolation has been studied primarily by two methods (to be reviewed later in this comment). Real-space renormalisation group and related methods are qualitatively useful, but typically do not produce accurate site or bond percolation thresholds, and sometimes are tricky to do properly. Numerical methods such as series expansions and Monte Carlo simulations are generally quite accurate, but require a considerable amount of computation. None of these approaches are convenient for the non-specialist to use, nor are results available in the literature for all lattices that might be of interest. For calculations using site-bond percolation as a model, it is desirable to have a relatively simple functional form for the phase boundary. Ideally, any description should also be applicable to general site-bond percolation problems with only a change of a few parameters. This comment describes an expression, developed empirically, that meets these criteria.

Consider a network of sites connected by bonds, for example on a two-dimensional square lattice. A site (or bond) is considered to be conducting if it is 'occupied'. If sites are randomly occupied with probability s, and all bonds are occupied, the network is conducting when s is greater than s_c, the site percolation threshold. If the bonds are randomly occupied and all sites are occupied, bond percolation occurs with threshold b_c. For site-bond percolation, both sites and bonds are independently randomly occupied.

The critical curve (phase boundary) for the site-bond problem can be defined as a function $b = b(s)$, which specifies the bond threshold for a particular site occupancy. Such a curve is shown in figure 1, which depicts a phase diagram for site-bond percolation on the simple cubic lattice as an example. The phase boundary is approximately hyperbolic, and has a similar appearance for all two-dimensional lattices in addition to the simple cubic lattice. As defined earlier, bond percolation occurs for $s = 1$, $b = b_c$, and site percolation for $b = 1$, $s = s_c$, so that the critical curve must satisfy the conditions $b(1) = b_c$ and $b(s_c) = 1$. The objective is to find an expression $b = b(s)$ that satisfies these requirements and agrees with critical curves produced by other methods.

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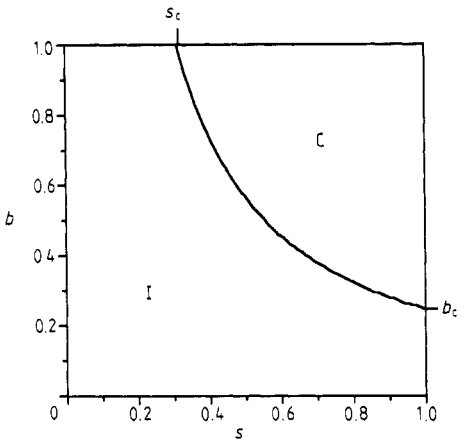

Figure 1. Schematic phase diagram for site-bond percolation on the 3D simple cubic lattice. The site-only and bond-only thresholds are labelled s_c and b_c. The conducting region is marked C, and the insulating region is marked I.

In searching for a general form for the critical curve, it was found that log-log plots of these curves are linear or nearly linear in all cases for which data could be extracted from the literature. Figure 2, a linear plot of $-\ln b$ against $-\ln s$ demonstrates this fact for several examples. For the purpose of maintaining clarity, not all of the data available for the lattices shown are included in the figure. Data for the triangular lattice (TR) were calculated with a precision of 2% from the real-space renormalisation equations given by Guttmann and Whittington [1]. For this case, $-\ln b$ against $-\ln s$ is linear within 5%. The square lattice data (SQ) were obtained by digitising graphical results given by Agrawal *et al* [2] based on a series expansion study. This example is linear within 2%, which was the accuracy of the digitisation process used. Chang and Odagaki [3] provide a polynomial fit to their Monte Carlo simulation of the simple

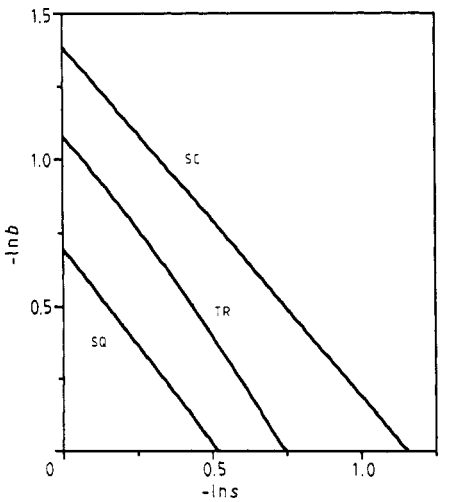

Figure 2. Logarithmic plot of the site-bond phase boundaries derived from several published sources: 2D triangular lattice (TR) from [1], 2D square lattice (SQ) from [2] and 3D simple cubic lattice (SC) from [3].

cubic lattice, which was used to generate curve SC in figure 2. The linearity is better than 1% for this case.

Real-space renormalisation results are available for the square lattice [1, 4] that are not included in figure 2, but which have the same degree of linearity as the data displayed for the triangular lattice. Kondor [5] gives results for the honeycomb and triangular lattices derived from a 'star-triangle transformation'. Deviations from linearity are much larger (10–15%) for this method, even though the site-only and bond-only thresholds obtained apparently are exactly correct for the triangular lattice. Other numerical results for the square lattice [3] and the simple cubic lattice [6] show very good (1–2%) linearity in $\ln b$ against $\ln s$.

The evidence cited above is overwhelming that a linear relationship between $\ln b$ and $\ln s$ is correct, or at least a very good approximation, for the site-bond phase boundary. The critical curve therefore may be expressed empirically as

$$bs^x = \text{constant} \tag{1}$$

or as

$$\ln b + x \ln s = \text{constant}. \tag{2}$$

The exponent and constant are determined by the requirement that (1) produces the correct site-only ($s = s_c$, $b = 1$) and bond-only ($s = 1$, $b = b_c$) thresholds. The model for the site-bond percolation phase boundary is given by

$$bs^x = b_c \tag{3}$$

$$x = \ln b_c / \ln s_c. \tag{4}$$

Values of the parameters s_c, b_c, and x are listed in table 1 for a number of two- and three-dimensional lattices [7–10].

As stated earlier, numerical studies give more accurate results for the site and bond thresholds than do renormalisation schemes, so are likely to be of similar accuracy for other points along the critical curve. For this reason (3) is compared with the

Table 1. Parameters used with $bs^x = b_c$ (3) to describe site-bond percolation phase boundaries.

	Lattice[a]	s_c	b_c	x
2D	HC	0.692[b]	0.6527[c]	1.178
	SQ	0.5928[d]	0.5000[c]	1.326
	TR	0.5000[c]	0.3473[c]	1.526
3D	DIA	0.4299[e]	0.3886	1.120
	SC	0.3119	0.2479	1.196
	BCC	0.2464	0.1795	1.226
	FCC	0.1998	0.1198	1.318

[a] HC, honeycomb; SQ, square; TR, triangular, DIA, diamond; SC, simple cubic, BCC, body centred cubic; FCC, face-centred cubic.
[b] From [7].
[c] Exact values from [8].
[d] From [9].
[e] All 3D thresholds from [10].

available numerical data only, since this can be expected to give a better indication of the accuracy of the model. Figure 3(*a*) shows the relative difference between data derived from the literature and the model for the square lattice. Curve A is the data extracted from Agrawal *et al* [2] that was used in figure 2, and curve B was obtained from the fit to Monte Carlo results given by Chang and Odagaki [3]. The model uses the parameters from table 1 with equation (3). In both cases, the model agrees with the literature results within 1% over most of the range of s. The deviations are larger at low s, near s_c, because the site thresholds calculated by Agrawal *et al* ($s_c = 0.595$) and by Chang and Odagaki (0.586) differ slightly from the value used for the model (0.5928). If their thresholds are used in the model, the fit is much better, with deviations of less than 1% that are primarily due to scatter in the derived data. The same situation is apparent in figure 3(*b*) for the simple cubic lattice. Curve C is the same data used in figure 2 from Chang and Odagaki, and curve D was taken from Heermann and Stauffer [6] by digitising their figures. As in the case of the square lattice, deviations generally are within 1% for most values of s and are larger near s_c. Agreement is improved by using thresholds from these sources instead of those from the table.

It should be emphasised that the model discussed above was developed empirically, and no theoretical or mathematical justification for it is offered here. The excellent quantitative agreement with numerical methods for the square and simple cubic lattices is a very strong indication that the model is correct for at least these two lattices. Numerical results for the other two- and three-dimensional lattices were not found, but the model still is in reasonable agreement with the renormalisation methods.

A (speculative) plausibility argument can be offered in support of the validity of the model. As far as threshold behaviour is concerned, only two parameters describe any particular regular lattice: the site coordination, z, and the spatial dimension, d. The thresholds s_c and b_c will be determined by z and d, so the thresholds may be taken as the two necessary parameters. If only two independent parameters are available, the critical curve should be describable by only two independent parameters. In other words, it should be universal in the sense that it should depend only on s_c and b_c, or, ultimately, on z and d. If the form is correct for one lattice, it should be correct for all lattices. Equation (3) would seem to be this universal form for the site-bond percolation phase boundary.

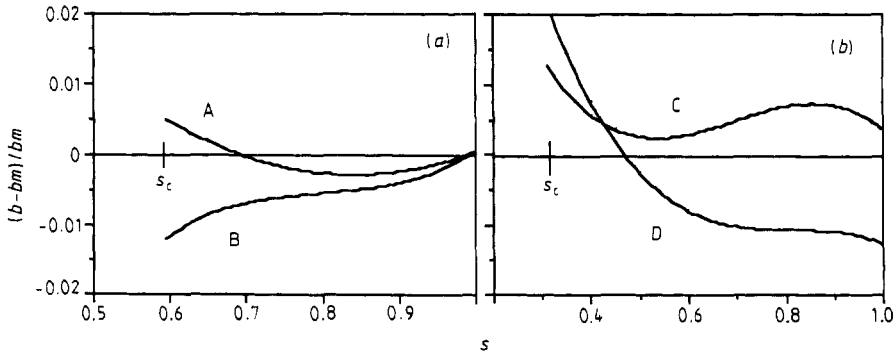

Figure 3. Comparison of the phase boundary model (3) and numerical results available in published literature for the 2D square lattice (*a*) and 3D simple cubic lattice (*b*). The quantity $(b - bm)/bm$ is the relative difference in bond threshold between the literature results and the model. Curves B and C were derived from [3], and curves A and D from [2] and [6] respectively.

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