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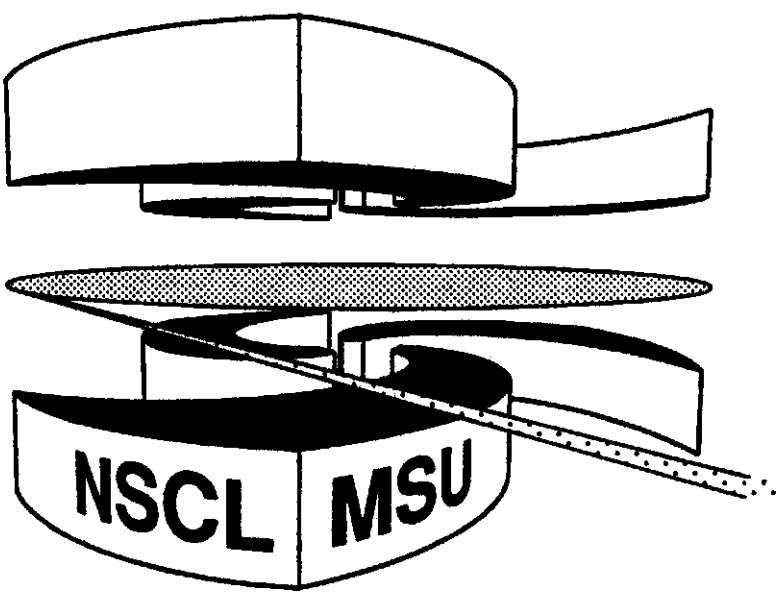


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# Phase Transitions in a Two-Component Site-Bond Percolation Model

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## Abstract

A method to treat a N-component percolation model as effective one component model is presented by introducing a scaled control variable $p_+$. In Monte Carlo simulations on $16^3$, $32^3$, $64^3$ and $128^3$ simple cubic lattices the percolation threshold in terms of $p_+$ is determined for N = 2. Phase transitions are reported in two limits for the bond existence probabilities $p_=$ and $p_{\neq}$. In the same limits, empirical formulas for the percolation threshold $p_+^c$ as function of one component-concentration, $f_b$, are proposed. In the limit $p_= = 0$ a new site percolation threshold, $f_b^c \simeq 0.145$, is reported.

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The percolation model goes back to Flory [1] who introduced it in the context of polymer gelation. Since then it has been used in a wide range of approaches and techniques [2–9]. In standard percolation models either bond or site percolation is dealt with [10,11]. Site-bond percolation [12,13] combines the two formulations, dealing with randomly occupied sites (vertices) and randomly existing bonds (open edges) connecting these sites. However in this version of the model only one active component exists, the other sites are considered unoccupied. A further generalization is to consider several components, which was done for site percolation as well as bond percolation by Zallen [14] and called polychromatic percolation. Zallen focused on the coexistence of percolating species in highly connected lattices, giving a criterion for the occurrence of a panchromatic regime where all species percolate. Site-bond percolation using two components was investigated previously by one of us [15] and applied to the question of the nuclear liquid gas phase transition. Site-bond percolation with several species was considered in [16] and an approximate percolation criterion was given.

In this Letter, we investigate a two component site-bond percolation model on a simple cubic lattice, focusing on two specific limits which exhibit novel behavior. Let us begin by describing the approach we have taken, in the general case of $N$ different component flavors. No assumption concerning topological dimensions or lattice structure is made. We have $N$ component concentrations $f_i$ with $\sum_{i=1}^{N} f_i = 1$ and different bond probabilities to connect all possible combinations of sites, resulting in $A_{par} = (N-1) + \binom{N+2-1}{2}$ free parameters $a_i$. The bonds have been assumed to be directionless, meaning that their probabilities only depend on the species of the sites they are connecting. We now want to know in which region of this $A_{par}$-dimensional parameter space an infinite network $C_\infty$ of connected bonds occurs, that is, where the probability for a given site to belong to the infinite network, $p_\infty(\{a_i\})$, is non-zero. The particular type of a bond shall be irrelevant in order for it to belong to the infinite network. For a system with $N \geq 3$ components, however, this approach is quite impractical. It would be preferable to be able to reduce the dependence of the order parameter, $p_\infty$, to one variable at fixed particle concentrations. We propose one such variable in following the

definitions of [15], generalizing them to $N$ components. In analogy to the bond existence probability used in ordinary one component bond percolation models, which gives the bond density in the system under observation, we introduce the scaled control parameter $p_+$:

$$p_+ = \sum_{i \geq j=1}^{N} \alpha_{ij} p_{ij}. \tag{1}$$

Here, the $p_{ij}$'s denote the probability for a bond to exist between two sites occupied by species $i$ and $j$ and $\alpha_{ij} = \alpha_{ji}$ is the probability that any given nearest neighbor edge is one that connects two sites of flavors $i$ and $j$:

$$\alpha_{ij} = 2 f_i f_j, \tag{2}$$

with the constraint that $\sum_{i \geq j}^{N} \alpha_{ij} = 1$.

For our simulation we consider a two component system on $16^3$, $32^3$, $64^3$ and $128^3$ simple cubic lattices. For simplicity we shall call one species blue, the other red. We now have four free parameters to vary: The fraction of one of the components, say of the blue sites, $f_b$ and three bond activation probabilities: $p_{bb}$ for bonds connecting two blue sites, $p_{rr}$ for bonds connecting two red sites and $p_{\neq}$ for $b$-$r$-bonds. However we shall set $p_{=} \equiv p_{bb} = p_{rr}$, introducing a symmetry in the system. This is motivated by considerations of, for example, isospin symmetry, where the $e^+e^+$ and $e^-e^-$ interactions are identical. Eqs. (1) and (2) now read

$$p_+ = \alpha_{\neq}\, p_{\neq} + \alpha_{=}\, p_{=}, \tag{3}$$

with $\alpha_{=} = (1 - \alpha_{\neq})$, and

$$\alpha_{\neq} = 2 f_b (1 - f_b), \tag{4}$$

respectively, where we have replaced the double indices by a more intuitive notation for only two components. Again the question is in which region of the three dimensional $p_{=}$—$p_{\neq}$—$f_b$ space an infinite network of bonds appears in the lattice. We defer the question of the concentration dependence to later and for the moment set $f_b$ to some fixed value, which

shall, for now, be $f_b = 0.5$. In the simulation the lattice is populated at random, without correlations, according to $f_b$ and bonds are formed for varied values of $p_=, p_{\neq} \in [0,1]$ using a Monte Carlo algorithm. The resulting cluster structure is analyzed using a cluster-find-algorithm described in [3] and $p_\infty(p_=, p_{\neq})$ is recorded. As always, a cluster is defined as a set of vertices connected by open edges. In Fig. 1 we show $p_\infty$ as a function of the two control parameters, $p_=$ and $p_{\neq}$, at a concentration of $f_b = 0.5$. We can see that $p_\infty$ changes from 0 (front corner) to 1 (back corner), with a critical line of a second order phase transition in the $(p_=, p_{\neq})$-plane. We now follow our previous consideration and analyze the same data in terms of the scaled control parameter $p_+$, the result of which is displayed in Fig. 2. Two distinct branches are seen, both in the shape of a second order phase transition. Figure 2 first suggests that $p_+$ is a good control parameter, as we only have these two universal scaled curves, but furthermore that another transition seems to take place in the system. Analysis of the data shows that the 'upper' branch constitutes of points with both $p_=$ and $p_{\neq}$ non-zero, whereas all points with $(p_= = 0, p_{\neq} \neq 0)$ and $(p_= \neq 0, p_{\neq} = 0)$ fall on the 'lower' branch. For other values of $f_b$ the same behavior is found, but then the two curves for the zero-limits in $p_=$ or $p_{\neq}$ are not the same. Also shown in Fig. 2 are the expectations from one component bond percolation theory, $p_\infty \propto (p_+ - p_+^c)^\beta$, (smooth lines). For the finite $(p_=, p_{\neq})$ regime the critical value $p_+^c$ has the same numerical value as the bond existence probability in one component bond percolation (aside from a small difference due to finite size effects), $p_+^c = 0.251 \pm 0.002$. As long as both bond-types are active, the system under observation here and the one component model show an identical phase transition behavior, which is consistent with the findings presented in [15]. In the zero-limits of $p_=$ or $p_{\neq}$, however, $p_+^c$ is shifted to $p_+^c = 0.280 \pm 0.002$. The critical exponent $\beta = 0.41$ from one component bond percolation theory is the same in both cases presented here, as shown in the double logarithmic plot in the inset of Fig. 2.

What causes the change of $p_+^c$ in the limits $p_= \to 0$ and $p_{\neq} \to 0$? We restrict ourselves to a discussion of $p_{\neq} \to 0$, as the same line of arguments applies in the other limit. For simplicity we first choose $p_= = 1$. Then setting $p_{\neq} = 0$ corresponds to a lattice in which all available

$bb$- and $rr$-edges are open, but all $br$-edges are closed. There will be an infinite network present, as usual identified with the biggest percolating cluster (with two components each above the site percolation threshold being present we could have two percolating clusters), with $p_\infty$ given by

$$p_\infty(p_\neq = 0) = f_b - \sum_{s=1}^{\infty-1} n_s^b \; s, \tag{5}$$

where $n_s^b$ is the number of $b$-clusters of size $s$ and the upper limit in the sum is meant to indicate that the infinite cluster is excluded. Letting $p_\neq = \epsilon = 1/N_{edges}$ introduces on average one $br$-bond in the lattice. This bond might, with some small probability, which is related to the number of perimeter edges of all finite clusters, connect two finite clusters. With a noticeably higher probability however, it will open an edge that connects the infinite cluster to the biggest $r$-cluster, $C^r_{max}$, with $|C^r_{max}| \approx |C_\infty|$. The infinite cluster can now consist of both $b$- and $r$-sites and $p_\infty$ reads

$$p_\infty(p_\neq = \epsilon) = 1 - \sum_{s=1}^{\infty-1} n_s \; s, \tag{6}$$

which, by rewriting $f_b$ in Eq. 5 as $f_b = 1 - \sum_{s=1}^{max} n_s^r \; s$, leads to a difference in $p_\infty$:

$$\begin{aligned} \delta_\infty(\epsilon) &= p_\infty(p_\neq = \epsilon) - p_\infty(p_\neq = 0) \\ &= \Big(\sum_{s=1}^{\infty-1} n_s^b \; s + \sum_{s=1}^{max} n_s^r \; s\Big) - \sum_{s=1}^{\infty-1} n_s \; s, \end{aligned} \tag{7}$$

with the property that $\lim_{\epsilon\to 0} \delta_\infty(\epsilon) \neq 0$ for all events where $C_\infty$ and $C^r_{max}$ are connected. Averaging over all events will yield some effective $\delta_\infty^{eff}$ with $0 < \delta_\infty^{eff} < \delta_\infty$. This leads to the conclusion that in the limit $p_\neq \to 0$ a first order phase transition takes place in $p_\infty$. The simulation results support this conjecture. Figure 3 shows these results, where the average was taken over events in which the number of $br$-bonds actually formed in the simulation, $n_{br}$, was non-zero. For values of $p_=$ other than 1 one still finds the same behavior, somewhat less pronounced due to smaller $|C_\infty|$ and $|C^r_{max}|$. The same holds for $f_b \neq 0.5$ where it is clear that the effect vanishes continuously in the limit of a one component bond percolation system: $f_b \to 0$ or $f_b \to 1$. Obviously the question arises what the behavior of $p_+^c$ is.

We found that for $p_{\neq} \to 0$ the percolation threshold $p_+^c$ continually changes to a new, concentration dependent value. In Fig. 4(a) we show this transition, which is of second order type. We also show a fit to the curve, which is of the form

$$p_+^c(p_=, p_{\neq} \to 0) = \frac{1}{(u + v\ p_{\neq})} + t, \tag{8}$$

where the fit parameters were found to be $u = 34.6 \pm 0.3$, $v = 1823 \pm 72$ and $t = 0.2462 \pm 0.0003$. It has to be noted that this formula only stands on empirical grounds, fits by exponential functions may also be useful. As stated earlier, the same line of thought is applicable to the $p_= \to 0$ limit and indeed do our simulations present the same results in the system with $f_b = 0.5$. For $f_b \neq 0.5$ this direct symmetry is broken, but qualitatively the results are still the same. Even for $f_b = 0.5$ they differ however with respect to the afore-mentioned dependence of $p_+^c$ on the concentration $f_b$ in the limits $p_= = 0$ and $p_{\neq} = 0$. For $p_+^c(f_b, p_{\neq} = 0)$ we find the functional form depicted in Fig. 4(b). The results shown are fits of $p_+^c$ to the scaling relation,

$$|p_+^c(L) - p_+^c| \propto L^{-1/\nu}, \tag{9}$$

as given in Ref. [10], where we kept $\nu$ fixed at 0.88 and lattice sizes $L = 16$, $L = 32$, $L = 64$ and $L = 128$ were taken into account. The simulation data is fitted with

$$p_+^c(f_b, p_{\neq} = 0) = \frac{2(f_b - \frac{1}{2})^2 + \frac{1}{2}}{h + m f_b}. \tag{10}$$

This is Eq. (3) with the purely empirical assumption of a hyperbola for $p_=^c(f_b)$, which is in agreement with the results of Heermann and Stauffer for a one component site-bond model [13]. Fitting the parameters to our simulation data results in $h = 4.007 \pm 0.002$ and $m = -4.428 \pm 0.005$. A comparison with the formula given by Heermann and Stauffer yields $h = 1/p_{bond}^c(0) = 4.019$ and $m = (1 - p_{bond}^c)/(p_+^c(f_{site}^c - 1)) = -4.386$, where $p_{bond}^c = 0.2488$ and $f_{site}^c = 0.3116$ are the percolation thresholds for one component bond- and site-percolation on a three dimensional simple cubic lattice, respectively. However, in contrast to the one component model, due to the symmetry introduced in the system, notably that

$p_= \equiv p_{bb} = p_{rr}$, we only have $f_b \in [0.0, 0.5]$ as independent regime here, with the interval $f_b \in [0.5, 1.0]$ being symmetric to the one shown here, with only the roles of blue and red sites being switched. This is a manifestation of the two components behaving like two superposed, non-interfering one component site-bond percolation systems and lets us conclude that the phase transition in $p_+^c$ for $p_{\neq} \to 0$ discussed above may be interpreted as an effective transition from a one component bond percolation model to a one component site-bond percolation model. For the case of the second limit discussed, $p_= \to 0$, the results are shown in Fig. 5. In Fig. 5(a) we go back to the bond existence probability $p_{\neq}$. Its critical value, as a function of the concentration, $p_{\neq}^c(f_b)$, is well reproduced with an exponential fit:

$$\varphi = p_{\neq}^c(f_b) = a \ \exp(-d \ f_b) \ + c \tag{11}$$

Fitting this empirical formula to the simulation data gives $a = 2.1 \pm 0.07$, $d = 10.9 \pm 0.2$ and $c = 0.547 \pm 0.002$. We define $f_b^c \equiv \varphi^{-1}(p_{\neq}{=}1)$ and numerically get $f_b^c \simeq 0.14$ from Eq. (11), whereas in an independent simulation we find $f_b^c = 0.1449 \pm 0.0003$, which again is a result from a fit to the scaling relation Eq. (9). The parameter $f_b^c$ can be regarded as a new threshold, which would correspond to the percolation threshold in a simple site percolation model in which nearest neighbors only belong to the same cluster if they are of opposite flavor, unlike the normal site percolation model which yields $f_{site}^c = 0.3116$. In Fig. 5(b) $f_b^c$ determines the critical point of the phase transition line $p_+^c(f_b, p_= = 0)$. Another argument in favor of a qualitatively new behavior arises by considering the density of accessible edges at the critical concentrations in the two models. For the one considered here it is given by $\alpha_{\neq}(f_b^c)$, see Eq. (4), for the usual site percolation model we might define one in an analogous manner: $\alpha_{site} = (f_{site}^c)^2$. By setting $\alpha_{\neq}(f_b^c) = \alpha_{site}$ one would expect $f_b^c$ to be 0.051 which stands in contradiction to our findings.

In concluding, we introduced a new way to treat N-component percolation. This approach was applied to a two component site-bond percolation model and new first order phase transitions of $p_\infty$ were reported in the limits $p_{\neq} \to 0$ and $p_= \to 0$. In the latter case we could furthermore establish a novel empirical formula for the percolation threshold as a

function of component concentration, whereas in the first earlier findings of a one component site-bond percolation model were found to apply in the two component model too. The field for future work in this area seems vast, one might, for example, try to apply the same method to multi-component systems on lattices of higher dimensions and/or higher connectivity. This approach should also find a broad range of possible applications. One might think of special networks or gelation phenomena with several components involved, which only interact with each other, as well as wetting phenomena. Furthermore an application to stock-market simulations seems possible and is being undertaken by the authors.

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# REFERENCES


[1] P. J. Flory, J. Am. Chem. Soc. **63**, 3083 (1941).

[2] M. F. Sykes and J. W. Essam, J. Math. Phys. **5**, 1117 (1964).

[3] W. Bauer, D. R. Dean, U. Mosel, and U. Post, Phys. Lett. **150 B**, 53 (1985); W. Bauer, U. Post, D. R. Dean, and U. Mosel, Nucl. Phys. **A 452**, 699 (1986); W. Bauer, Phys. Rev. C **38**, 1297 (1988).

[4] S. Galam and A. Mauger, Phys. Rev. E **53**, 2177 (1996).

[5] S. C. van der Marck, Intl. J. Mod. Phys. C **9**, 529 (1998).

[6] S. Galam and A. Mauger, Phys. Rev. E **56**, 322 (1997).

[7] T. Gharib, W. Bauer and S. Pratt, Phys. Lett. B **444**, 231 (1998); W. Bauer and A. Botvina, Phys. Rev. C **52**, R1760 (1995).

[8] M. Sahimi, *Applications of Percolation Theory* (Taylor and Francis, London, 1994).

[9] R. Cont and J. P. Bouchaud, preprint cond-mat/9712318.

[10] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, Revised 2nd ed. (Taylor and Francis, London, 1994).

[11] G. Grimmett, *Percolation*, (Springer Verlag, New York, 1989).

[12] A. Coniglio, H. E. Stanley, and W. Klein, Phys. Rev. Lett. **42**, 518 (1979).

[13] D. W. Heermann and D. Stauffer, Z. Phys. **44**, 339 (1981).

[14] R. Zallen, Phys. Rev. B **16**, 1426 (1977)

[15] G. Kortemeyer, W. Bauer, and G. J. Kunde, Phys. Rev. C **55**, 2730 (1997); W. Bauer, in *Proceedings of the Workshop on Nuclear Matter in Different Phases and Transitions, Les Houches, France* (1999, to be published).

[16] A. S. Ioselevich, Phys. Rev. Lett. **74**, 1411 (1995).

[17] C. D. Lorenz, R. M. Ziff, Phys. Rev. E. **57**, 230 (1998).

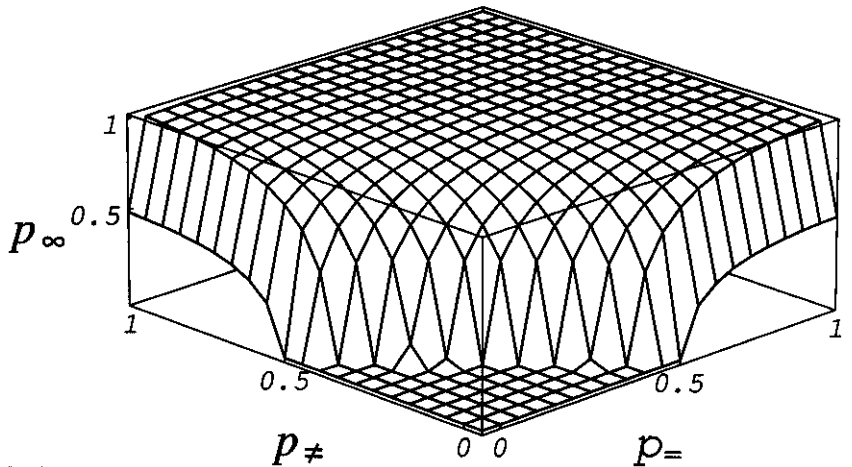


FIG. 1. Probability to belong to the infinite cluster, $p_\infty$, in a simple cubic two component site-bond percolation lattice of size $128^3$ as a function of the two parameters, $p_=$ and $p_{\neq}$, calculated for a fraction of the blue species of $f_b = 0.5$.

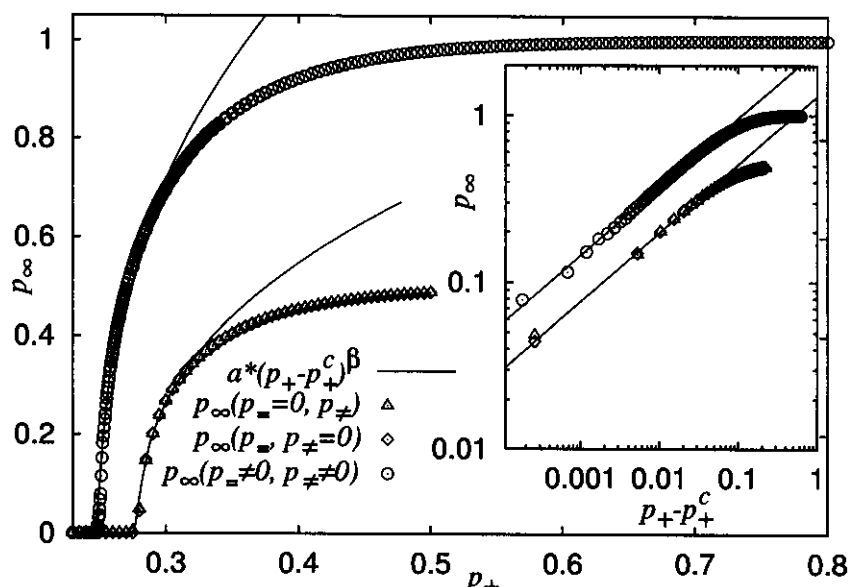


FIG. 2. Probability to belong to the infinite cluster, $p_\infty$, as a function of the scaled control parameter, $p_+$, in a $128^3$ simple cubic lattice with $f_b = 0.5$, for values of $p_=, p_{\neq} \in [0,1]$, fitted with $p_\infty \propto (p_+ - p_+^c)^\beta$ (solid line). Here $p_+^c \simeq 0.251$ for the 'upper' branch, $p_+^c \simeq 0.280$ for the 'lower' branch and $\beta = 0.41$ in both cases. The inset shows the same data in a double logarithmic representation.

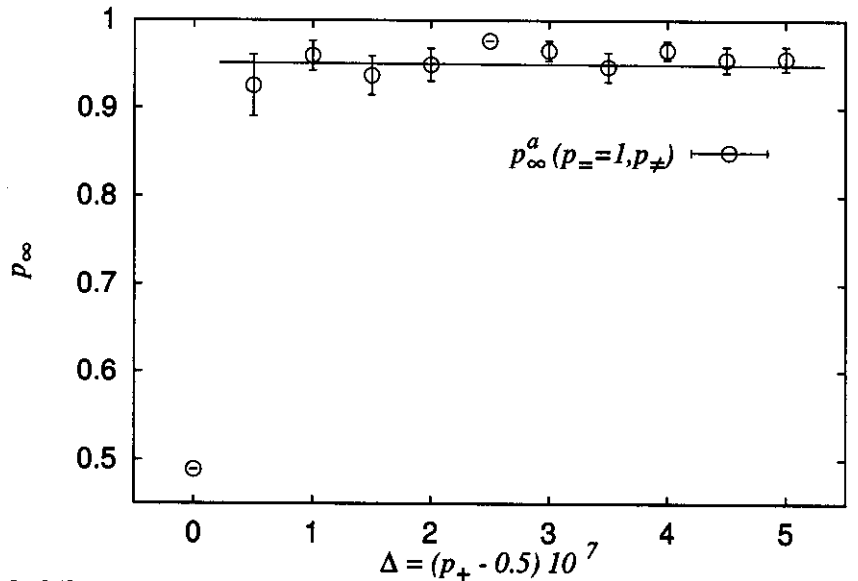


FIG. 3. Probability to belong to the infinite cluster, $p_\infty$, as a function of the scaled control parameter $p_+$, in a $128^3$ simple cubic lattice with $f_b = 0.5$, at fixed $p_= = 1$ for varied $p_\neq$. 50 independent simulation events where taken into account and the average was taken over events in which the number of *br*-bonds actually formed in the simulation, $n_{br}$, was non-zero.

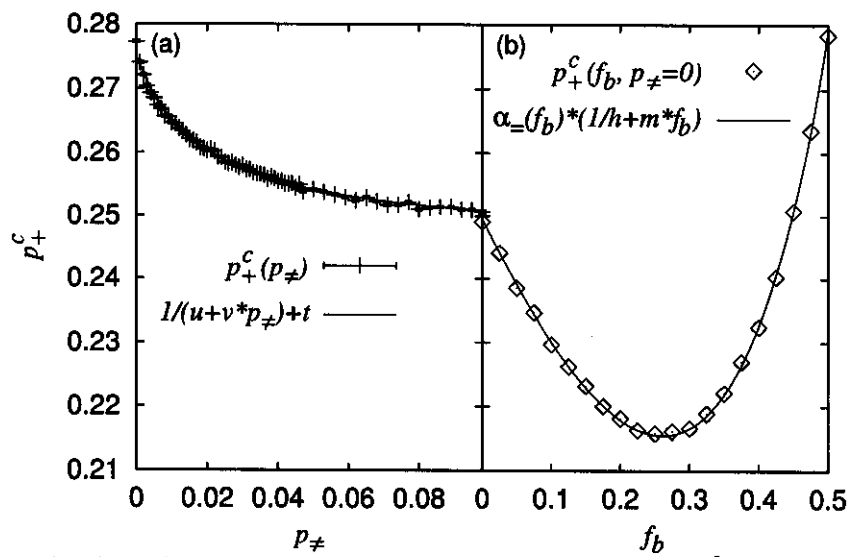


FIG. 4. Critical value of the scaled control parameter, $p^c_+$, in a $128^3$ simple cubic lattice with $f_b = 0.5$, (a) plotted as a function of $p_\neq$, and (b) plotted as a function of the fraction of blue sites, $f_b$, in the limit $p_\neq = 0$ and obtained by a fit to the scaling law $|p^c_+(L) - p^c_+| \propto L^{-1/\nu}$. The errors, estimated as described in [5], are smaller than the symbol sizes in (b).

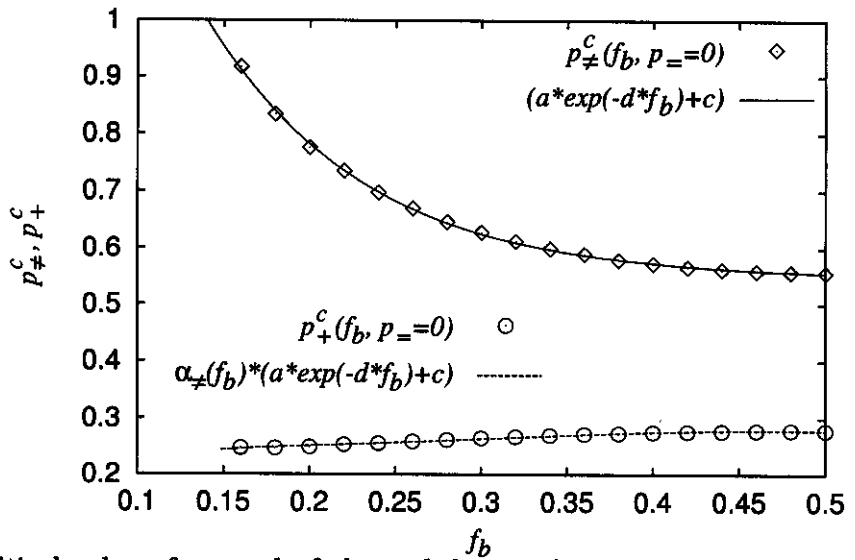


FIG. 5. Critical value of $p_{\neq}$ and of the scaled control parameter, $p^c_{\neq}$ and $p^c_+$, plotted as a function of the fraction of blue sites $f_b$ in the limit $p_{\neq} = 0$. The data has been obtained by a fit to $|p^c_+(L) - p^c_+| \propto L^{-1/\nu}$. Again the errors, estimated as described in [5], are smaller than the symbol sizes.