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LETTER TO THE EDITOR

Universality at the three-dimensional percolation threshold

Dietrich Stauffer†, Joan Adler‡§ and Amnon Aharony§

† Institute for Theoretical Physics, Cologne University, 50939 Köln, Germany
‡ Physics Department, Technion, Haifa 32000, Israel
§ School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

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Abstract. The fraction of samples spanning a lattice at its percolation threshold is found via simulations of bond and site-bond percolation to have a universal value of about 0.42 in three dimensions. The ratio of shift (of the finite to infinite size threshold) to width of the threshold distribution is also compatible with universality. Lattices with up to 1001^3 sites and/or very good statistics were needed to obtain clear results in these Monte Carlo tests; preliminary studies with smaller lattices were inconclusive.

The renormalization group description [1] of the percolative phase tradition was recently corrected by Ziff [2], whose arguments were criticized and generalized by Aharony and Hovi [3] with emphasis in two dimensions; here we check them numerically in three dimensions. Consider a d-dimensional lattice, of linear size L. If a random fraction p of the bonds between nearest neighbour sites is occupied, then there is a probability $R_{\mathrm{L}}(p)$ that a particular sample contains a connected cluster which connects two opposite ends of the lattice. Here we follow rule R_1 of [1], in which one considers spanning only in one fixed direction, leaving the other boundaries free. For infinite L, $R_{\mathrm{L}}(p)$ is equal to 0 (or 1) for p below (or above) the percolation threshold p_{c}. The value of R_{L} at p_{c}, $R_{\mathrm{L}}(p_{\mathrm{c}})$, has been the topic of several recent papers [2, 3]. R_{L} was called the crossing probability by Langlands *et al* [4], and the spanning probability in [2]. A while ago, Reynolds *et al* [1] suggested an approximate real space renormalization group, based on the recursion relation $p' = R_b(p)$, where b was the length rescale factor. This recursion relation implies that p_{c} is given by the solution of $p_{\mathrm{c}} = R_b(p_{\mathrm{c}})$, and therefore that $R_L(p_{\mathrm{c}})$ is not universal. In contrast, recent work [2–4] showed that $R_L(p_{\mathrm{c}})$ is universal, equal to $\frac{1}{2}$ for several two-dimensional (2D) lattices with both bond and site percolation. In the present paper we consider this issue for some 3D cases. As a byproduct we also re-evaluate the percolation threshold for 3D bond percolation.

At finite large L, the derivative $\mathrm{d}R_L/\mathrm{d}p$ has a sharp peak close to p_{c}. This derivative may be interpreted as the distribution function of the threshold concentration p at which particular realizations of the sample percolate [5]. Defining averages via $\langle A\rangle = \int \mathrm{d}p A(\mathrm{d}R_L(p)/\mathrm{d}p)$, this implies that $p_{\mathrm{av}}(L)\langle p\rangle$ approaches p_{c} and that the squared width, $\Delta^2 = \langle (p - p_{\mathrm{av}})^2\rangle$, approaches zero as $L \to \infty$. Below we evaluate both the shift $(p_{\mathrm{c}} - p_{\mathrm{av}})$ and the width Δ, and compare their L-dependence with the theoretical predictions. A simple prediction, that ignores corrections to scaling, is that one expects $R_L(p)$ to depend on p and L only via the scaled variable $L/\xi \sim L|p - p_{\mathrm{c}}|^{\nu}$, where ξ is the percolation correlation length [5]. This would imply that both $[p_{\mathrm{av}}(L) - p_{\mathrm{c}}]$ and $\Delta(L)$ decay as $L^{-1/\nu}$. However, adding correction terms and considering some specially symmetric 2D cases, Ziff [2] showed that the former difference decays faster, as $L^{-1/\nu-1}$. Aharony and Hovi [3] then generalized this argument, and showed that there also exist terms of order $L^{-1/\nu-\theta}$, where θ comes from confluent corrections. Basically, Aharony and Hovi showed that $R_L(p)$ obeys the scaling form

$$R_L(p) = F(AtL^{1/\nu}, B_i\omega_i L^{-\theta_i}) \tag{1}$$

where $t = p - p_c$ and ω_i represents irrelevant variables. The function $F(x, y_i)$ is universal, and only the scale factors A and B_i depend on details of the lattice. Equation (1) immediately implies that when L approaches infinity, $R_L(p_c)$ approaches the universal limit $F(0, 0)$. Another direct consequence of (1) is that the scales of both $[p_{av} - p_c]$ and Δ contain the scale factor A, and therefore that in the limit $t \to 0$, $L \to \infty$ the ratio of these two quantities must approach a universal limit. For the special 2D cases studied by Ziff [2], this ratio approaches zero. In the present letter we check both $R_L(p_c)$ and this ratio in 3D, and confirm that both have non-trivial universal values.

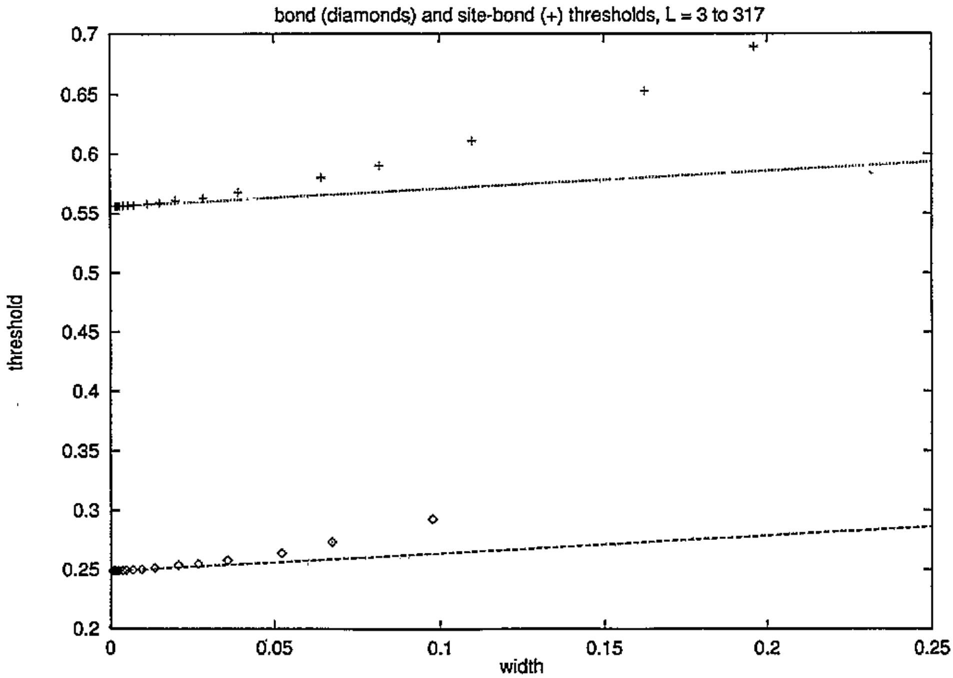

Figure 1. Threshold versus width for simple cubic bond and site-bond percolation, $L = 3$ to 1001. Averages from 10 to 10^4 samples.

Our specific procedure is to check for a given sequence of random numbers at which occupation probability p a spanning cluster first appears, call p_{av} the average over this p for different sequences of random numbers and Δ its RMS deviation (width). To reduce the chances for programming errors and to check universality between several cases, we studied site-bond percolation with a fraction x of sites occupied; we looked at the pure bond percolation limit $x = 1$ and at $x = \frac{1}{2}$ mostly. Using standard percolation algorithms [5] in

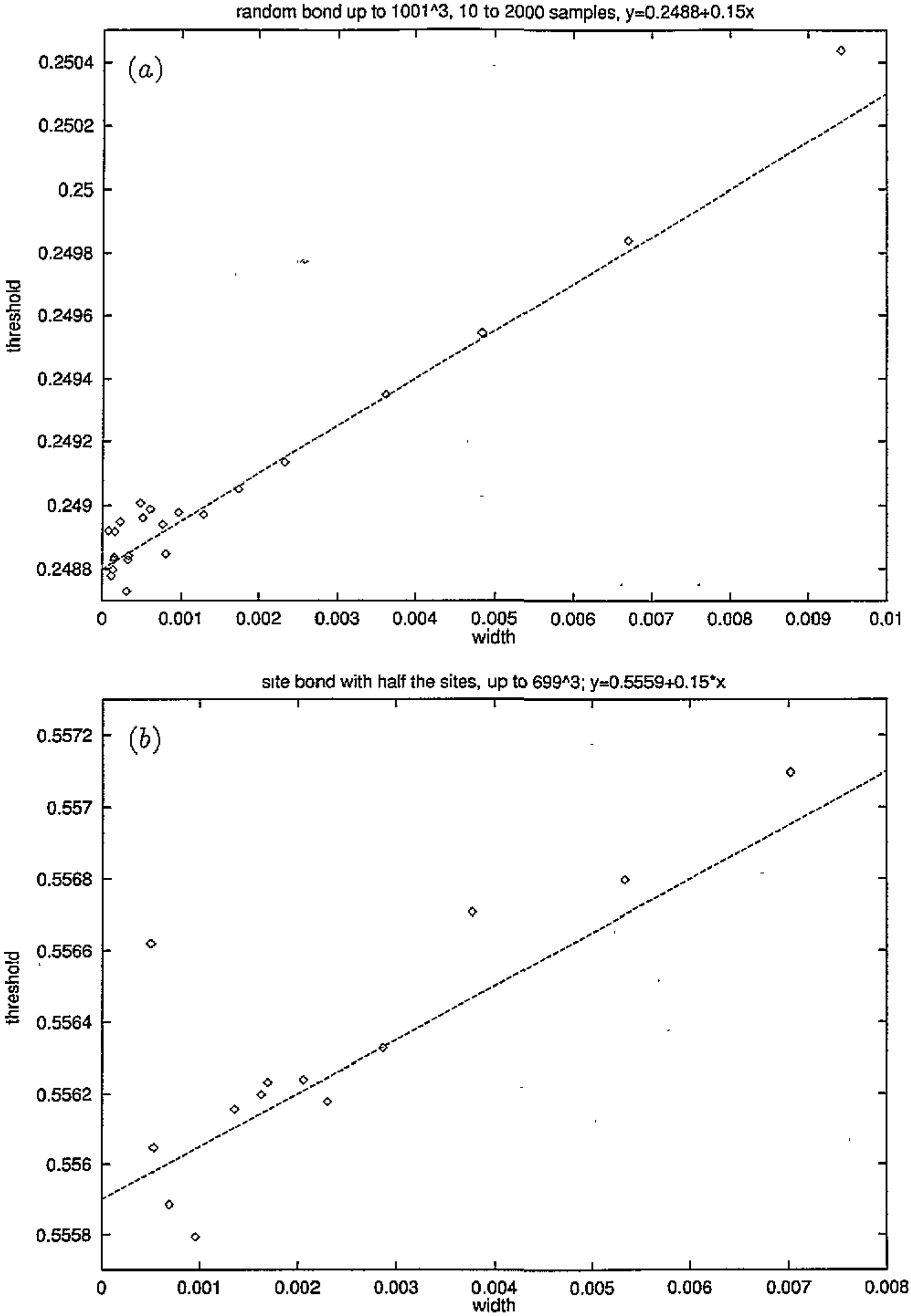

Figure 2. Enlarged view of large-lattice data from figure 1. (a) refers to bond percolation, (b) to site-bond percolation. The straight lines have the same slope 0.15 and are thus compatible with universality. The ten and four leftmost points in (a) and (b), respectively, refer to ten samples only and $L > 300$ and thus have large error bars of order 0.0001 and 0.0002; for smaller lattices the statistics are much better (more than 2000 runs for $L < 200$) and the error bars smaller, as seen in the figure.

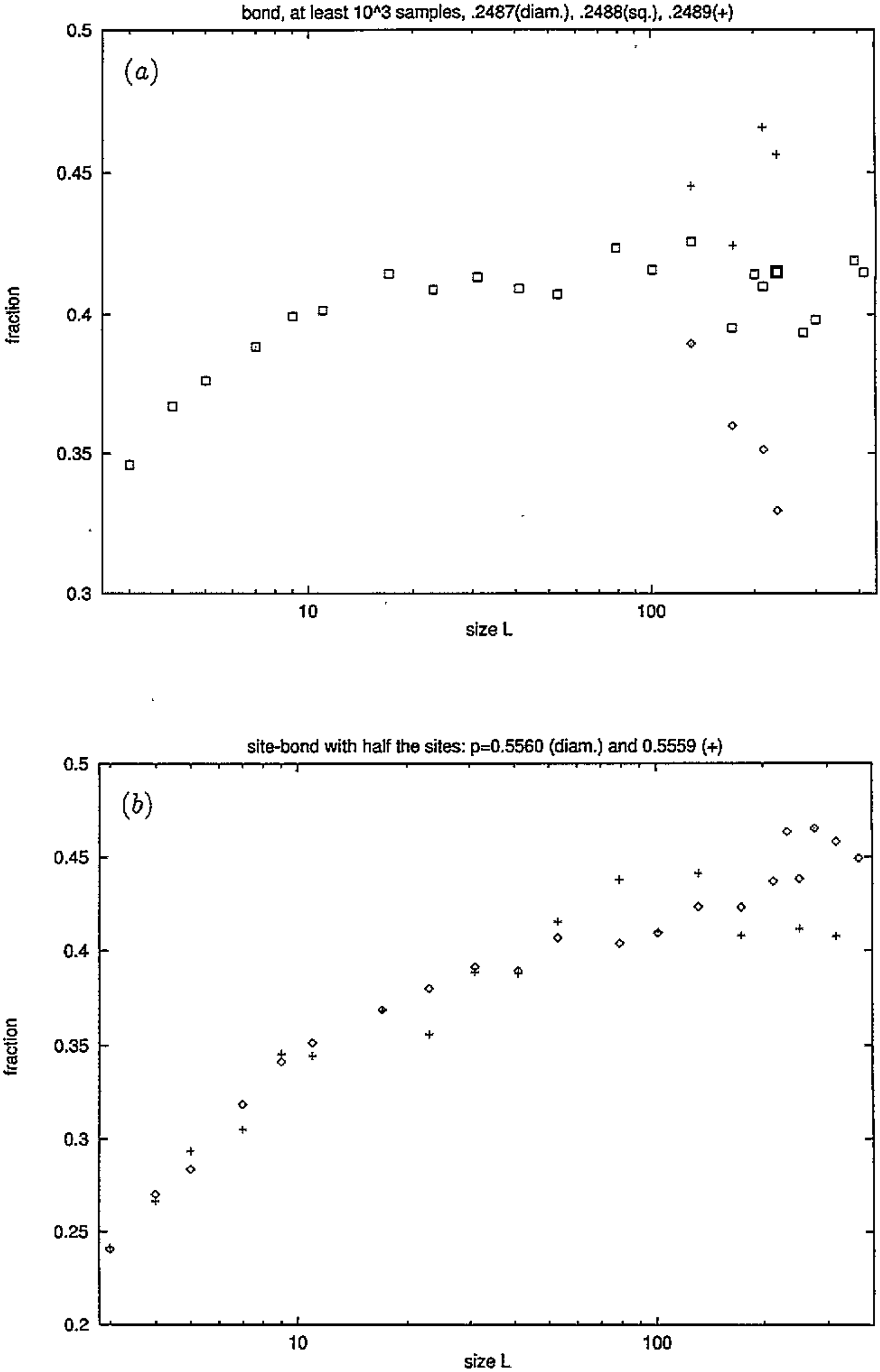

Figure 3. Fraction of spanning samples at the threshold for infinite lattices, for bond (a) and site-bond (b) percolation. The agreement in the plateau value confirms numerically the universality of the critical spanning fraction.

$L \times L \times L$ cubes, we varied p for a fixed sequence of random numbers, until we found the threshold at which a cluster percolates from top to bottom for this sequence. For site-bond percolation, details of the threshold distribution depend on whether we allow for a different site distribution for each different set of bond random numbers, or take the same sites for all different bond configurations; we took the first choice (theory predicts that universal features, like the ratio of $[p_{\mathrm{av}} - p_{\mathrm{c}}]$ to Δ, should not depend on this choice). Thousands of different random number sequences were averaged over to give the mean value $p_{\mathrm{av}}(L)$ and its standard deviation $\Delta(L)$. In figure 1 we plot the threshold width for both simple-cubic bond and site-bond percolation. These functions exhibit a definite curvature which we interpret as resulting from strong corrections to scaling: for intermediate size lattices the shift $[p_{\mathrm{av}} - p_{\mathrm{c}}]$ is not yet proportional to the width Δ. Restricted to $L \geqslant 23$ for bond and $L \geqslant 79$ for site-bond percolation, the same data are plotted in figure 2 on a finer scale. This shows that the straight line $p_{\mathrm{av}} - p_{\mathrm{c}} = 0.15\Delta$ is a reasonable approximation in both cases, with $p_{\mathrm{c}} = 0.2488$ and 0.556, respectively. The latter number corresponds to site occupation $x = \frac{1}{2}$. Thus the deviation $[p_{\mathrm{av}} - p_{\mathrm{c}}]$ is roughly proportional to the width Δ, as assumed for a long time [5] and *not* as in the special two-dimensional case of Ziff [2]. (Roughly the data fit $(p_{\mathrm{av}} - p_{\mathrm{c}})/\Delta = 0.15 + 3\Delta$ for $\Delta < 0.1$, but a correction term with a somewhat smaller power of Δ is not excluded.)

With a simpler program, we also checked how often the cube percolates for a fixed p equal to the infinite-lattice $p_{\mathrm{c}} = 0.2488$ and 0.556; this fraction $R_L(p_{\mathrm{c}})$ is shown in figure 3 to approach about 0.42 for *both* cases, clearly different from the thresholds $p_{\mathrm{c}} = 0.249$ and 0.556. This confirms the universality of $F(0, 0)$, and shows that the violation of the belief $R_L(p_{\mathrm{c}}) = p_{\mathrm{c}}$ is *not* restricted to Ziff's special cases. The data in figure 3 were plotted versus $\log L$, to emphasize the plateau at large L. For small L, plots of $R_L(p_{\mathrm{c}})$ versus $1/L$ are roughly straight, consistent with a leading correction of order $1/L$ as predicted by Ziff [2].

We now consider applications of these calculations to the question of percolation thresholds. In figure 3(b), the fractions for $p = 0.5560$ but not those for 0.5559 seem to increase for the largest lattices, indicating that the true threshold is slightly lower than 0.556 for the site-bond case, as also suggested by figure 2(b). Similar spanning fractions were obtained at $x = 0.8$ and $p = 0.321$. For pure bond percolation, the different trial values 0.2487, 0.2488 and 0.2489 shown in figure 3(a) suggest $p_{\mathrm{c}} = 0.2488 \pm 0.0001$. Figure 3($a$) shows that, already for the moderate lattice sizes used here, the bond percolation threshold is below the value 0.2493 claimed by Wilke, Stauffer and Zabolitzky [6], and compatible with 0.2488 of Grassberger, Adler *et al* and Ziff and Stell [7]. The reason for the discrepancy is unclear, but the old simulations used a sophisticated efficient program whereas the present version was written to be more primitive and reliable and already in 1988 confirmed the lower value [8]. After completing these calculations we received a communication from R M Ziff proposing the value 0.555 88 for site-bond percolation, more precise but in good agreement with our value.

Thus our three-dimensional data confirm the general predictions from the scaling theory, and do not exhibit the special features which were observed in two dimensions. In particular, the critical spanning fraction $R_L(p_{\mathrm{c}})$ is a universal number near 0.42 and thus cannot agree with the non-universal p_{c}. Simulations in higher dimensions are in preparation.

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