## Percolation and cluster structure parameters: The radius of gyration

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# Percolation and cluster structure parameters: The radius of gyration 

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Received 14 April 1997, in final form 27 June 1997


#### Abstract

The squared radius of gyration of percolation clusters are determined in terms of the clusters' second spatial moments using the enhanced Hoshen-Kopelman algorithm for square and triangular lattices containing $2.025 \times 10^{9}$ sites. Correlation length exponents and related exponents as well as their corresponding amplitudes are calculated in terms of the squared radius of gyration above and below the percolation threshold. A coefficient for cluster compactness that is based on the squared radius of gyration of a cluster is introduced. That coefficient is compared with a similar coefficient of compactness that is based on the cluster cyclomatic number.


## 1. Introduction

Since the introduction of percolation theory, the focus of cluster analysis in Monte Carlo simulation has been on quantities that can be derived from cluster sizes [1]. Cluster structure or shape information has received somewhat less attention, possibly, because the computational tools for calculating structure parameters are not as powerful as those that are used for determining cluster sizes. Cluster structure calculations usually involve relatively small lattices when compared with cluster size calculations which very often employ lattices containing $10^{9}$ sites or more. For example, Rapaport [2] reported cluster size calculations for a lattice containing $4.225 \times 10^{11}$ sites.

A very important cluster structure parameter is the squared radius of gyration, which is a measure for the mean distance between two sites belonging to the same cluster. Stauffer and Aharony [1] suggested a relationship between the radius of gyration and the fractal dimension of the lattice. They also suggested relationships between the radius of gyration and the correlation length and other related squared distance parameters. Other researchers have provided us with examples of computed cluster structure parameters, which include perimeters [3], correlation length [4], backbone perimeter [5], and spanning lengths [6]. A more recent study focuses on exponents for the end-to-end distance distribution between two cluster sites at criticality [7].

Quandt and Young [8] calculated the gyration tensor to determine the cluster asphericity parameters of Rudnic and Gaspari [9] for percolation and Ising clusters. They applied the Hoshen-Kopelman (HK) [10] algorithm to identify clusters. Yet, in their calculations, they only studied relatively small percolation clusters of sizes 5-4096.

Domb and Stoll [11] introduced the cyclomatic number as a structure parameter. They used the cyclomatic number, which represents the number of independent cycles in a cluster, to define a coefficient of cluster compactness.
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Recently, Hoshen et al [12] introduced the enhanced HK (EHK) algorithm for the structural analysis of clusters in binary lattices. The EHK algorithm was further enhanced for multiple colour image processing [13]. This enhanced algorithm can be used to calculate various cluster structure parameters in large lattices with the computational efficiency of the original HK algorithm [10]. The original HK algorithm makes a single pass through the lattice inspecting each site sequentially and assigning it with a cluster label. Each cluster in the lattice is identified by one or more labels. The EHK algorithm generalizes the HK method of cluster size calculation to the calculation of structural parameters such as spatial moments, cluster bounding rectangles and perimeters of all clusters in the lattice in a single pass [12]. To enable the EHK analysis of very large lattices while storing only a small fraction of the lattices in the computer's memory, we have used the label recycling method, denoted as option (c) in [10].

Using the EHK algorithm, in section 2, we provide results for the squared radius of gyration calculations for lattices containing $2.025 \times 10^{9}$ sites where the squared radius of gyration is determined from the clusters' spatial moments. We use the squared radius of gyration to calculate the correlation length and other parameters as suggested by Stauffer and Aharony [1]. In section 3, we introduce a cluster compactness coefficient, which is based on the squared radius of gyration, and compare it with the cyclomatic number coefficient of Domb and Stoll [11]. In section 4, we discuss our computation results.

## 2. The squared radius of gyration

A general expression for cluster spatial moments, $M_{k}$, in $d$ dimensions is

$$
\begin{equation*}
M_{k}(m(1), m(2), \ldots, m(d))=\sum_{i \in k} \prod_{\mu=1}^{d} x_{\mu}^{m(\mu)}(i) \tag{1}
\end{equation*}
$$

where $x_{\mu}(i)$ denotes the $\mu$ th coordinate of the $i$ th site of the $k$ th cluster and $m(\mu)$ is the exponent for the $x_{\mu}$ coordinate. When all $m(\mu)=0$, (1) represents the zero moment of the cluster. This moment denotes the cluster size. The first cluster moment, which defines the cluster's centre of mass, for the $\mu$ th coordinate is

$$
\begin{equation*}
M_{k}(m(1)=0, m(2)=0, \ldots, m(\mu)=1, \ldots, m(d)=0) \tag{2}
\end{equation*}
$$

In a similar fashion, the second spatial cluster moment can be defined. In two dimensions, this would correspond to $x^{2}, y^{2}$ and $x y$ terms.

Using the cluster moments, we can calculate the squared radius of gyration, $R_{s}^{2}$, given by:

$$
\begin{equation*}
R_{s}^{2}=\frac{1}{2 s^{2}} \sum_{i, j}\left|\boldsymbol{r}_{i}-\boldsymbol{r}_{j}\right|^{2} \tag{3}
\end{equation*}
$$

where $s$ is the size of the cluster, $\boldsymbol{r}_{i}$ and $\boldsymbol{r}_{j}$ are the positions of sites $i$ and $j$ belonging to the cluster. The double summation is carried over all $i$ and $j$ sites of the cluster. It can be shown that $R_{s}^{2}$ can be given in terms of the cluster first and second moments [12]:

$$
\begin{equation*}
R_{s}^{2}=\frac{1}{s^{2}} \sum_{\mu=1}^{d}\left[s X_{\mu}^{(2)}-\left(X_{\mu}^{(1)}\right)^{2}\right] \tag{4}
\end{equation*}
$$

where $X_{\mu}^{(1)}=\sum_{i} x_{\mu}(i)$ is the first moment and $X_{\mu}^{(2)}=\sum_{i} x_{\mu}^{2}(i)$ is the second moment.
In the remainder of this section, we shall use the EHK algorithm calculation of the squared radius of gyration to test the various relationships for the radius of gyration given


Figure 1. $\ln \left(R_{s}^{2}\right)$ versus $\ln (s)$ for $p=0.592$ and for cluster sizes $100000>s>30000$ for $45000 \times 45000$ lattice.

Table 1. $D^{*}$ values for some $p$ values for a square lattice.

| $p$ | Number <br> of clusters | $D^{*}$ |
| :--- | :--- | :--- |
| 0.580 | 1001 | $0.887 \pm 0.022$ |
| 0.585 | 4064 | $1.230 \pm 0.005$ |
| 0.590 | 4125 | $1.715 \pm 0.004$ |
| 0.592 | 1975 | $1.782 \pm 0.005$ |

by Stauffer and Aharony [1]. They suggest that at the percolation threshold, the following relationship exists between $R_{s}^{2}$ and $s$

$$
\begin{equation*}
R_{s}^{2} \propto s^{1 / D} \tag{5}
\end{equation*}
$$

where $D$ is the fractal dimension.
To test relationship (5), using the EHK algorithm, we computed $R_{s}^{2}$ values for clusters on a $45000 \times 45000$ simulated square lattice. Figure 1 displays the result of this computation for $p=0.592$ and for cluster sizes $100000>s>30000$. The values of the exponent $D^{*}$, which were determined from the slope $T\left(D^{*}=T^{-1}\right)$ of the line corresponding to a logarithmic transformation of (5), are given in table 1 for $p=0.58,0.585,0.59,0.592$. (We denote the exponents as $D^{*}$ to distinguish them from $D$, which is defined for $p_{c}$.) Clearly, the $D^{*}$ values increase as the percolation threshold is approached. At $p=0.592$ the mean value of $D^{*}$ is 1.782 indicating a slow convergence to the $D_{\text {exact }}$ value of $\frac{91}{48} \approx 1.896$ [1].
$D^{*}$ and other parameters reported in this paper were calculated using linear regression analysis. The error bars of these parameters were derived from the standard deviations in the linear regression coefficients [14]. For example, the error bar $\Delta D^{*}$ for the exponent $D^{*}$ is $T^{-2} \Delta T$ where $\Delta T$ is the error bar for the gradient $T$ of the regression line.

A Windows 95166 MHz Pentium ${ }^{\circledR}$ PC was used for all EHK algorithm computations. The algorithm was implemented in $C$. The computation time for each Monte Carlo run on a $45000 \times 45000$ lattice took approximately 60 min and consumed about 3 MB of RAM. In all simulations free boundary conditions were used. In the simulations, we used a pseudorandom number generator suggested by Knuth [15]. That generator has a pseudorandom number sequence cycle that is at least $2^{55}-1$ long.

Stauffer and Aharony [1] suggested three different definitions of a lattice averaged squared radius given in terms of $R_{s}^{2}$. These include the correlation length, $\xi^{2}$, and two other radii, which we denote as $\xi_{2}^{2}$ and $\xi_{3}^{2}$, where

$$
\begin{align*}
\xi^{2} & =\frac{2 \sum_{s}\left\langle R_{s}^{2}\right\rangle s^{2} n_{s}}{\sum_{s} s^{2} n_{s}}  \tag{6a}\\
\xi_{2}^{2} & =\frac{2 \sum_{s}\left\langle R_{s}^{2}\right\rangle s n_{s}}{\sum_{s} s n_{s}}  \tag{6b}\\
\xi_{3}^{2} & =\frac{2 \sum_{s}\left\langle R_{s}^{2}\right\rangle n_{s}}{\sum_{s} n_{s}} . \tag{6c}
\end{align*}
$$

Below $p_{c}$ the summation is carried over all clusters. Above $p_{c}$, the contribution of the largest cluster is excluded from the summation. $n_{s}$ denotes the number of clusters of size $s$. $\left\langle R_{s}^{2}\right\rangle$ stands for the mean squared radius of gyration over all clusters of size $s$. Near $p_{c}$, the following relationships are expected to hold, $\xi=\xi_{1, W}\left|p-p_{c}\right|^{-v}, \xi_{2}=\xi_{2, W}\left|p-p_{c}\right|^{-(\nu-\beta / 2)}$ and $\xi_{3}=\xi_{3, W}\left|p-p_{c}\right|^{-J} . v$ and $\beta$ are the critical exponents for the correlation length and the infinite cluster probability, respectively. $J$ stands for a proposed exponent for ( $6 c$ ). The subscript $W$ for the amplitudes $\xi_{1, W}, \xi_{2, W}$ and $\xi_{3, W}$ is set to $B$ if $p<p_{c}$ and is set to $A$ if $p>p_{c}$.

To calculate the amplitudes and exponents for $\xi, \xi_{2}$ and $\xi_{3}$, 92 Monte Carlo runs were made on square and triangular lattices containing $45000 \times 45000$ sites below and above $p_{c}$. Table 2 provides a summary for these run sequences. To ensure that pseudorandom number sequences do not overlap within a run sequence, the last random number seed of a run was used to generate a new seed for the next run. Square boundaries were used for the square lattice simulations and rhombus boundaries were used for the triangular lattice simulation. In the calculation, we used $p_{c}=0.5$ for the triangular lattice, and $p_{c}=0.592746$ for the square lattice [1]. Figure 2 gives a $\log -\log$ plot for $\xi, \xi_{2}$ and $\xi_{3}$ for the square lattice data below $p_{c}$. The amplitudes $\xi_{I, W}$ and their error bars are determined from the intercept $V$ of the regression line, such that $\xi_{I, W}=\exp (V)$ and $\Delta \xi_{I, W}=\exp (V) \Delta V$ where $I=1,2,3$ and $\Delta V$ is the statistical error for $V$ [14].

Table 2. Simulation run sequences.

| Lattice | Data points | $p$ range |
| :--- | :--- | :--- |
| square | 32 | $0.52-0.58$ |
| square | 19 | $0.601-0.624$ |
| triangular | 22 | $0.425-0.48$ |
| triangular | 19 | $0.51-0.5325$ |



Figure 2. $\ln (R)$ versus $\ln (D p)$ where $D p=\left|p_{c}-p\right|$ for 32 runs, $p=0.52-0.58$ (some $p$ values are repeated) and $45000 \times 45000$ lattice size. When $R=\xi$, corresponding to ( $6 a$ ), data points shown as $\times$ and - denotes the regression line. When $R=\xi_{1}$, corresponding to ( $6 b$ ), data points are shown as $\square$ and -- denotes the regression line. When $R=\xi_{2}$, corresponding to ( $6 c$ ), data points shown as $\Delta$ and --- denotes the regression line.

Table 3. Lattice mean squared radii exponents and amplitudes for $(6 a)-(6 c)$ for square and triangular lattices.

|  |  |  | Below $p_{c}$ |  |  | Above $p_{c}$ |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Lattice <br> radius | Lattice <br> type | Exponent | Computed <br> exponent | $\xi_{I, B}$ |  | Computed <br> exponent | $\xi_{I, A}$ |
| $\xi$ | square | $v$ | $1.320 \pm 0.002$ | $0.539 \pm 0.004$ |  | $1.39 \pm 0.07$ | $0.12 \pm 0.03$ |
| $\xi_{2}$ | square | $v-\beta / 2$ | $1.233 \pm 0.001$ | $0.385 \pm 0.001$ | $1.05 \pm 0.01$ | $0.13 \pm 0.01$ |  |
| $\xi_{3}$ | square | $J$ | $0.390 \pm 0.006$ | $0.845 \pm 0.019$ |  | $0.33 \pm 0.01$ | $0.36 \pm 0.01$ |
|  |  |  |  |  |  |  |  |
| $\xi$ | triangular | $v$ | $1.343 \pm 0.002$ | $0.460 \pm 0.003$ |  | $1.35 \pm 0.05$ | $0.12 \pm 0.02$ |
| $\xi_{2}$ | triangular | $v-\beta / 2$ | $1.244 \pm 0.001$ | $0.348 \pm 0.001$ |  | $1.02 \pm 0.01$ | $0.14 \pm 0.01$ |
| $\xi_{3}$ | triangular | $J$ | $0.359 \pm 0.010$ | $1.085 \pm 0.034$ | $0.32 \pm 0.01$ | $0.44 \pm 0.01$ |  |

The results for the exponents, their amplitudes and error bars for square and triangular lattices above and below $p_{c}$ are summarized in table 3 . We should note that the statistical error bars for both the square and triangular lattices were larger above $p_{c}$ than below it. The computed $v$ exponent values for both the square and triangular lattices below and above $p_{c}$ are scattered around 1.35 which is close to $\nu_{\text {exact }}=\frac{4}{3} \approx 1.333$ [1]. In table 3 we observe that below $p_{c} v-\beta / 2 \approx 1.23$ for the square and triangular lattices, and that above $p_{c}$

Table 4. Results for $p_{c}$ and amplitudes, $\xi_{1, W}$, for (7) and (8) for square and triangular lattices.

|  | Data points <br> range | $p_{c}{ }^{\mathrm{a}}$ | $\xi_{1, W}{ }^{\mathrm{a}}$ | $\xi_{1, W}{ }^{\mathrm{b}}$ |
| :--- | :--- | :--- | :--- | :--- |
| Lattice | below $p_{c}$ | $0.5930 \pm 0.0001$ | $0.522 \pm 0.001$ | $0.516 \pm 0.004$ |
| square | above $p_{c}$ | $0.594 \pm 0.001$ | $0.13 \pm 0.01$ | $0.14 \pm 0.01$ |
| square | $0.4996 \pm 0.0001$ | $0.471 \pm 0.001$ | $0.475 \pm 0.004$ |  |
| triangular | below $p_{c}$ | $0.501 \pm 0.001$ | $0.14 \pm 0.01$ | $0.15 \pm 0.01$ |
| triangular | above $p_{c}$ | 0.1 |  |  |

${ }^{\text {a }}$ Value determined using (7).
${ }^{\mathrm{b}}$ Value determined using (8).
$v-\beta / 2 \approx 1.03$. Yet for both lattices, these values differ by 0.2 .
It is worth noting that below $p_{c}, v_{\text {exact }}-\beta_{\text {exact }} / 2=\frac{91}{72} \approx 1.264$ is close to the calculated values of 1.233 and 1.244 for the square and triangular lattices given in table 3. Furthermore, $D=d-\beta / v=d-2+2(v-\beta / 2) / v$. Since $d=2, D=2(v-\beta / 2) / v$. Using the below $p_{c}$ values of $v$ and $(\nu-\beta / 2)$ from table 2 , we obtain $D=1.868$ for the square lattice and $D=1.853$ for the triangular lattice which compares rather well with $D_{\text {exact }}=\frac{91}{48} \approx 1.896$.

For the proposed exponent $J$, we note that for both square and triangular lattices below and above $p_{c}, J \approx 0.4$, which differs from the value of 0 suggested in [1].

Using our numerical results and setting $v$ to $\nu_{\text {exact }}$, we can calculate $p_{c}$. We transform $\xi=\xi_{1, W}\left|p_{c}-p\right|^{-v}$ to

$$
\begin{equation*}
p=p_{c}+Q \xi^{-1 / v} \tag{7}
\end{equation*}
$$

where $Q=-\xi_{1, B}^{1 / v}$ for $p_{c}>p$ and $Q=\xi_{1, A}^{1 / v}$ for $p>p_{c}$. In (7), both $p_{c}$ and $Q$ are unknown, and we set $v$ to $v_{\text {exact }}$. We can calculate $p_{c}$ and $Q$ from the intercept and gradient of $p$ versus $\xi^{-1 / \nu}$. The error bars for $\xi_{1, W}$ are $\nu|Q|^{\nu-1} \Delta Q$ where $\Delta Q$ is the statistical error for $Q$. Using linear regression analysis for (7) and assuming $v=v_{\text {exact }}$ and employing data points of table 2, we calculated $p_{c}$ and $\xi_{1, w}$. Table 4 presents results for $p_{c}$ and $\xi_{1, W}$ in columns 3 and 4 , respectively.

If $p_{c}$ is known in addition to $\nu_{\text {exact }}$, we can calculate $\xi_{1, W}$ using the following expression:

$$
\begin{equation*}
\xi_{1, W}=\xi\left|p_{c}-p\right|^{v} \tag{8}
\end{equation*}
$$

Setting $v=v_{\text {exact }}$, and $p_{c}=0.5$ for the triangular lattice and $p_{c}=0.592746$ for the square lattice in (8), we calculate $\xi_{1, W}$. Results for this calculation are presented in column 5 of table 4.

The calculated values for the square lattice for the amplitudes, $\xi_{1, B}$, below $p_{c}$, are 0.539 (table 3), and 0.522 (table 4 column 4) and 0.516 (table 4 column 5); for the triangular lattice they are 0.460 (table 3), 0.471 (table 4 column 4) and 0.475 (table 4 column 5). They are close to the value of 0.52 calculated by Aharony and Stauffer [16] for both the square and triangular lattices, which is different from the value of 0.63 given by Corsten et al [17]. Furthermore, the amplitude ratios $\xi_{1, B} / \xi_{1, A}$ for both the square and triangular lattices is about 4 which is also consistent with [16,17]. Chayes et al [18] gave a ratio of 2 instead of 4 by using a different definition of the correlation length.

## 3. Bounds on the radius of gyration

The squared radius of gyration, $R_{s}^{2}$, is a useful cluster structure quantity. It is a measure for the mean square distance between two cluster sites and, therefore, it is a measure for cluster compactness. Yet, just knowing that a given cluster has some $R_{s}^{2}$ value does not tell
us how compact or ramified the cluster in question is. In a similar fashion to Domb and Stoll [11], who proposed a coefficient of compactness, $\lambda$, based on the cyclomatic number, we could define cluster compactness relative to the upper and lower bounds of $R_{s}^{2}$.

The upper bound, $R_{s, \max }^{2}$, for $R_{s}^{2}$ occurs when the cluster is linear. Since $R_{s}^{2}$ is an invariant quantity under translation (and rotation), we can place a linear cluster of size $s$ on the $x$-axis at $x=1$. Using the summation formulae for $1+2+, \ldots,+s$ and $1^{2}+2^{2}+, \ldots,+s^{2}$, and (4), we obtain

$$
\begin{equation*}
R_{s, \max }^{2}=\frac{s^{2}-1}{12} \tag{9}
\end{equation*}
$$

For large $s, R_{s, \text { max }}^{2}$ can be written as

$$
\begin{equation*}
R_{s, \max }^{2}=\frac{s^{2}}{12} \tag{9a}
\end{equation*}
$$

where (9) and ( $9 a$ ) are true for linear clusters in any dimension.
To determine $R_{s, \text { min }}^{2}$, the lower bound for $R_{s}^{2}$, in two dimensions, we assume that the most compact cluster of size $s$ is bounded by a circle of radius $r$, whose area is equal to the area covered by the cluster. For a square lattice, given that the distance between nearest neighbours is 1 , the density of sites is also 1 . Therefore, we have $s=\pi r^{2}$. For a large $s$, we change the summation in (4) into integration and assume that the centre of mass for the cluster is at the origin. We obtain

$$
\begin{equation*}
R_{s, \min }^{2}=\frac{1}{s} \int_{0}^{2 \pi} \mathrm{~d} \theta \int_{0}^{r} \rho^{2} \rho \mathrm{~d} \rho=\frac{\pi r^{4}}{2 s}=\frac{s}{2 \pi} \tag{10}
\end{equation*}
$$

We can also calculate a similar $R_{s, \text { min }}^{2}$ for a simple cubic lattice for the compact cluster bounded by a sphere. We use now (4) for a sphere whose centre is at the origin. We replace summation by integration for $X_{\mu}^{(2)}$ and noting that the volume of the sphere is $s=4 \pi r^{3} / 3$, we obtain

$$
\begin{equation*}
R_{s, \min }^{2}=\frac{1}{s} \int_{0}^{\pi} \mathrm{d} \theta \int_{0}^{2 \pi} \mathrm{~d} \phi \int_{0}^{r} \rho^{2} \sin \theta \rho^{2} \mathrm{~d} \rho=\frac{4 \pi r^{5}}{5 s}=\frac{3}{5}\left(\frac{3 s}{4 \pi}\right)^{2 / 3} \tag{11}
\end{equation*}
$$

We assumed again that the density of sites is 1 . For other lattice types, the density of sites would be higher or lower than 1 depending on the density of sites in a unit square (or cube). However, the exponent of $s$ would only depend on the dimension of the lattice.

Equations (10) and (11), apply to a large $s$ only. For small clusters, we employ an algorithm to compute $R_{s, \min }^{2}$. This algorithm is based on a recursive representation of (4). To do that, we express $R_{s}^{2}$ in the coordinate system of the centre of the mass of the cluster, so that $R_{s}^{2}$ simplifies to

$$
\begin{equation*}
R_{s}^{2}=\frac{1}{s} \sum_{\mu=1}^{d} \sum_{i} x_{\mu, i}^{2} \tag{12}
\end{equation*}
$$

$x_{\mu, i}$ is the $\mu$ th coordinate of the $i$ th site of the cluster. Using (4) and adding one more site to our cluster, we obtain

$$
\begin{equation*}
R_{s+1}^{2}=\frac{1}{(s+1)^{2}} \sum_{\mu=1}^{d}\left[(s+1) X_{\mu}^{(2)}-\left(X_{\mu}^{(1)}\right)^{2}\right] \tag{13}
\end{equation*}
$$

Writing (13) in terms of the centre of mass of the original cluster of size $s$, we get a recursive relationship for $R_{s}^{2}$ :

$$
\begin{equation*}
R_{s+1}^{2}=s\left[\frac{R_{s}^{2}}{s+1}+\frac{\sum_{\mu=1}^{d} x_{\mu, s+1}^{2}}{(s+1)^{2}}\right] \tag{14}
\end{equation*}
$$



Figure 3. Squared radius of gyration for the compact cluster ( $\mathrm{SRG}(\mathrm{min})), R_{s, \min }^{2}$, versus cluster size $s$ for a square lattice, denoted as two dimensional; and cubic lattice, denoted as three dimensional. Full curves denote algorithm (14) results. Broken curves denote approximate results given by (10) and (11) for square and cubic lattices, respectively.
where $x_{\mu, s+1}$ is the $\mu$ th coordinate of the new cluster site $s+1$ given in the coordinate system of the centre of mass of the $s$-sized cluster.

We now use recursively (14) to determine $R_{s, \min }^{2}$. The algorithm starts from a single site at the origin. It then inspects all empty neighbouring sites around that site such that $\sum_{\mu=1}^{d} x_{\mu, 2}^{2}$ is minimized. When it finds a site that minimizes (14), the algorithm adds it to the cluster. The search process is repeated around the cluster for an empty site that minimizes $\sum_{\mu=1}^{d} x_{\mu, 3}^{2}$ etc. Every time $\sum_{\mu=1}^{d} x_{\mu, s+1}^{2}$ is minimized, we make sure that we minimize it in terms of the coordinates of the centre of the mass of the previous cluster.

The justification for the algorithm is that at every iteration, we minimize $R_{s}^{2}$. However, such a minimum may be only a local minimum and not a global one. So, at this point, we should consider the algorithm to be a heuristic algorithm. Yet, when we compare the algorithm results with the approximate formulae, (10) and (11), for $R_{s, \text { min }}^{2}$, we obtain good matches for $s>40$ as shown in figure 3 .

To measure cluster compactness, we define $e$ as a coefficient of compactness:

$$
\begin{equation*}
e=\frac{\left(R_{s}^{2}\right)^{-1}-\left(R_{s, \max }^{2}\right)^{-1}}{\left(R_{s, \min }^{2}\right)^{-1}-\left(R_{s, \max }^{2}\right)^{-1}} \tag{15}
\end{equation*}
$$

The value of $e$ ranges from 0 , for the linear cluster, to 1 , for the most compact cluster. For large $s$, our simulations suggest that for most clusters $\left(R_{s, \text { min }}^{2}\right)^{-1}>\left(R_{s}^{2}\right)^{-1} \gg\left(R_{s, \max }^{2}\right)^{-1}$ so that $e \approx R_{s, \text { min }}^{2} / R_{s}^{2}$. Figure 4 displays $e$ for several $p$ values for clusters grouped by size. We observe that as the cluster size increases for a given $p$, the ratio $e$ decreases, indicating


Figure 4. Cluster compactness coefficient, $e$, plotted versus cluster size groups $i$ such that $2^{i} \leqslant s<2^{i+1}$ for $p=0.57,0.58,0.5875,0.59,0.5925$ for $45000 \times 45000$ lattices.
that the larger clusters are more ramified. On the other hand, clusters of a given size group become more compact as $p$ increases.

At this point, it would be useful to compare the coefficient $e$ with the coefficient $\lambda$ given by Domb and Stoll [11]

$$
\begin{equation*}
\lambda=\frac{b-s+1}{\left(s^{1 / 2}-1\right)^{2}} \tag{16}
\end{equation*}
$$

In (16), $b$ represents the number of bonds in the cluster. $b-s+1$ is the cyclomatic number representing the number of independent cycles in the cluster and $\left(s^{1 / 2}-1\right)$ represents the cyclomatic number for the most compact cluster of size $s$. The values of both $e$ and $\lambda$ range from 0 to 1 . However, the value of 0 for $\lambda$ does not distinguish between a linear cluster or a tree-like cluster. In contrast, $e=0$ applies only to linear clusters. For tree-like clusters and other clusters, $e>0$. When a cluster achieves maximum compactness, both $\lambda$ and $e$ are equal to 1 . For large clusters, $\lambda=1$ for both compact circular clusters and compact square clusters. $e=1$ for only compact circular clusters. Using (15), (9a) and (10) for compact square clusters, we obtain $e=(3-3 / s) /(\pi-3 / s) \approx 3 / \pi$.

## 4. Discussion

With the help of the EHK algorithm, we approached the issue of cluster structure by studying the squared radius of gyration that is derived from the first and second spatial moments of the cluster. We used the squared radius of gyration to evaluate the correlation length and related parameters. We had a very good linear fit for the correlation length curve where
$v=1.320 \pm 0.002$ for the square lattice and $v=1.343 \pm 0.002$ for the triangular lattice below $p_{c}$. These values are close to the exact value of $v$ of $\frac{4}{3} \approx 1.333$. Since the statistical error bars are relatively small (0.002), systematic errors are the likely source for the differences between the calculated $v$ values and $v_{\text {exact }}$. Examples of sources for systematic errors are pseudorandom number generators, the ranges of values of $p$ used in the simulation, and the finite distance of $p$ from the threshold. Nevertheless, because both calculated $v$ values for the square and triangular lattices were determined by the same method, the reasons for the 0.023 difference between these two values ( 11.5 error bars) requires further study.

The finite sizes and boundary shape of the lattices is likely to be another source of systematic errors. It appears that the boundary effects are more pronounced for large clusters cut off by the boundary. A simple example illustrates this point. At $p=1$ in two dimensions, the squared correlation length for a square lattice with finite square boundaries is $\xi^{2}=s / 6$. On the other hand, according to (10), the squared correlation length for a square lattice bounded by a finite circle is $\xi^{2}=s /(2 \pi)$. The large clusters are significant contributors to the numerator of $(6 a)$, and when they are cut, the value of the correlation length could be significantly affected. There are several approaches that could be used to address the problem. In one approach, we could remove the contributions of all clusters that touch the lattice boundary as was described in [16] for the Leath [19] algorithm calculations. Alternatively, we could use cyclic boundary conditions to extend the clusters across the boundary. Another approach would be to use only smaller $p$ values so that there would be fewer large clusters stretching across the boundary.

The focus of this paper has been on low-order cluster spatial moments. Since the EHK algorithm can calculate higher moments for large lattices, the question is what new physical information can be derived from these higher-order moments. While raw moments are not very useful quantities by themselves, quantities that can be derived from them such as the squared radius of gyration are useful. For higher moments to become useful, there is a need to find quantities similar to the radius of gyration and express them in terms of these higher moments. These quantities should be defined with respect to the centre of mass of the cluster, thus, making them invariant to translation.

## Acknowledgment

I would like to thank D Stauffer for his valuable help, comments and his suggestion for the study of the critical exponents amplitudes.

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