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Percolation in two-dimensional lattices. I. A technique for the estimation of thresholds

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We put forward a relatively simple method to estimate reliable percolation thresholds p_c of two-dimensional (2D) lattices both for the bond and site problem. On the basis of this method, we actually evaluate p_c for several 2D lattices by analyzing the results which we obtain from Monte Carlo simulations. Our method enables us to achieve three significant figures for p_c even when the system size N is less than 300×300 and the increment Δp of the concentration p of intact bonds or sites is 0.002. We ascertain that our method works both for the bond and site problem, both for periodic and nonperiodic lattices, and both for lattices with single-valued and mixed-valued coordination.

I. INTRODUCTION

It was only about 30 years ago when Broadbent and Hammersley[1] first introduced the concept of percolation into the realm of science. Since then, this concept has literally *percolated* into a remarkably vast area of science. The number of papers published per year on percolation exceeded three hundred by 1987 and keeps increasing. (For reviews of percolation, see, for instance, Refs. 2 to 7.) Among various reasons why percolation is very popular, the following three are the leading factors.

In the first place, percolation is an interesting mathematical quiz which is comparatively easy to approach and yet reasonably telling, thus being appropriate for brain exercises. The second point is that the ideas of percolation are applied to many problems of completely different types of fields ranging from natural sciences to sociological phenomena. The very first theme of Broadbent and Hammersley[1] was the motion of gas molecules through the maze of pores in carbon granules filling a gas mask. The infection of tree diseases in an orchard,[6] the spread of a forest fire,[8] and the propagation of rumors[7] are popularly mentioned examples. Even when we confine our discussions to physics alone, the list includes topics at a macroscopic level such as electrical conduction in a mixture[9] as well as topics at a microscopic level[10] such as magnetic properties, classical localization, and hopping of electrons. It is also pointed out that some theoretical explanations for the appearance of high-T_c superconductivity are also based upon the concept of percolation. As a matter of fact, examples of problems for which the concept of percolation plays an important role are too numerous to enumerate.

The third reason why percolation is widely studied lies in the fact that percolation serves as a relatively tractable model for the investigation of critical phenomena in general.[11,12] Among other things, it is easy to construct an intuitive picture of critical phenomena near the percolation threshold, and consequently the examination of critical behaviors in the percolation problem provides us with clues to a better understanding of phase transitions observed in more subtle systems.

Despite some intensive efforts to establish the concrete grounds of percolation theory, problems which have been solved by mathematically rigorous arguments[13] are rather limited, and even the scaling hypothesis which characterizes critical phenomena is still hardly beyond a matter of conjecture. In fact, it is the power of computers that has made percolation theory what it is today. The central themes of percolation which need further analyses are (1) determination of the reliable values of percolation thresholds for various structures, that is, for various ways of connectivity of atoms and (2) confirmation of the existence of "*universality*" in the sense that the critical exponents are dimensional invariants, depending only on the dimension d of lattices and therefore being independent of the details of the structure of each lattice.[6,14–17] We concern ourselves with the former theme[18] in the present paper while the latter theme will be treated in the succeeding paper[19] on the basis of Stauffer's cluster number hypothesis.[6]

Except for some lucky lattices which happen to have special topological advantages, percolation thresholds have to be estimated numerically by means of computer simulations. Naturally, the larger the system size to study, the more accurate the values of the threshold obtained therefrom. Accordingly, there seems to be no end to the desire for the increase of the system size in most of the computer simulations of this kind. But in practice, it is far more desirable to have a method by which we could achieve a reasonably accurate value of the threshold from the study of *finite-size* systems without making the system size very large. In addition, it is nicer if we could somehow get an idea about the error bar for the value of the threshold determined thereby.

Under this situation, it is a purpose of this paper to make a proposal concerning the estimation of thresholds

as well as of their error bars for percolation in two-dimensional (2D) lattices. We also carry out Monte Carlo (MC) simulations of percolation, analyze their results using the technique we propose, and derive percolation thresholds of several 2D lattices.

We explain the scheme of our proposal concerning the estimation of thresholds in Sec. II and concerning the estimation of errors bars in Sec. III. The method of MC simulations and results are presented at length in Sec. IV while a summary is found in Sec. V.

II. EFFECTIVE THRESHOLD

What is percolation anyway? Imagine a set of N sites, pick up M sites in a completely random manner out of the N sites, and put an atom on each of the M sites. We call a site with an atom on it an "occupied" site while a site without an atom on it an "empty" site. Then, we connect each pair of nearest-neighbor occupied sites by a bond and ask if we can find a cluster—a group of occupied sites connected by bonds, each between a pair of nearest-neighbor occupied sites—which extends from one side to the opposite side of the system, say from top to bottom or from left to right, for a given value of $p \equiv M/N$. When we find such a cluster, we say that this cluster "percolates" through the lattice. This problem is generally named "site percolation."[2-7]

On the other hand, we can also define "bond percolation" as follows. We connect, by a bond, each pair of nearest-neighbor sites (here, sites to be considered being all the sites in a system), denote the total number of bonds by N, and pick up M bonds in a completely random fashion out of the N bonds. We call each of the M bonds thus picked up an "intact" bond while each of the other $(N-M)$ bonds which are not chosen is named a "broken" bond. Here again, we ask a question whether or not there exists a cluster composed of connected intact bonds which penetrates from one side to the opposite side of the lattice (say from top to bottom or from left to right) for a given value of $p \equiv M/N$. If such a cluster exists, we call it a "percolating cluster."

It is also possible to connect, by a bond, a pair of second- and further-neighbor occupied sites. This is named "site percolation" with further neighbors. A counterpart for bond percolation is also defined by connecting, by a bond, a pair of nearest-second- and further-neighbor sites out of all sites in a lattice and thereafter remove some of the bonds thus constructed. Both the site and bond percolation with further neighbors lead to results quantitatively modified but qualitatively of no difference from those of the initial percolation which is defined by nearest-neighbor bonds alone. Therefore, we confine ourselves to the latter case in this paper.

A. Threshold

The central idea of percolation theory is the following assertion; when both N and M become infinite under the condition that p is kept finite, we find for a given lattice the critical percolation concentration or the percolation threshold, denoted by p_c, such that there always exists one percolating cluster for $p \geq p_c$ while there exists no percolating cluster at all for $p < p_c$. The important point is that, as long as the structure of the background lattice is the same, the value p_c is always the same in spite of the random configuration of a percolating cluster which varies from sample to sample.

It is generally difficult to determine, analytically, the value of the threshold p_c for a given lattice. But for some special and lucky types of lattices, geometrical considerations enable us to derive thresholds exactly. To date, exact thresholds are known for a square, triangular, and honeycomb lattice concerning the bond problem and for a triangular and kagomé lattice concerning the site problem. Some details of these exact calculations will be given in what follows if necessary.

B. Rightward and downward percolating clusters

The idea underlying our method is the analysis of the probability $R = R_N(p)$ that a lattice composed of N elements percolates at concentration p, elements being either sites or bonds. Here we study the following three definitions:

$R_N^R(p)$: the probability that we find a rightward percolating cluster , (2.1a)

$R_N^D(p)$: the probability that we find a downward percolating cluster , (2.1b)

$R_N^A(p)$: the average of $R_N^R(p)$ and $R_N^D(p)$ given by the relation , (2.1c)

$$R_N^A(p) \equiv \tfrac{1}{2}[R_N^R(p) + R_N^D(p)] .$$

In our MC work, $R_N^X(p)$ for $X = R$ or D is determined for each "discrete" value of p in a given type of lattice of a given size N. In order to express $R_N^X(p)$ as a function of "continuous" p values, it is convenient if we could fit $R_N^X(p)$ to some approximate function through the least-mean-square method. The curve fitting is carried out using the error function because $dR_N^X(p)/dp$ is expected to behave like the Gaussian distribution as[6,7]

$$\frac{dR_N^X(p)}{dp} = \frac{1}{\sqrt{2\pi}\Delta_N^X} \exp\left[-\frac{1}{2} \left[\frac{p - p_c^X(N)}{\Delta_N^X} \right]^2 \right] , \tag{2.2}$$

where $p_c^X(N)$ is the concentration at which the slope of $R_N^X(p)$ is the largest and Δ_N^X is the standard deviation from $p_c^X(N)$. The function $R_N^X(p)$ thus defined is the error function which has properties that

$$R_N^X(p)=\tfrac{1}{2} \text{ at } p=p_c^X(N) , \tag{2.3a}$$

that

$$\text{the slope of } R_N^X(p) \text{ is largest at } p=p_c^X(N) , \tag{2.3b}$$

and that

$$[R_N^X(p)-\tfrac{1}{2}] \text{ is an odd function with respect to } [p-p_c^X(N)] , \tag{2.3c}$$

where $X=R$ or D.

Discussions to follow remain unaltered as long as $R_N^X(p)$ fulfills the properties as stated by Eqs. (2.3a)–(2.3c), although the form given by Eq. (2.2) is mathematically most reasonable.

While the definition of a percolation threshold is clear cut when the system size N is infinite, this is not the case when N is finite. Let us define that the effective threshold for each kind of percolation is given by $p_c^X(N)$ in a system of size N. Either when the symmetry of a lattice has some appropriate property or when the system size N is large enough so that the symmetry of a lattice does not matter, we have $p_c^R(N)=p_c^D(N)$ and $\Delta_N^R=\Delta_N^D$. When this is the case, we denote an effective threshold by

$$p_c^A(N)\equiv p_c^R(N)=p_c^D(N) .$$

We assert in the rest of this section that $p_c^A(N)$ thus determined for finite size N serves as a very good approximation for the percolation threshold of an infinite lattice.

C. Dual lattice and matching lattice

For any 2D lattice, it is always possible to define its *dual lattice*.[13] When an initial lattice $\mathcal{L}$ is given, its dual lattice $\mathcal{L}^d$ is constructed by assigning one and only one site of $\mathcal{L}^d$ with each cell (the smallest polygon made of bonds) of $\mathcal{L}$ and connecting a pair of these new sites of $\mathcal{L}^d$ if they belong to neighboring cells of $\mathcal{L}$ which share a bond of $\mathcal{L}$. In this way, it becomes possible to realize the situation that each bond of $\mathcal{L}^d$ intersects one and only one bond of $\mathcal{L}$. It is also easy to see that the whole story is vice versa in the above procedure; that is, one and only one site of $\mathcal{L}$ is assigned with each cell of $\mathcal{L}^d$ and each bond of $\mathcal{L}$ intersects one and only one bond $\mathcal{L}^d$. In other words, when $\mathcal{L}^d$ is a dual lattice of $\mathcal{L}$, then $\mathcal{L}$ is a dual lattice of $\mathcal{L}^d$.

From this definition of a dual lattice, we can easily conclude that, if there exists a rightward percolating cluster of bonds in an initial lattice $\mathcal{L}$, a downward percolating cluster of bonds in its dual lattice $\mathcal{L}^d$ cannot form, and this is again vice versa. This naturally leads to a relationship,[13]

$$p_c(\infty\text{:bond};\mathcal{L})+p_c(\infty\text{:bond};\mathcal{L}^d)=1 . \tag{2.4}$$

A *matching lattice* $\mathcal{L}^m$ is constructed by drawing, in addition to the bonds of the initial lattice $\mathcal{L}$, all possible diagonal lines in each cell (polygon) of $\mathcal{L}$. From a straightforward geometrical observation, it follows that if there exists a rightward percolating cluster of sites in an initial lattice $\mathcal{L}$, a downward percolating cluster of sites in its matching lattice $\mathcal{L}^m$ is prohibited, and vice versa. Then, the relation

$$p_c(\infty\text{:site};\mathcal{L})+p_c(\infty\text{:site};\mathcal{L}^m)=1 \tag{2.5}$$

is satisfied.

Both Eqs. (2.4) and (2.5) are the well-known relations for infinite lattices. In the following, we discuss problems of similar kinds for finite systems. Since what a dual lattice is to bond percolation as what a matching lattice is to site percolation, we mainly discuss the relation between an initial lattice and its dual lattice concerning the bond problem, but it must always be remembered that the same argument holds with the relation between an initial lattice and its matching lattice concerning the site problem.

From now on, we employ the description as follows. When we discuss bond percolation, we denote by p the concentration of intact bonds in an initial lattice $\mathcal{L}$, and by q the concentration of intact bonds in its dual lattice $\mathcal{L}^d$. This, of course, is similar to saying that, when we discuss site percolation, we denote by p the concentration of occupied sites in an initial lattice $\mathcal{L}$ and by q the concentration of occupied sites in its matching lattice $\mathcal{L}^m$.

Suppose we draw both initial lattice $\mathcal{L}$ and its dual lattice $\mathcal{L}^d$ in the same plane. In the first place, for a given value of p, we choose $M=pN$ bonds in a random manner out of total N bonds in $\mathcal{L}$, and decide these M bonds to be intact. Then at each intersection of a bond of $\mathcal{L}$ and a bond of $\mathcal{L}^d$, we assume that a bond of $\mathcal{L}^d$ is intact if a bond of $\mathcal{L}$ is broken, and that a bond of $\mathcal{L}^d$ is broken if a bond of $\mathcal{L}$ is intact. This inevitably leads to

$$p+q=1 . \tag{2.6}$$

From the definitions (2.1), it is ready to show

$$R_N^R(p;\mathcal{L})+R_N^D(q;\mathcal{L}^d)=1 . \tag{2.7}$$

Using Eq. (2.7) and the property of $R_N^X(p)$ as described by Eqs. (2.3), we can prove that

$$p_c^R(N;\mathcal{L})+q_c^D(N;\mathcal{L}^d)=1 , \tag{2.8}$$

and a similar relation with R and D interchanged. Note that the well-known relations (2.4) and (2.5) for infinite systems are realized when the limit of $N\to\infty$ is taken in Eq. (2.8) because, in this limit, the effective thresholds of all kinds (i.e., both for the rightward and downward percolation) become identical. In other words, Eq. (2.8) which we have derived here for finite systems is the counterpart of Eq. (2.4) or (2.5) for infinite systems.

D. Some simple lattices of two dimension

Now, on the basis of Eqs. (2.1)–(2.8), let us study percolation in several simple lattices. In particular, we are going to show that, for each of the following cases discussed in Sec. II D 1–4, $p_c^A(N)$ for finite size N as defined in Sec. II B is identical with the exact threshold $p_c^A(\infty)$ of an infinite system.

1. Bond percolation in a square lattice

A square lattice is called "self-dual" since the dual lattice of a square lattice is again a square lattice. Then, Eq.

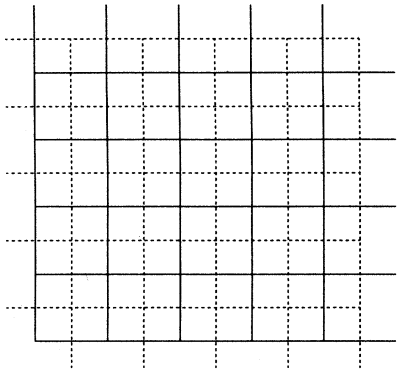

FIG. 1. A square lattice of size 5×5 (solid lines) and its dual lattice (broken lines). When boundaries are chosen this way, Eq. (2.9) holds right even for very small N.

(2.4) immediately gives $p_c(\text{bond;square})=\frac{1}{2}$.[13] It is easy to see that a square lattice of finite size $N\equiv L\times L$ is also self-dual when appropriate care is taken of the boundaries of the lattice (see Fig. 1). Accordingly, we have $q_c^X(N)=p_c^X(N)$, $X=R$ or D. Besides, the symmetry of a square lattice guarantees that

$$p_c^R(N)=p_c^D(N)=p_c^A(N)\ .$$

Then, it follows directly that

$$p_c^A(N\text{:bond;square})=p_c(\infty\text{:bond;square})=\tfrac{1}{2}\ , \quad (2.9)$$

which means that the effective threshold $p_c^A(N)$ as defined in Sec. II B for finite-size N is equal to the threshold $p_c(\infty)$ of an infinite system.

2. *Bond percolation in a triangular and honeycomb lattice*

For a triangular and honeycomb lattice which are mutually dual, the technique of the star-triangle transformation provides us with exact thresholds as[13]

$$p_c(T)\equiv p_c(\infty\text{:bond;triangular})=2\sin\left[\frac{\pi}{18}\right]\simeq0.347\,296\ , \quad (2.10)$$

$$p_c(H)\equiv p_c(\infty\text{:bond;honeycomb})=1-2\sin\left[\frac{\pi}{18}\right]\simeq0.652\,704\ . \quad (2.11)$$

When $p=p_c(T)$ and $q=p_c(H)$, the star-triangle transformation proves that the connectivity of vertices in one of these lattices is identical with that in the other lattice. It follows then that

$$R_N^X(p_c(T);\text{triangular})=R_N^X(p_c(H);\text{honeycomb}),\quad (X=R \text{ or } D)\ . \quad (2.12)$$

Now, let us regard a triangular lattice as initial and a honeycomb lattice as its dual. (Our argument needs no modification even when we take the description the other way around.) When these concentrations $p_c(T)$ and $p_c(H)$ are inserted in Eq. (2.7), we get

$$R_N^R(p_c(T);\text{triangular})+R_N^D(p_c(H);\text{honeycomb})=1\ , \quad (2.13)$$

and a similar equation with R and D interchanged. From Eqs. (2.12) and (2.13), we have for a triangular lattice,

$$R_N^A(p_c(T))\equiv\tfrac{1}{2}[R_N^R(p_c(T))+R_N^D(p_c(T))]=\tfrac{1}{2}\ , \quad (2.14)$$

which leads to

$$p_c^A(N\text{:bond;triangular})=p_c(\infty\text{:bond;triangular})\ , \quad (2.15a)$$

$$p_c^A(N\text{:bond;honeycomb})=p_c(\infty\text{:bond;honeycomb})\ , \quad (2.15b)$$

for finite-size N. Here again, the effective threshold $p_c^A(N)$ of finite-size N as defined in Sec. II B is identical with the exact threshold $p_c(\infty)$ in a triangular and honeycomb lattice.

3. *Site percolation in a triangular lattice*

Since we cannot draw any further diagonal line in a triangle, a triangular lattice is self-matching, which directly yields[13]

$$p_c(\infty\text{:site;triangular})=\tfrac{1}{2}\ . \quad (2.16)$$

Following the argument analogs to that for bond percolation in a square lattice, we can readily show that

$$p_c^A(N\text{:site;triangular})=p_c(\infty\text{:site;triangular})=\tfrac{1}{2}\ . \quad (2.17)$$

4. *Site percolation in a kagomé lattice*

A *covering lattice* $\mathcal{L}^c$, which is obtained by locating a site of $\mathcal{L}^c$ at the center of each bond of an initial lattice $\mathcal{L}$ and connecting, by a bond, two sites of $\mathcal{L}^c$ if and only if the corresponding two bonds of $\mathcal{L}$ meet at a site of $\mathcal{L}$. Note that, when the coordination number of an initial lattice is z, that of its covering lattice is $2(z-1)$. In this

way, the connectivity of an initial lattice is perfectly retained in its covering lattice.

Consequently, we readily obtain the relation

$$p_c(\text{site};\mathcal{L}^c)\equiv p_c(\text{bond};\mathcal{L}) . \tag{2.18}$$

Since a kagomé lattice as illustrated in Fig. 1(a) is the covering lattice of a honeycomb lattice, we have

$$p_c(\infty\text{:site;kagomé})=p_c(\infty\text{:bond;honeycomb}) \tag{2.19}$$

Since the initial-covering topology holds even in lattices of finite sizes when an appropriate care is taken of the boundaries of the lattices, we can derive from Eq. (2.15b),

$$p_c^A(N\text{:site;kagomé})=p_c(\infty\text{:site;kagomé}) . \tag{2.20}$$

5. *Other lattices*

We have shown in the above that, for five cases where some special aspects of lattice topology enable us to evaluate exact thresholds for infinite lattices, the same aspects of topology help us to show that, even when system size N is small, the effective threshold $p_c^A(N)$ of each lattice is, in principle, identical with the threshold of a corresponding infinite lattice. Concerning lattices other than those mentioned above, it is neither to derive an exact threshold nor to prove that the effective threshold $p_c^A(N)$ serves as a good approximation of the exact threshold. Our prediction, however, is that, even though we cannot give a concrete proof for other lattices right now, the effective threshold $p_c^A(N)$ for finite N, as defined in the first part of this section, would be reasonably close to the percolation threshold of an infinite system. Actually, in sections to follow, we show by MC simulations that this is the case both for bond and site percolation in all the lattices we study.

III. EXTRAPOLATION TO INFINITY

The percolation threshold p_c of an infinite lattice, when it is not obtained exactly, is normally estimated through the following two steps: (1) to calculate the effective threshold $p_c(N)$ for finite size N *by some definition,* and (2) to extrapolate $p_c(N)$ into the limit of $N\to\infty$ *based upon some rule.* As for the first step, we have just proposed one definition of the effective threshold $p_c^A(N)$ in the preceding section. As for the second step, we make use of a relation due to scaling hypothesis,[11,12] the relation being for the correlation length ξ as expressed

$$\xi\propto|p-p_c|^{-\nu} , \tag{3.1}$$

where ν is a critical exponent which is analytically shown to be $\frac{4}{3}$. When $p=p_c^X(N)$, the correlation length ξ reaches to the linear dimension $L\equiv\sqrt{N}$ of the lattice. Then we have

$$|p_c^X(N)-p_c|\propto L^{-1/\nu} \tag{3.2a}$$

or

$$p_c^X(N)=p_c+A^X L^{-1/\nu} , \tag{3.2b}$$

where A^X is some constant, positive or negative, and superfix X denotes the type of a percolating cluster.

It is also important to know the accuracy of p_c thus determined. We assert that we measure the degree of accuracy or the error bar in the following way. That is to say, we introduce two probabilities for a lattice of finite-size N:

$R_N^L(p)$: the probability that we find a cluster which percolates both in a rightward direction and in a downward direction , (3.3a)

$R_N^U(p)$: the probability that we find either a rightward percolating cluster or a downward percolating cluster . (3.3b)

Here, I denotes "*intersection*" and U, "*union.*" From this definition we can write

$$I=R\cap D , \tag{3.4a}$$

$$U=R\cup D , \tag{3.4b}$$

$$R_N^A(p)\equiv\tfrac{1}{2}[R_N^R(p)+R_N^D(p)]=\tfrac{1}{2}[R_N^I(p)+R_N^U(p)] . \tag{3.5}$$

The initial-dual relation for bond percolation (or the initial-matching relation for site percolation) also exists;

$$\begin{aligned} &R_N^I(p;\mathcal{L})+R_N^U(q;\mathcal{L}^d \text{ or } \mathcal{L}^m)=1 , \\ &p+q=1 . \end{aligned} \tag{3.6}$$

Again from definition,

$$R_N^L(p)\le R_N^A(p)\le R_N^U(p) , \tag{3.7}$$

where the equal signs hold in the limit of $N\to\infty$. We assume that the effective threshold for $R_N^L(p)$ or $R_N^U(p)$ is also obtained from the error function derived from Eq. (2.2) with $X=I$ or U. Then, it follows that

$$p_c^I(N)\ge p_c^A(N)\ge p_c^U(N) , \tag{3.8}$$

where the equal signs hold for $N\to\infty$.

By making use of Eq. (3.2), we obtain three values of thresholds $p_c^A(\infty)$, $p_c^I(\infty)$, and $p_c^U(\infty)$, which are the extrapolations, respectively, from $p_c^A(N)$, $p_c^I(N)$, and $p_c^U(N)$ to $N\to\infty$. Our assertion in the previous section amounts to saying that $p_c^A(\infty)$ gives a good approximation to the percolation threshold of an infinite system. Our assertion in this section is that the largest of $|p_c^I(\infty)-p_c^A(\infty)|$ and $|p_c^A(\infty)-p_c^U(\infty)|$ serves as a measure for the accuracy of $p_c^A(\infty)$. There may be other ways of estimating the error bar; e.g., the error bar may be calculated from the root-mean-square deviation in the curve fitting by means of

Eq. (3.2b). Compared with this kind of estimation, the advantage of our method as stated above lies in that it is concerned with the values $p_c^X(\infty)$ with $X = A$, I, and U extrapolated into infinity.

IV. MONTE CARLO SIMULATIONS

Now we are ready to carry out MC simulations of percolation. We first construct a desired lattice composed of N elements (either sites or bonds). Then each MC run consists of the following two steps: (1) a random choice of M elements out of the N elements, and (2) the cluster analysis first to determine the number n_s of s clusters, an s cluster being a cluster composed of s connected elements, for all values of s, and then to see if there exists a percolating cluster. This percolating cluster could be R, D, I, or U.

The construction of a desired lattice is easy when the lattice under consideration is regular and periodic, while it is not an easy task to construct a Penrose lattice especially when N is large. One of the present authors (Sakamoto[20]) has invented a quick algorithm to obtain a Penrose lattice of any size by means of the deflation technique. The first step of each MC run—choosing M elements by means of random numbers—is the quintessence of MC simulations. The second step of the cluster analysis for a large system is exceedingly troublesome and time consuming (or equivalently money consuming) unless some smart treatment is employed,[6,21] which we have managed to achieve (the details of the cluster analysis will be found elsewhere).[22]

In the construction of a desired lattice, we prepare a lattice which contains somewhat larger number of sites than a desired number N. Thereafter, we cut out a portion of a square shape containing approximately N sites. We use this portion not only for the study of site percolation but also for the study of bond percolation. Since the

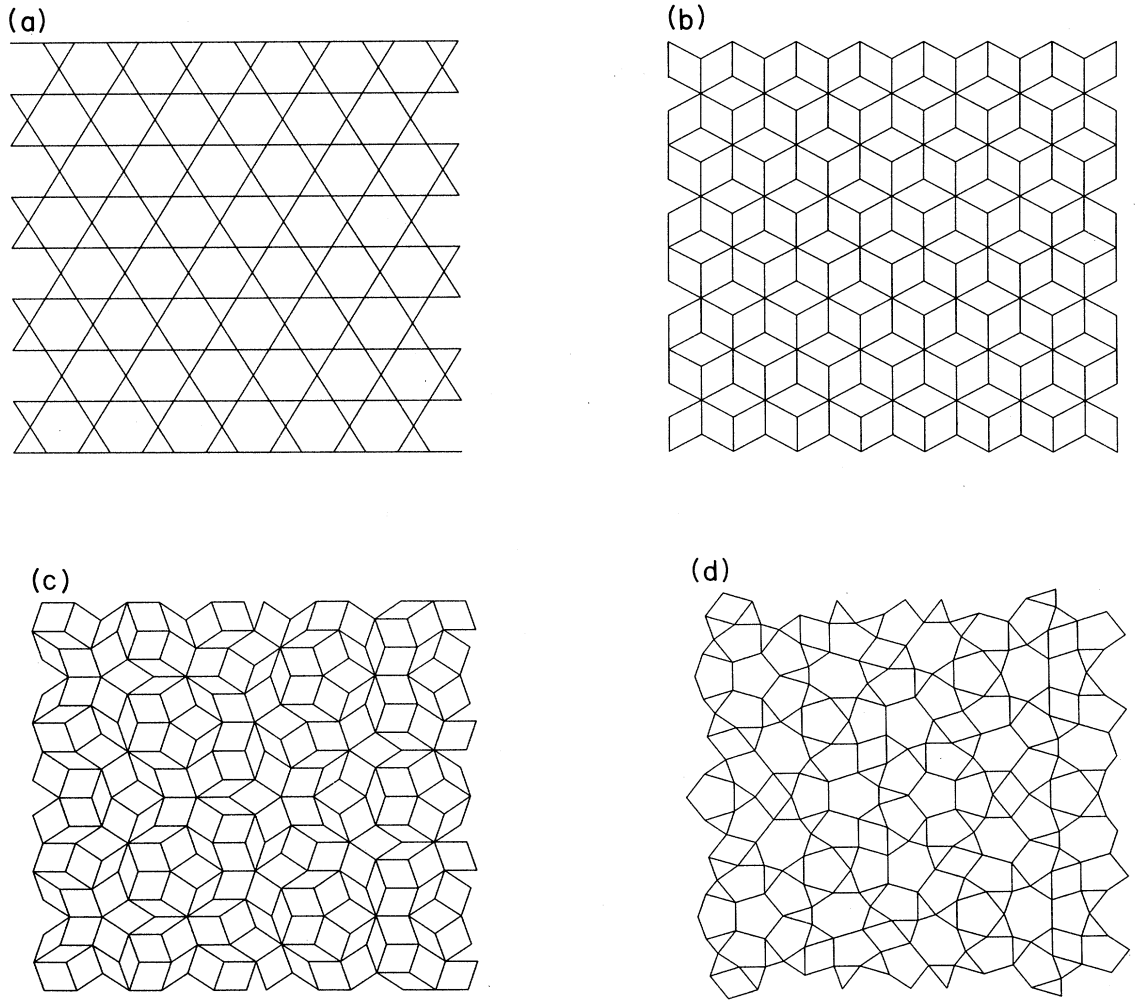

FIG. 2. Some two-dimensional lattices; (a) kagomé, (b) dice, (c) Penrose tiling, and (d) dual lattice of Penrose.

number of bonds in a lattice with the coordination number z is $z/2$ times the number of sites, the number of bonds in the above-described portion is about $zN/2$. Consequently, the accuracies of our results to be presented in what follows are expected to be higher for bond percolation than for site percolation.

Then, it is necessary to calculate $R_N^X(p)$ as a function of p for $X=R$, D, I, and U. In simulations, we shall be concerned with systems which are large enough so that the effects of the boundary conditions are negligibly small and the relation $R_N^R(p)=R_N^D(p)$ holds approximately. The method to determine $R_N^X(p)$ for a given p is described

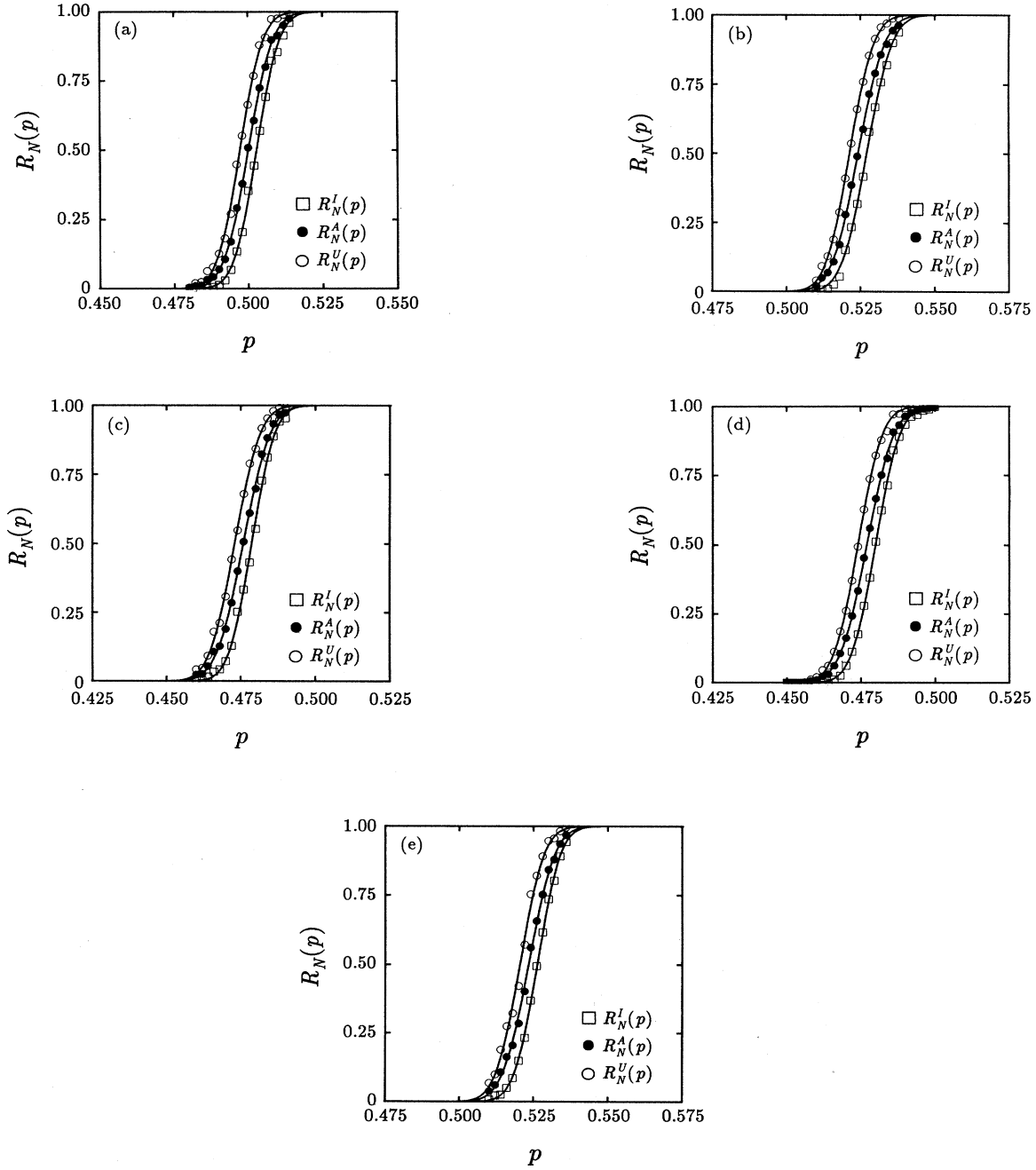

FIG. 3. Probabilities $R_N^A(p)$ (solid circles), $R_N^I(p)$ (open squares), and $R_N^U(p)$ (open circles) for the bond problem with $N\simeq 100\,000\simeq 310\times 310$. The corresponding curves are obtained by the least-mean-square fitting on assuming the error function. Note that the scale on the p axis is very minute. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

as follows.

(i) Carry out n runs of MC simulations, and find out the number m of runs for which a percolating cluster of the desired type exists.

(ii) Define $R_N(p)$ by m/n.

We perform steps (i) and (ii) for different values of p with increment Δp. In our simulations, we choose concentrations p with each interval of $\Delta p = 0.002$, and carry out 500 MC runs at each concentration. Owing to the relation (2.14) and $R_N^R(p) = R_N^D(p)$, the size of the ensemble for $R_N^A(p)$ is twice as large, being 1000 in this case.

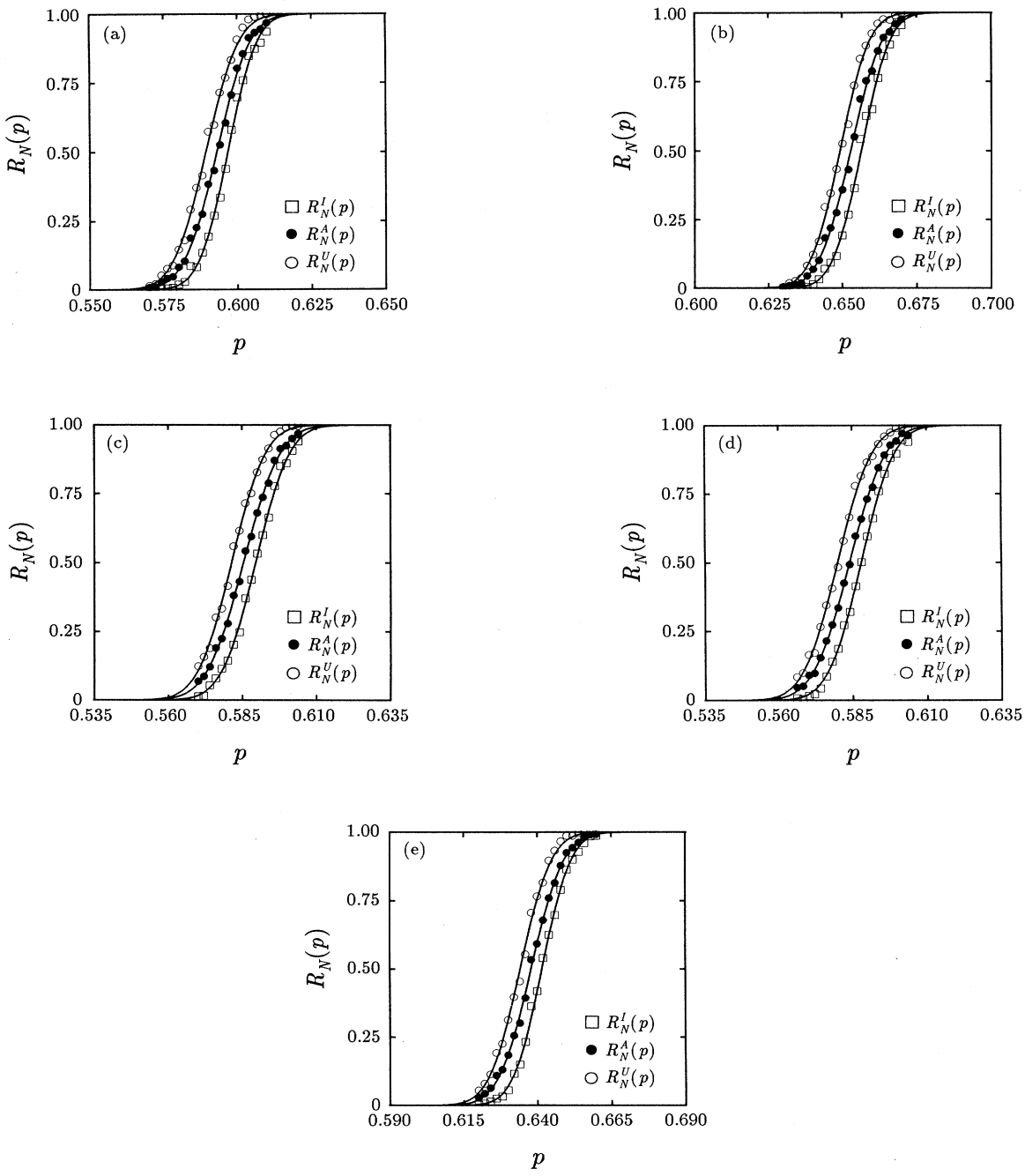

FIG. 4. Probabilities $R_N^A(p)$ (solid circles), $R_N^I(p)$ (open squares), and $R_N^U(p)$ (open circles) for the site problem with $N \simeq 50\,000 \simeq 230 \times 230$. The corresponding curves are obtained by the least-mean-square fitting on assuming the error function. Note that the scale on the p axis is very minute. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

The results thus obtained give information of $R_N^X(p)$ at discrete values of p. It is therefore necessary to carry out curve fitting assuming the error function related to Eq. (2.2) in order to evaluate $p_c^X(N)$ and Δ_N^X. We use the least-mean-square method for curve fitting.

We study both bond and site percolation in 2D lattices such as square, triangular, honeycomb, kagomé, dice, Penrose, and a dual lattice of Penrose. The first three lattices are periodic while Penrose tiling and a dual lattice of Penrose are quasiperiodic. Exact shapes of the last four lattices are given in Fig. 2. The coordination number z is single valued in a square, triangular, honeycomb, kagomé lattice, and in a dual lattice of Penrose, while z is mixed valued in a dice lattice which has $z=3$ and 6 and

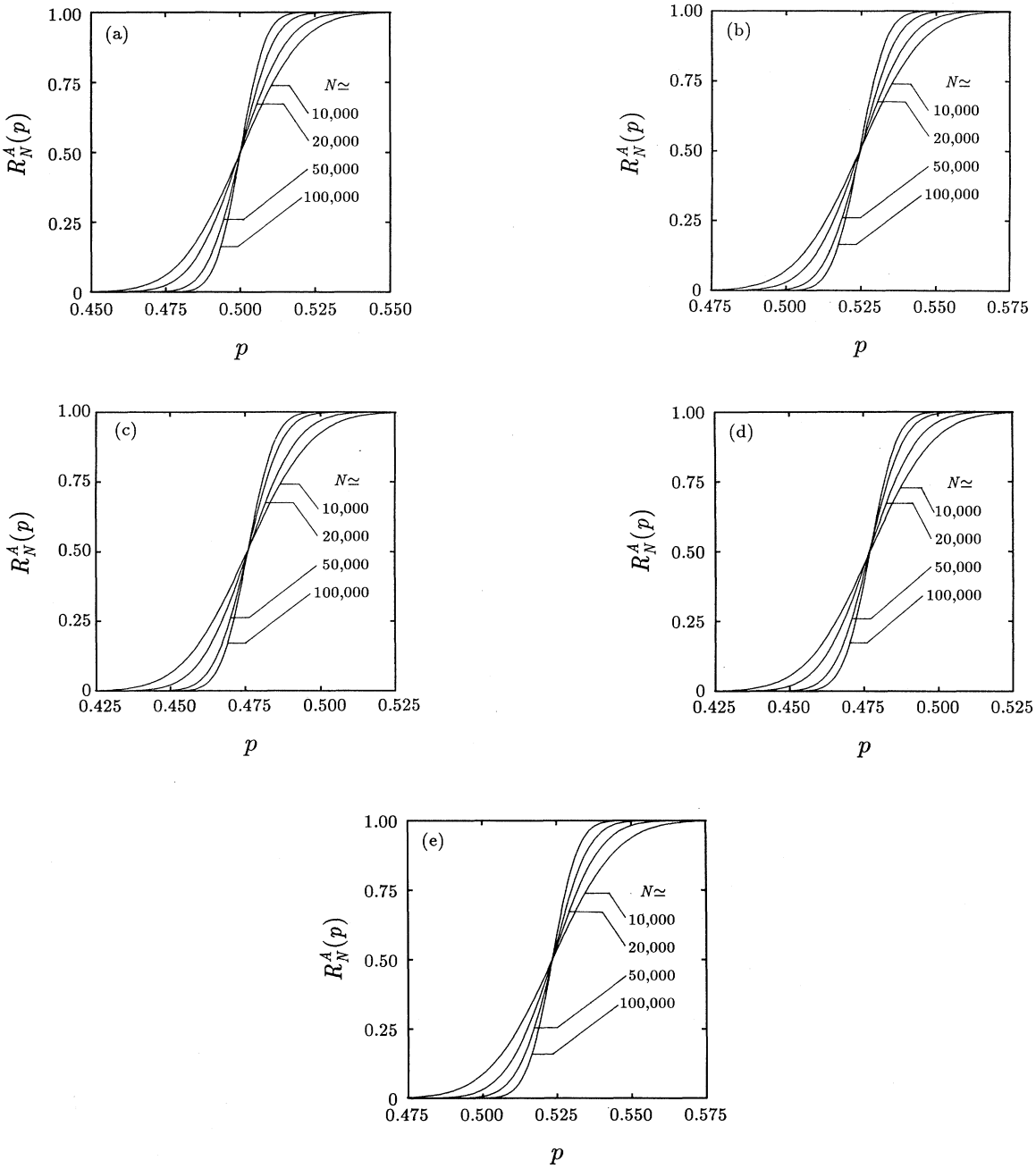

FIG. 5. Probabilities $R_N^A(p)$ of the bond problem as expressed by the error function for several values of N. $N\simeq 10\,000(\simeq 100\times 100)$; $N\simeq 20\,000(\simeq 140\times 140)$; $N\simeq 50\,000(\simeq 230\times 230)$; and $N\simeq 100\,000(\simeq 310\times 310)$. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

in Penrose tiling which has $z=3$, 4, 5, 6, and 7. We show detailed results for five lattices—square, kagomé, dice, Penrose, and a dual lattice of Penrose.

In Fig. 3, we illustrate by solid circles, open squares, and open circles, three probabilities $R_N^A(p)$, $R_N^I(p)$, and $R_N^U(p)$, respectively, of bond percolation which we have evaluated by the procedures stated above. The corresponding results for site percolation are given in Fig. 4. The best curve fittings for $R_N^A(p)$, $R_N^I(p)$, and $R_N^U(p)$ are achieved for five lattices as shown in Figs. 3 and 4. Fittings are remarkable, especially in the region where $R_N^X(p)\simeq 0.5$.

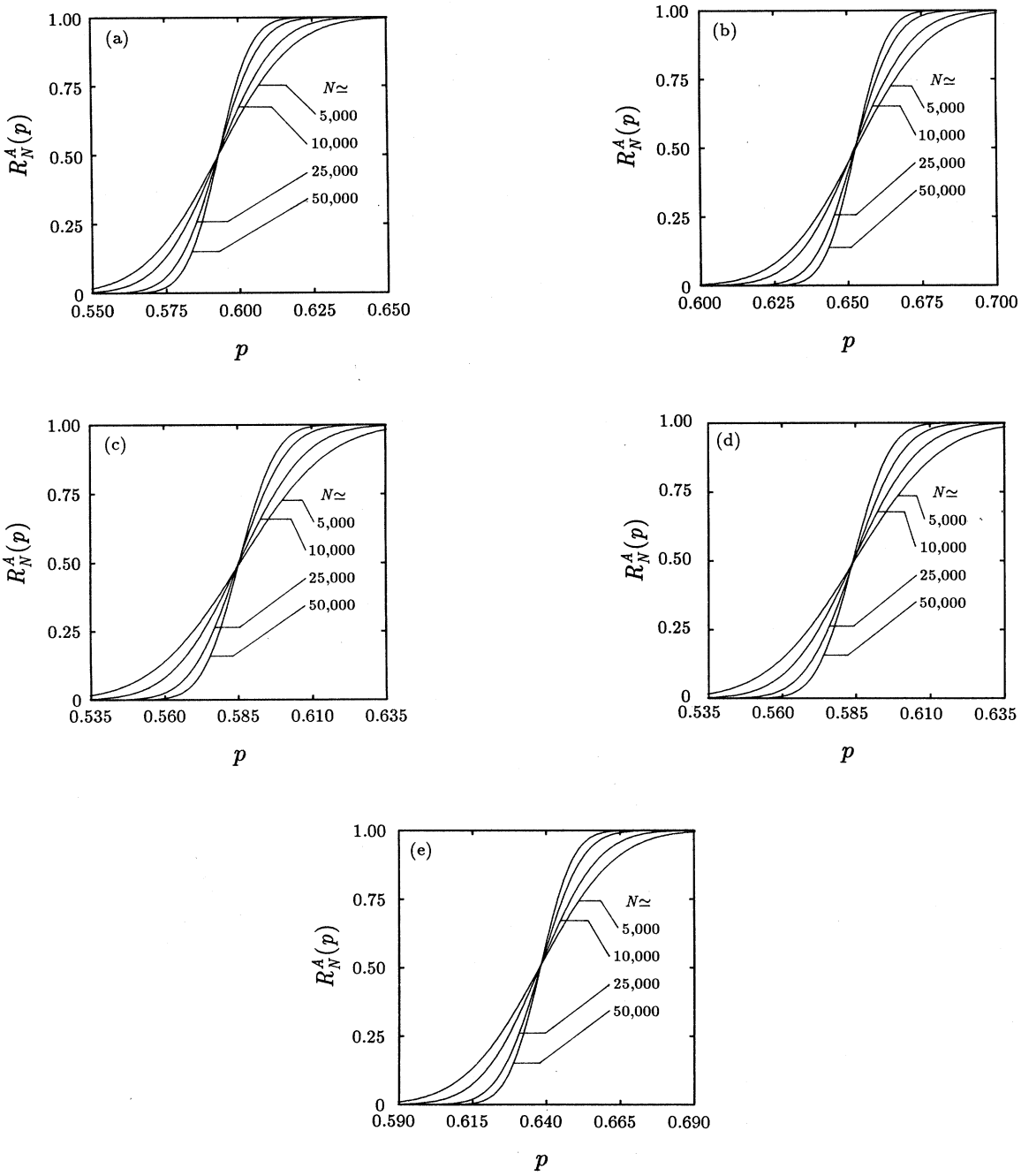

FIG. 6. Probabilities $R_N^A(p)$ of the site problem as expressed by the error function for several values of N. $N\simeq 5000(\simeq 70\times 70)$; $N\simeq 10\,000(\simeq 100\times 100)$; $N\simeq 25\,000(\simeq 160\times 160)$; and $N\simeq 50\,000(\simeq 230\times 230)$. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

The size dependence of $R_N^A(p)$ is presented in Fig. 5 for bond percolation and in Fig. 6 for site percolation. In each of the ten figures in Figs. 5 and 6, we can clearly observe that the point at which $R_N^A(p)=0.5$ behaves like the so-called fixed point. This fact lends support to our assertion in Sec. II that, even when the system size N is not very large, $p_c^A(N)$ is very close to the threshold p_c of an infinite lattice.

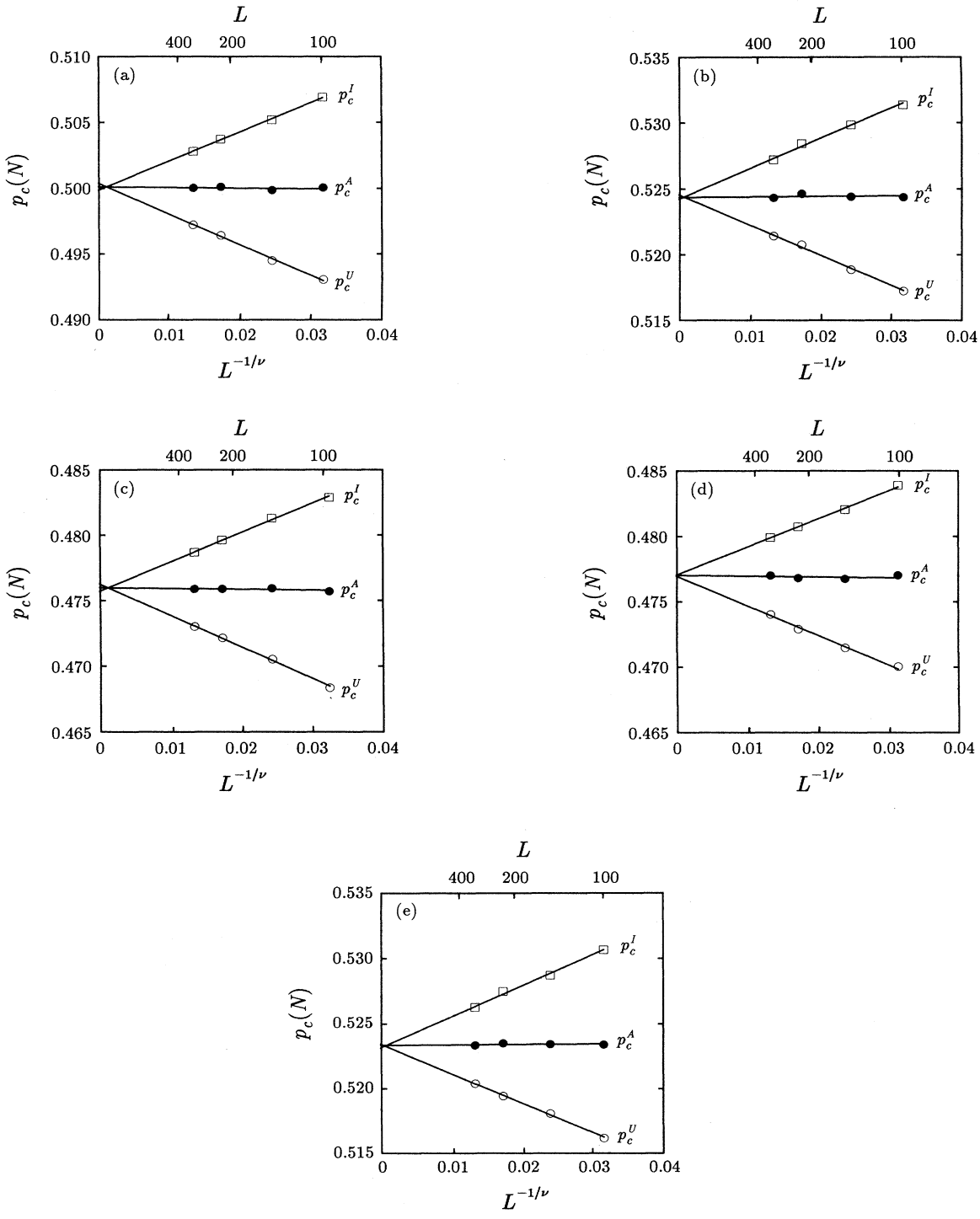

FIG. 7. Three thresholds $p_c^A(N)$, $p_c^I(N)$, and $p_c^U(N)$ of the bond problem vs $L^{-1/\nu}(=N^{-1/2\nu})$. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

In fact, the agreement among values for different N is highly impressive as demonstrated in Table I where the values of $p = p_c^A(N)$ which satisfy $R_N^A(p) = \frac{1}{2}$ are listed. Even when $N \simeq 5000$ or $L \simeq 70$ for site percolation, $p_c^A(N)$ gives three significant figures and the error in the fourth digit is ± 0.0003. It is rather remarkable to be able to achieve the accuracy as high as this from simulations of a system with the size of 70×70.

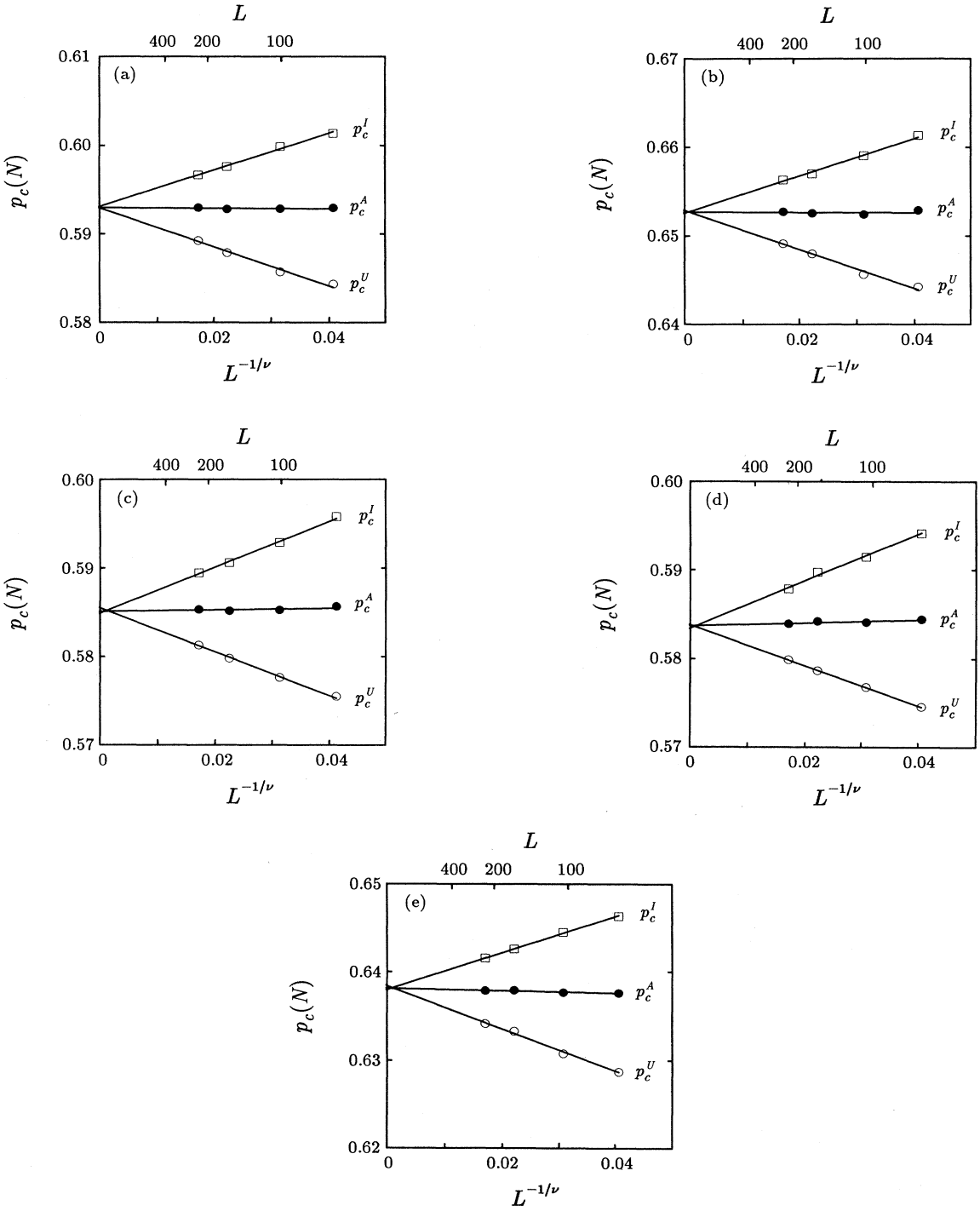

FIG. 8. Three thresholds $p_c^A(N)$, $p_c^I(N)$, and $p_c^U(N)$ of the site problem vs $L^{-1/\nu}(=N^{-1/2\nu})$. (a) square; (b) kagomé; (c) dice; (d) Penrose; and (e) dual lattice of Penrose.

TABLE I. Thresholds $p_c^A(N)$ of the bond and site problem for five different lattices with various sizes N.

	$N \simeq$	Square	Kagomé	Dice	Penrose	Dual of Penrose
Bond	10 000	0.5000	0.5244	0.4757	0.4770	0.5234
	20 000	0.4999	0.5244	0.4759	0.4768	0.5234
	50 000	0.5001	0.5246	0.4759	0.4768	0.5235
	100 000	0.5000	0.5243	0.4759	0.4770	0.5233
Site	5000	0.5929	0.6529	0.5857	0.5845	0.6376
	10 000	0.5928	0.6524	0.5853	0.5841	0.6377
	20 000	0.5928	0.6526	0.5852	0.5842	0.6379
	50 000	0.5930	0.6527	0.5854	0.5840	0.6379

The situation is visually expressed in Fig. 7 for bond percolation and in Fig. 8 for site percolation. Among other things, let us note that $p_c^A(N)$ gives a perfect horizontal line in any of the ten figures shown in Figs. 7 and 8. As for the error bars, the extrapolations from three lines $p_c^A(N)$, $p_c^I(N)$, and $p_c^U(N)$ versus $L^{-1/\nu}$ are almost equivalent to one another, the differences being very small. The differences $|p_c^I(\infty)-p_c^A(\infty)|$ and $|p_c^A(\infty)-p_c^U(\infty)|$ give the error bar which is less than 0.0003.

We have decided to show all these figures because we want to emphasize that our assertion concerning $p_c^A(N)$ turns out to be correct for a wide variety of cases—both for bond and site percolation, both for periodic and nonperiodic lattices, and both for single-valued and mixed-valued coordination.

Another important point is that our method does not require precise values of critical exponents in the process of estimating percolation thresholds. This is obvious from Figs. 7 and 8 since, in each case, $p_c^A(N)$ is almost constant for various sizes N as long as $N \gtrsim 5000$, the corresponding line being practically horizontal. Naturally, the same feature survives for any value of critical exponent ν. This is a great advantage of our method compared to most of the previous methods by which both a percolation threshold and the critical exponents must be searched such that they are consistent among themselves. Therefore, many trials and errors were undergone in previous methods while our method is perfectly free from this trouble.

Percolation thresholds thus determined are listed in Table II both for bond and site percolation. For lattices whose percolation thresholds have previously been derived either by exact analyses[13,23–28] or by computers,[6,7,29] we can compare our results with those previous values and we can readily see that agreement is outstanding. This fact indicates that those percolation thresholds

TABLE II. Thresholds p_c derived from our simulations compared with previous results. As explained in the test, our results for the threshold are derived by making use of the finite-size scaling where 500 MC runs are performed for each p of each size, the largest being 100 000 bonds and 50 000 sites.

			Previous results	
	Lattice	Our result	Theoretical	Numerical
Bond	Square	0.5001±0.0003	0.5[a]	
	Kagomé	0.5244±0.0002	0.524429[b]	
	Dice	0.4760±0.0003	0.475591[b]	
	Penrose	0.4770±0.0001		0.483±0.005[c]
	Dual of Penrose	0.5233±0.0002		
	Triangular	0.3473±0.0002	0.347 291[a]	
	Honeycomb	0.6527±0.0002	0.652 704[a]	
Site	Square	0.5930±0.0001		0.593±0.005[d]
	Kagomé	0.6527±0.0002	0.652 704[a]	
	Dice	0.5851±0.0004		
	Penrose	0.5837±0.0003		
	Dual of Penrose	0.6381±0.0003		

[a]Exact, Ref. 13.
[b]Pott's model, Ref. 24.
[c]20 MC runs for 90 000 bonds, Ref. 31.
[d]MC, Ref. 29.

that we have evaluated here for the first time (e.g., thresholds for dice, Penrose, and dual lattice of Penrose) are very reliable. Note also that, for each set of dual lattices, thresholds in Table II satisfy Eq. (2.4).

All these beautiful circumstantial evidences suggest that our method as explained in Sec. II extracts important and correct information from the analysis of finite lattices of rather small sizes, and this situation seems to hold true in almost any kind of 2D lattices including disordered systems.

V. SUMMARY

We have proposed a new method for evaluating the percolation thresholds in 2D lattices from the study of finite systems. We have also introduced a method for estimating the error bars of the percolation thresholds thus obtained. We have applied these methods of ours to the study of bond and site percolation in some 2D systems on the basis of Monte Carlo simulations. The results achieved therefrom definitely prove that our method is excellent.

The outline of our method, its applications and the results obtained are summarized as follows.

(1) We define probabilities $R_N^X(p)$ for finding a percolating cluster of type X which could be *rightward*, *downward*, *average*, *intersection*, or *union*.

(2) Using MC simulations, we calculate $R_N^X(p)$.

(3) Assuming the error function for $R_N^X(p)$, we carry out curve fitting by the least-mean-square method to derive the effective threshold $p_c^X(N)$ and the standard deviation Δ_N^X.

(4) We assert that $p_c^A(N)$ for finite N yields a true value close to the percolation threshold p_c of an infinite system.

(5) Another assertion here is that the upper and lower bound $p_c^I(N)$ and $p_c^U(N)$ of the effective threshold are given from $R_N^I(p)$ and $R_N^U(p)$, respectively, and that the error bar Δp_c of the threshold is estimated by the largest of $|p_c^I(\infty)-p_c^A(\infty)|$ and $|p_c^A(\infty)-p_c^U(\infty)|$.

(6) Values of thresholds are actually derived for several 2D lattices. These values are shown to be reliable; the reliability of the thresholds is guaranteed by the small error bars of 0.0003 at most estimated by the method as stated in (5). The thresholds obtained confirm the initial-dual relationship expressed by Eq. (2.4).

(7) From the analysis of the results of our computer simulations, we ascertain that the above assertion of ours holds right both for bond and site percolation in all the lattices we have studied. This implies that our method works both for the bond and site percolation, both for periodic and nonperiodic lattices, and both for single-valued and mixed-valued coordination.

For future study, it would be interesting to investigate the modified effective-medium approximation (EMA) for thresholds,[9,30] because the lowest-order EMA gives the threshold for bond percolation to be $p_c=2/z$ which is exact in a square lattice and a fairly good approximation for any of the other lattices. Research along this line is in progress.

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