Percolation on two- and three-dimensional lattices

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(Received 6 December 2002; revised manuscript received 5 February 2003; published 25 April 2003)

In this work we apply a highly efficient Monte Carlo algorithm recently proposed by Newman and Ziff to treat percolation problems. The site and bond percolations are studied on a number of lattices in two and three dimensions. Quite good results for the wrapping probabilities, correlation length critical exponent, and critical concentration are obtained for the square, simple cubic, hexagonal close packed, and hexagonal lattices by using relatively small systems. We also confirm the universal aspect of the wrapping probabilities regarding site and bond dilution.

DOI: 10.1103/PhysRevE.67.046119 PACS number(s): 05.10.Ln, 02.70.−c, 05.70.Jk, 64.60.Ak

I. INTRODUCTION

Among the several methods for treating disordered systems and geometrical problems, percolation theory is certainly one of the most important. Due to its similarities with transitions that occur in many other systems (not only physical, but biological, social, etc.), percolation has been used in studies within a large variety of fields. Forest fires [1], biological evolution [2,3], epidemics [4], social influence [5], and dilute magnetism [6] are only a few examples of the wide applicability of this theory, as well as percolation (e.g., in porous media) itself [7].

Although easily defined, percolation presents theoretical and computational difficulties. For instance, the percolation threshold for the site problem on a simple square lattice is not known exactly. Therefore, approximate solutions are necessary, and much effort has been dedicated in this direction. From the theoretical point of view, one can utilize mean-field [8,9] and renormalization group [10–13] techniques, among others. In particular, computer simulations constitute a powerful tool in this area, since their application to percolation is simpler than for many other problems in statistical physics [14]. Typically, one can obtain a valid configuration by simply populating sites (or bonds) in a given lattice. To measure quantities of interest, such as the percolation threshold or the mean cluster size, it is necessary to identify all clusters in the configuration. For this purpose, many algorithms have been developed, the best known perhaps being that devised by Hoshen and Kopelman [15]. Other algorithms, like hull generation [16,17], can also be used, but only to answer some specific questions. More recently, Newman and Ziff proposed a new algorithm [18], which is general and quite efficient, both in its computational requirements and in its accuracy. Although the algorithm can be used to obtain any observable of the problem, in their papers they have used it to calculate the so-called wrapping probabilities to investigate a number of aspects of the problem. For example, using exact values of the wrapping probabilities, a high-precision result for the site percolation threshold on the square lattice was obtained [18].

Unfortunately, for most lattices, one does not know the exact wrapping probabilities and, in using them, the problem must be tackled in a different way. One of the wrapping probabilities—$R_L^{(1)}$, which is the probability that a cluster wraps around one specified axis, but not around the other ones—is particularly useful. In this case it is not necessary to know its exact value at the critical concentration for the infinite system, since it has a maximum from which the critical point can be obtained. The method, however, is indeed capable to properly estimate the other wrapping probabilities which do not exhibit a maximum (in such cases there is just a crossing region close to the critical threshold). On the other hand, as we will see below, there are still some probabilities in dimensions higher than two that present, besides the maximum, a crossing region from where critical behavior is also achieved.

In this work we compute the percolation threshold and the correlation length exponent, as well as the set of the unknown wrapping probabilities using the Newman-Ziff algorithm. These quantities are evaluated by employing the usual finite-size scaling as well as a cell-to-cell scheme [19]. After summarizing the Newman-Ziff approach in the following section we describe, in Sec. III, the method that enables us to evaluate such geometrical quantities and we apply it to site and bond percolations on the square, simple cubic, HCP (hexagonal close-packed), and simple hexagonal lattices. Concluding remarks are given in the final section.

II. THE NEWMAN-ZIFF ALGORITHM

To determine the percolation transition, this algorithm uses the wrapping probability $R_L(p)$, which, for a given site (or bond) occupation p, is basically the probability that a cluster wraps around a system with periodic boundary conditions on a lattice of linear dimension L. This wrapping can, however, be defined in various manners, each with its own probability. For instance, on two-dimensional lattices one has: (i) $R_L^{(h)}$ and $R_L^{(v)}$, the probabilities that a cluster wraps around the system in the horizontal or vertical direction, respectively (on a square lattice these quantities are equal); (ii) $R_L^{(e)}$, the probability that the cluster wraps around the lattice *either* horizontally *or* vertically (or both); (iii) $R_L^{(b)}$ for wrapping in *both* horizontal *and* vertical directions; (iv) $R_L^{(1)}$ for wrapping around *one* specified direction but *not* the other one. Different lattices can allow for further geometrical

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choices for $R_L(p)$. For example, on a simple cubic lattice, besides $R_L^{(1)}$, we can define $R_L^{(2)}$ as the probability that there exists a cluster that wraps the system in two directions, but not around the third one. Analogously to $R_L^{(b)}$, we have $R_L^{(3)}$ for wrapping around the three directions.

In order to evaluate these quantities it is necessary to generate many independent realizations of the algorithm, each of them consisting of the following steps.

(1) Initially, all sites are empty.

(2) Sites are chosen to be occupied at random.

(3) When a new site is added, one must check all its neighbors to verify if the new site forms an isolated cluster (all neighbors empty) or if it joins together two or more clusters. In the first case, we need to do nothing. In the latter, we have to update the cluster listing. Clusters are stored in a tree structure, with one site of each cluster considered the *root* site. All sites in a given cluster, other than the root, have a pointer to some other site in the same cluster, such that by following a succession of such pointers one can ultimately reach the root. In order to join two clusters we simply add a pointer from the root of the smaller cluster to the root of the larger one.

(4) Each time step (3) is repeated, we evaluate the quantities of interest Q_L^n as a function of the number n of occupied sites. Q_L^n may be any of the wrapping probabilities R_L. Let n' be the number of occupied sites for which percolation first occurs in a given realization. Q_L^n represents the fraction of realizations in which n' is less than or equal to n. Using all Q_L^n's so evaluated, it is possible to calculate the function $Q_L(p)$ for all possible values of p in the range between 0 and 1 by a convolution with the binomial distribution [18]:

$$Q_L(p)=\sum_n \binom{N}{n} p^n(1-p)^{N-n}Q_L^n. \tag{1}$$

For the bond percolation problem, we just replace sites by bonds in the above steps.

The evaluation of the statistical errors can be done in a conventional fashion. As discussed in Ref. [18] the standard deviation of the binomial distribution (1) is given by

$$\sigma_{Q_L(p)}=\sqrt{\frac{Q_L(p)[1-Q_L(p)]}{\mathcal{N}_{\mathrm{MCS}}}}, \tag{2}$$

where $Q_L(p)$ in the above equation has been taken as the mean value of the corresponding wrapping probability and $\mathcal{N}_{\mathrm{MCS}}$ is the number of Monte Carlo steps per site.

As an illustration, we show in Figs. 1(a) and 1(b) the wrapping probabilities $R_L^{(h)}$ and $R_L^{(1)}$ as a function of the concentration p of occupied sites for square lattices of different sizes. The exact values $R_\infty(p_c)$ of these quantities for an infinite square system were derived by Pinson [20] and Ziff [21]. In Ref. [18] it has been used these exact values to obtain an estimate for the percolation threshold p_c. For each system size L, one determines the p value yielding a wrapping probability equal to exact critical value. This p value

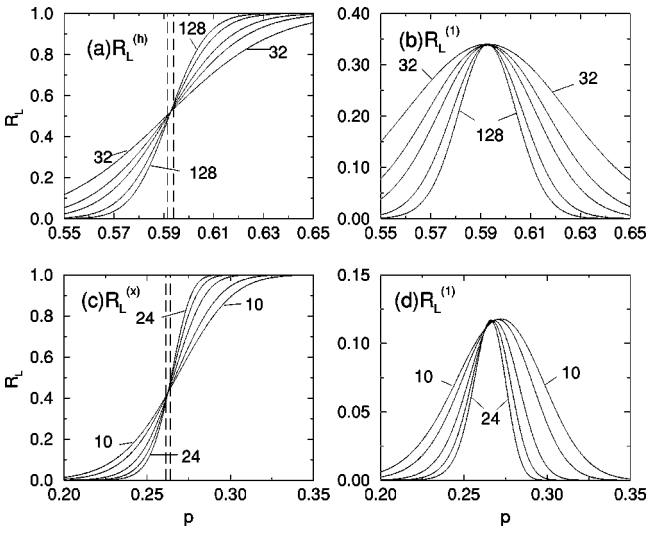

FIG. 1. Wrapping probabilities R_L as a function of occupation probability for site percolation on: square lattices (a) $R_L^{(h)}$ and (b) $R_L^{(1)}$; and hexagonal lattices (c) $R_L^{(x)}$ and (d) $R_L^{(1)}$. For the square lattice the data have been obtained by taking 4.0×10^5 MCS and lattice sizes $L=32$, 48, 64, 96, 128. For the hexagonal lattice the data have been obtained by taking 5.0×10^5 MCS and lattice sizes $L=10$, 12, 16, 20, 24. In all figures the error bars were omitted for a better visualization. Vertical dashed lines represent the lowest and the greatest values of p we have utilized for evaluating wrapping probabilities.

provides the estimate of p_c^L for that L. In the critical region, one knows that the estimates p_c^L converge to the threshold p_c according to

$$p_c^L-p_c\sim L^{-\theta-1/\nu}. \tag{3}$$

For square systems, using the known value 4/3 of the exponent ν and $\theta=2$, as obtained in Ref. [18], we have $p_c^L-p_c\sim L^{-11/4}$. By a finite-size scaling, Newman and Ziff obtained $p_c=0.592\,746\,21(13)$ for the infinite system. This procedure is more complicated in higher dimensions. Since neither θ nor ν are known, one has to vary the scaling exponent to obtain a straight line. In Ref. [18], it was found that the estimates of the percolation threshold for a simple cubic lattice scale as L^{-2}. Thus, it seems to be not so easy to determine ν and θ separately by this method.

One has to note [Fig. 1(b)] that $R_L^{(1)}$ is different from the other probabilities, as it exhibits a maximum. In this case, p_c^L can be estimated from the position of this maximum. $R_L^{(1)}$ is then of particular utility in systems, for which the exact values are not known. We will see, moreover, that all the other wrapping probabilities can also be used to estimate the percolation threshold, as well as the correlation length critical exponent, on any lattice. There are, in addition, some quantities like $R_L^{(2)}$ in three dimensions which exhibit both a maximum and a crossing region.

III. APPROACH AND RESULTS

We have applied the Newman-Ziff algorithm to site percolation on the two-dimensional (2D) square, the three-

TABLE I. Lattice sizes and run lengths (MCS) used in this work. The smallest and largest figures correspond to the total number of sites or bonds. In parentheses we have the corresponding lattice size L.

Lattice	Smallest	Largest	MCS (units of 10^5)
		Site percolation	
Square	1 024(32)	16 384(128)	4.0
Hexagonal	4 096(16)	21 952(28)	1.0–10.0
Cubic	4 096(16)	21 952(28)	1.0–2.0
		Bond percolation	
Square	2 048(32)	32 768(128)	2.0–4.0
HCP	768(4)	20 736(12)	5.0
Cubic	12 288(16)	52 728(26)	0.1–0.5

dimensional simple hexagonal and simple cubic (3D) lattices, and to bond percolation on square (2D), simple cubic, and HCP (hexagonal close-packed) lattices. Table I gives the system and sample sizes used in our study.

Before discussing the results, we analyze the standard deviation of some particular quantities. Figure 2 shows the relative error of $R_L^{(v)}$ for the square lattice and $R_L^{(x)}$ for the hexagonal lattice as a function of L, at the critical concentration. Apart from a strong dependence with small L, we clearly see that for larger lattice sizes the relative error is almost independent of L, as predicted by Eq. (2) and previously stressed by Newman and Ziff [18], even for the three-dimensional hexagonal lattice. Similar behavior is found for other wrapping probabilities, other three-dimensional lattices, as well as for the bond problem in different lattice structures.

Let us now discuss the evaluation of the critical exponent, the percolation threshold, and the wrapping probabilities. In order to get an idea of the performance of the present approach, we will first apply it to the problem in two dimensions where the exact (or more accurate) results are available. From Fig. 1(a) one sees that the derivative of $R_L^{(h)}$ at the critical concentration increases as the lattice size increases. In fact, one expects that the maximum derivative of any wrapping probability not exhibiting a maximum scales as [22]

$$\left(\frac{dR_L}{dp}\right)_{max} \sim L^{1/\nu}. \tag{4}$$

Thus, the critical exponent ν can be estimated without any consideration of the critical concentration p_c by taking the scaling behavior of the derivatives of the thermodynamic quantities R_L. They can be straightforwardly computed from relation (1)

$$\frac{dQ_L}{dp} = \sum_n \left[\binom{N}{n} np^{n-1}(1-p)^{N-n} - \binom{N}{n}(N-n)p^n \times (1-p)^{N-n-1} \right] Q_L^n. \tag{5}$$

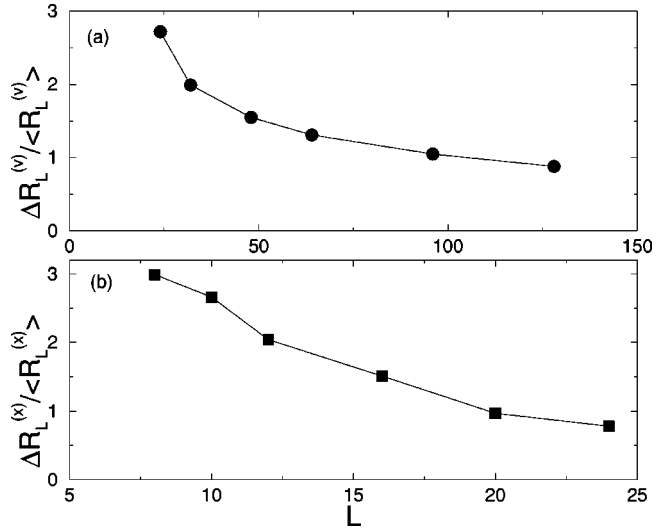

FIG. 2. (a) Relative error of $R_L^{(v)}$, where $\Delta R_L^{(v)} = \sigma_{R_L^v}$ for site percolation on the square lattice. (b) Relative error of $R_L^{(x)}$, where $\Delta R_L^{(x)} = \sigma_{R_L^x}$ for site percolation on the hexagonal lattice.

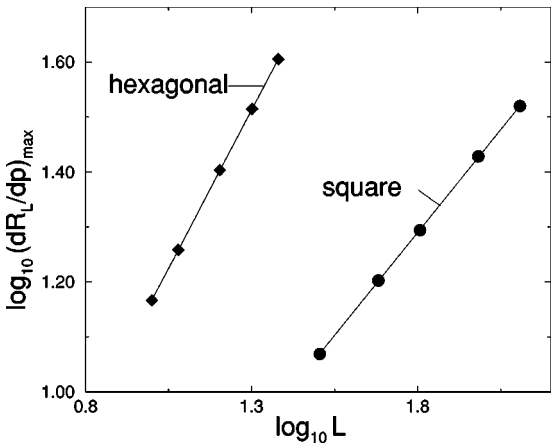

FIG. 3. Maximum derivative of wrapping probabilities ($R_L^{(v)}$ for site percolation on the square lattice and $R_L^{(x)}$ for site percolation on the hexagonal lattice) as a function of system size. Error bars are smaller than the symbol sizes. Linear regression of the data gives $\nu = 1.334(4)$ for the square lattice and $\nu = 0.866(1)$ for the hexagonal lattice.

In Fig. 3 we plot, on $\log_{10}$ scales, the maximum value of the derivative of $R_L^{(v)}$ as a function of system size, for site percolation on the square lattice (the hexagonal lattice will be discussed later); a linear fit yields $\nu^{(v)} = 1.334(4)$. Other quantities give independent estimates of the exponent (the corresponding data are too close to those of $R_L^{(v)}$ to be distinguished on the scale of Fig. 3). We find $\nu^{(h)} = 1.331(2)$; $\nu^{(b)} = 1.339(4)$; and $\nu^{(e)} = 1.327(1)$. Combining these four estimates we obtain $\nu = 1.333(5)$, in very good agreement with the exact result 4/3.

Figure 4 illustrates the approach for evaluating the critical concentration, as well as the wrapping probabilities at p_c, applied again to the site percolation problem on the square lattice, through a cell-to-cell estimate. For a fixed probability occupation p, we compute the specified wrapping probability

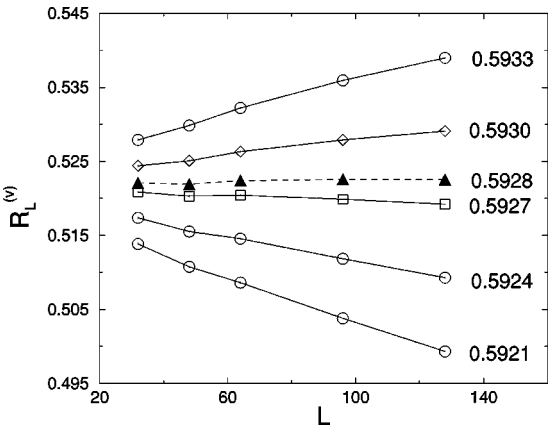

FIG. 4. Wrapping probability $R_L^{(v)}$ as a function of the lattice size L for site percolation on square lattices. Different lines correspond to different concentrations p. The best constant horizontal line is represented by full triangles yielding $p_c=0.5928(2)$ and $R_L^{(v)}=0.523(4)$. Error bars are smaller than the symbol sizes.

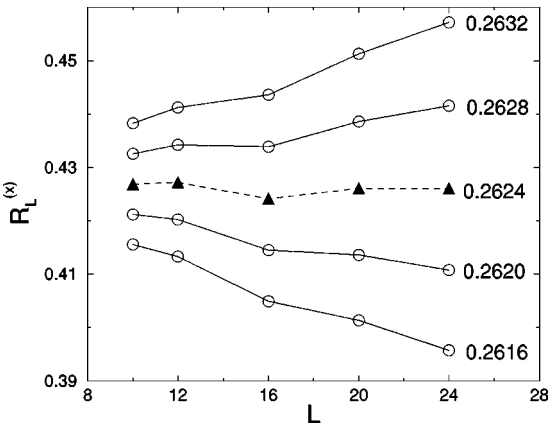

FIG. 5. Wrapping probability $R_L^{(x)}$ as a function of the lattice size L for site percolation on hexagonal lattices. Different lines correspond to different concentrations p. The best horizontal line is represented by full triangles, yielding $p_c=0.2624(4)$ and $R_L^{(x)}=0.429(5)$. Error bars are smaller than the symbol sizes.

as a function of the lattice size. Figure 4 shows $R_L^{(v)}$ as a function of L. For $p<p_c$, $R_L^{(v)}$ decreases with increasing lattice size. For $p>p_c$, it increases. Exactly at p_c one expects the wrapping probability to be independent of system size. Thus, by varying p in the critical region and searching for a constant $R_L^{(v)}$ we obtain an estimate for p_c. The vertical dashed lines in Fig. 1(a) represent the limits on the p values studied. From the data for $R_L^{(v)}$, in Fig. 4, we have then $p_c=0.5928(2)$ and $R_L^{(v)}=0.523(4)$. Combining this estimate with those coming from the other quantities we obtain the values listed in Table II. The results are quite close to the exact or expected ones, despite the small systems (sizes up to 128×128) and short runs (see Table I). Table II also gives the results obtained from the present procedure to the bond percolation problem (which is easily implemented in the algorithm) with an excellent estimate of the known critical concentration. Moreover, the wrapping probabilities, within the error bars, are the same for site and bond problems, confirming the universal character of these quantities.

Having demonstrated the good performance of the method in cases where exact results are available, we studied some three-dimensional lattices where data are not so ubiquitous in the literature. In particular, we treat the simple cubic, simple hexagonal, and the HCP (hexagonal close-packed) lattices. To our knowledge, there are no results available for the wrapping probabilities on such geometries as well as no indication of their universal aspect regarding site and bond dilution.

As an example, we show in Figs. 1(c) and 1(d) the wrapping probabilities $R_L^{(x)}$ and $R_L^{(1)}$ as a function of p for various lattice sizes, for site percolation on the simple hexagonal lattice. The corresponding scaling behavior of the derivative of $R_L^{(x)}$ is depicted in Fig. 3; an estimate for the critical exponent ν may be extracted from these data. In Fig. 5 we show the estimate for p_c as well as the value of the wrapping probability $R_L^{(x)}$. The combined results are listed in Table III together with the values for the simple cubic lattice and those obtained for the bond percolation on the HCP and simple cubic lattices. One can clearly see that the wrapping probabilities are distinct for different geometries, as is the critical concentration. Not only are our p_c estimate comparable to the values obtained previously, but the critical exponents found here are close to the expected result for this universality class, namely, $\nu=0.83(5)$ from series [23], $\nu=0.88(1)$

TABLE II. Results for site and bond percolation on the square lattice. Errors in parentheses affect the last digits. For each case, the first row shows the results described in Sec. III and for the second row those from the modified approach briefly discussed in Sec. IV (in the latter method the exact value for the exponent ν) is used.

	Two dimensions						
Lattice	$R^{(h)}$	$R^{(v)}$	$R^{(e)}$	$R^{(b)}$	ν	p_c (this work)	p_c
Site	0.517(4)	0.523(4)	0.692(3)	0.347(4)	1.333(5)	0.592 7(1)	0.592 7 [a]
	0.521(9)	0.524(6)	0.695(7)	0.353(5)		0.592 9(3)	0.592 7 [a]
Bond	0.521(2)	0.518(3)	0.691(3)	0.351(2)	1.331(3)	0.499 95(15)	1/2 [b]
	0.517(11)	0.519(13)	0.684(16)	0.348(6)		0.499 8(4)	1/2 [b]
Exact [a]	0.5211	0.5211	0.6905	0.3516	4/3		

[a]Reference [18].
[b]Reference [24].

TABLE III. Results for site (s) percolation on hexagonal and simple cubic lattices and for bond (b) percolation on simple cubic and HCP lattices. Errors in parenthesis affect the last digits.

	Three dimensions							
Lattice	$R^{(x)}$	$R^{(y)}$	$R^{(z)}$	$R^{(e)}$	$R^{(3)}$	ν	p_c (this work)	p_c
Hexagonal (s)	0.429(5)	0.332(5)	0.183(4)	0.467(6)	0.120(3)	0.867(14)	0.262 5(2)	0.262 3(2) [a]
Simple cubic (s)	0.254(5)	0.255(5)	0.254(5)	0.456(7)	0.078(3)	0.877(12)	0.311 5(3)	0.311 6063(9) [b]
Simple cubic (b)	0.265(6)	0.266(6)	0.265(6)	0.471(8)	0.084(4)	0.868(11)	0.249 0(2)	0.248 8126(5) [c]
HCP(b)	0.331(6)	0.443(6)	0.093(3)	0.561(7)	0.052(3)	0.848(33)	0.120 3(2)	0.119 9(2) [a]

[a]Reference [25].
[b]Reference [26].
[c]Reference [28].

[7], $\nu=0.8765(16)$ [26] and $\nu=0.893(40)$ [27] from Monte Carlo simulations.

The data of Table III are, up to our knowledge, quite new for these three-dimensional lattices. A byproduct of the present results concerns the universality of $R_L(p_c)$ at the percolation threshold. One can clearly see that for site or bond percolation the wrapping probabilities of the simple cubic lattice are, within the error bars, the same (as well as for the problem in two dimensions depicted in Table II). This is in quite good agreement with the expected universal aspect previously obtained for the spanning probability in general dimensions and with both free and periodic boundary conditions [29].

Another interesting aspect of the three-dimensional lattices is the behavior of the quantity $R_L^{(2)}(p)$ giving the probability of wrapping around two directions and not around the third direction. Figure 6 shows such behavior for the simple cubic site diluted problem. In this case one can obtain an estimate of the critical concentration not only from the position of its maximum but also from the crossings at p_c. It is noted, however, that a more accurate value is achieved from the analysis of the crossings (as done in Fig. 5) than from the location of its maximum. The same behavior occurs for other lattice structures.

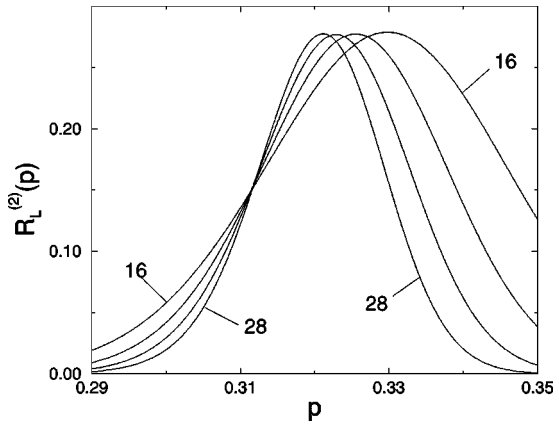

FIG. 6. Wrapping probability $R_L^{(2)}(p)$ as a function of p for the site percolation on the simple cubic lattice. From the position of the peaks one estimates $p_c=0.3171(3)$ and from the procedure of the crossing region one gets $p_c=0.3116(3)$.

IV. CONCLUDING REMARKS

We have seen that the results obtained using the present method are in good agreement with the exact (when available) or expected ones. It is important to note that this procedure has been implemented using relatively small systems and short Monte Carlo runs; better results could be achieved in larger-scale simulations. In addition, from the computed wrapping probabilities at p_c for the square and simple cubic lattices one can also confirm their universal aspect regarding site and bond dilution. The same should hold, of course, for the other lattice geometries.

A slightly modified version of the present procedure, not using the cell-to-cell estimate, can also be applied to problems on two-dimensional lattices. Instead of tuning p, one can tune one of the R_L in the critical region. For a given quantity R_L (say, for example $R_L^{(h)}$) we fix it at a specified value R^* on the vicinity of the critical point, and proceed analogously to Newman and Ziff's original approach. Observe that R^* is in this case a first estimate for $R_\infty(p_c)$. One can then compute, for each L, the intercept between the function $R_L(p)$, previously evaluated, with the fixed R^*. Each of these intercepts gives an estimate for p_c^L, which is expected, for two-dimensional systems, to scale as $L^{-\phi}$ with $\phi=11/4$. Therefore, plotting p_c^L vs $L^{-11/4}$ for different values of R^*, we can estimate the true R_∞ as well as the percolation threshold by looking for the value of R^* that yields the best straight line. Table II reports the critical values so obtained for the two-dimensional lattice. The results are quite good and comparable to those obtained in the preceding section for both the wrapping probabilities and the critical concentration. However, the errors are in general considerably larger. In three dimensions this procedure can be implemented only if we know the exponent ϕ beforehand.

ACKNOWLEDGMENTS

Fruitful discussions with R. Dickman, D. P. Landau, and S.-H. Tsai are gratefully acknowledged. This research was supported in part by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Fundação Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), and Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG) (Brazilian Agencies).

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