Chapter 5

Percolation of objects with finite spatial sizes

5.1 Introduction

In the last chapter we have discussed the site percolation problem on a lattice [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. It has been observed that this is an example of continuous phase transition phenomena, associated with a unique percolation threshold. There exist a number of scaling relations for the cluster distribution near this threshold, where the critical exponents are universal. One important point to note here is that the object percolating through the lattice is itself a point object, and it resides on a single lattice site. A physical example would be the classical transport of electrons in a solid, where electrons are treated as point objects.

However, there also exist objects of interest which have finite spatial extent. The transport of granular materials is one such problem. Another example is the flow of vehicular traffic in a randomly grown habitation. This problem has the additional feature that not only the objects (in this case the vehicles) but also the obstacles have finite sizes. As one more instance, an interesting experiment has been reported recently [16] on the transport properties of the Fe-doped ceramic La$_{0.75}$Ca$_{0.25}$Mn$_{1-x}$Fe$_x$O$_3$. It has been observed that at a concentration of about 4% ($x \approx 0.04$) of Fe ions the
resistivity of the material jumps up by a factor of about 22. The results indicate that at this concentration and above the Fe impurities may be prohibiting the transport of magnetic polarons which are objects with finite spread [17, 18]. It is possible to interpret these experimental observations as a percolation transition for the polarons. We discuss the details of this experiment and its percolation model in a separate section later in this chapter.

It would thus seem relevant to talk about a percolation problem on a lattice where the percolating objects have finite sizes. We have already come across one problem involving finite-sized objects, the 'Swiss cheese model' for continuum percolation as mentioned in the last chapter. In this chapter we introduce, to our knowledge for the first time, a new type of percolation model in which the finite-sized objects are defined on a lattice [20, 21]. In addition to the possible applications as mentioned in the preceding paragraph, this problem has its own theoretical appeal. We have discussed universality in the last chapter, in which it was mentioned that the critical exponents decide the universality class to which the system belongs. In the present context, it is interesting to explore if the critical exponents, and hence the universality class, depend on the size and/or the shape of these percolating objects (we shall see later that for a one dimensional lattice at least one exponent does not have this dependence).

We have numerically investigated the problem of percolation of finite-sized objects on two lattices: A two dimensional square lattice, and a three dimensional simple cubic lattice. Let us first consider the two dimensional square lattice.

5.2 Two dimensional square lattice

5.2.1 The system

We take a two dimensional square lattice and randomly 'disallow' (or assign 'empty' state to) its sites with a certain probability $q$. We define our percolating object as a
spatially extended entity of linear size $r$ (in lattice units) consisting of $n(r)$ neighboring allowed sites. We now say that such an object can percolate in the lattice only if none of its $n(r)$ sites overlap with any of the disallowed sites. This means that for such an object to move, the channel must have a minimum width of the order of $r$. Then one can study the standard percolation problem for such an object, such as estimating the threshold, the infinite cluster, the critical exponents etc. As is evident, this system has two parameters: $q$ and $r$, unlike the problem of point object percolation which has a single parameter $p$ (the concentration).

5.2.2 The complementary problem

One can also study the following complementary problem. Let us place obstacles of radius $r$ containing the same $n(r)$ sites with a suitably defined center at random locations with probability $q$. We now treat the remaining sites as 'allowed' (or 'occupied') and study the standard site percolation problem for point objects (the points here represent the centers of the percolating objects).

It can be seen that the two problems are essentially equivalent if the following conditions are met: Firstly, the centers of the finite-sized objects or obstacles lie on a lattice site and not on an empty space between neighboring sites. Secondly, the objects or obstacles themselves have the same underlying symmetry as that of the lattice. Finally, the obstacles are allowed to overlap. As mentioned in the following subsection, we shall be considering the percolating objects with spherical symmetry having radius $r$ (in lattice units). All the above three conditions are automatically fulfilled for these objects with their geometrical centers lying on lattice sites. We have observed that it is numerically more convenient to study the problem with obstacles as it involves less computer runtime. Therefore, we make use of the abovementioned equivalence rule to study this complementary problem for all the calculations presented in this chapter.
5.2.3 The percolating object

We consider the percolating objects as circular disks with different radii \( r \) and their centers on the lattice sites. We concentrate on the first five radii \( r = 1, \sqrt{2}, 2, \sqrt{5}, \text{and} \sqrt{8} \) (in lattice units), and call them type 1, 2, 3, 4, and 5 objects respectively. The first three columns of Table 5.1 list these objects and the number \( n(r) \) of allowed sites contained in them. The point object percolation case \( r = 0 \) with the corresponding \( n(r) = 1 \) is also shown here for comparison, which we accordingly call the 'type 0' object.

Table 5.1: The quantities \( n(r), q_c, q_c^l, p(q_c, r), \beta, \gamma, D \) and \( \tau \), for different radii \( r \) in two dimensional square lattice. With \( r > 0 \) error margins for \( q_c, \beta, \gamma, D \) and \( \tau \) are \( \pm 0.0001, \pm 0.01, \pm 0.1, \pm 0.01 \) and \( \pm 0.05 \) respectively.

<table>
<thead>
<tr>
<th>Type</th>
<th>( r )</th>
<th>( n(r) )</th>
<th>( q_c )</th>
<th>( q_c^l )</th>
<th>( p(q_c, r) )</th>
<th>( \beta )</th>
<th>( \gamma )</th>
<th>( D )</th>
<th>( \tau )</th>
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</thead>
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<td>-</td>
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</tr>
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<td>0.087</td>
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<td>2.39</td>
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<td>2.04</td>
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</tbody>
</table>

We define a cluster for this system as a group of allowed sites with the following properties: centers of the percolating objects can be placed on these sites, and, these sites are connected through their nearest neighbors. We say that a lattice is percolating for a given \( q \) and \( r \) when there exists at least one cluster spanning the lattice end to end (a so called 'infinite cluster'). We define the threshold probability \( q_c \) such that for \( q > q_c \) the lattice ceases to be percolating. It is obvious that \( q_c \) is a function of the radius \( r \). It is to be noted that in Chapter 4 we have defined the threshold \( p_c \) for the point object percolation problem through the probability \( p \) of occupancy, whereas here the threshold \( q_c \) is defined through the probability \( q \) of disallowance (or emptiness).
5.3 Results and discussion

Let us now present the results obtained for the two dimensional square lattice. We have employed periodic boundary conditions for our system. This is necessary, since otherwise the finite-sized objects are not well-defined at and near the lattice boundary. Most of the data are taken for lattices with linear sizes \( L = 10, 20, 40, 80, 160, 320, 640, 1280, 2560, \) and \( 5120, \) and on two occasions we have gone as high as \( L = 10240, \) and once even \( 50000. \) The probability \( q \) is varied between 0 and 1. For each such value of \( q, \) the data are averaged over \( 100000, 50000, 20000, 10000, 5000, 2000, 500, 200, 100, 50, 20, \) and \( 4 \) number of realizations of randomly generated disallowed sites, corresponding to the values of \( L \) mentioned above.

5.3.1 Percolation threshold \( q_c \)

In order to obtain the percolation threshold \( q_c, \) we gradually increase \( q \) from zero to unity and estimate, for each \( q, \) the number of realizations of the lattice which support a percolating (or infinite) cluster. Let \( F^{(2)}(q) \) denote this number, normalized by the total number of realizations (superscript '2' denotes the lattice dimensionality). Fig. 5.1 shows the variation of \( F^{(2)}(q) \) with \( q, \) for different lattice sizes \( L \) and for the type 1 \((r = 1)\) object. We observe that the plot exhibits an approach towards a step function of the form

\[
F(q) = \begin{cases} 
1 & \text{for } q < q_c, \\
0 & \text{for } q > q_c,
\end{cases}
\]

as \( L \) increases to \( \infty \) (this function is without a superscript since this is a common feature for a lattice of any dimension). This behavior remains essentially the same for all other values of \( r \) that we have considered, with the difference that the threshold \( q_c \) reduces as \( r \) increases, which can be seen in Table 5.1.

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Figure 5.1: Plot of percolating fraction $F^{(2)}(q)$ versus $q$, for different lattice sizes $L$ and with $r = 1$ (type 1). $L = 2560$ graph not shown for clarity.

The data of Fig. 5.1 obey a finite (lattice) size scaling relation, near the threshold $q_c$, of the form

$$F^{(2)}(q, L) \rightarrow L^{-b} F(L^a | q - q_c|),$$

(5.2)

where $a$ and $b$ are the scaling exponents, and $F$ is the scale-independent function given by (5.1). By trying out different values of $a, b$ and $q_c$, we observe that for a proper combination of these three, all the graphs of Fig. 5.1 indeed collapse onto a single function which is almost a step function of the form (5.1). This can be seen in Fig. 5.2. Similar scaling is observed for all other types of objects. The fourth column of Table 5.2 shows the values of $a, b$ and $q_c$ for different values of $r$, that we have obtained by the above method. We also mention the associated error margins. Thus
we get an estimate of $q_c$. The same values appear in the fourth column of Table 5.1. Table 5.2 shows that both the threshold $q_c$ and the exponent $a$ exhibit a monotonic decrease in their values as the radius $r$ of the objects increases, whereas the exponent $b$ remains equal to zero for all $r$.

One can also obtain $q_c$ in another way. Fig. 5.1 shows that the graphs are approximately linear for values of $F^{(2)}(q)$ between 0.3 and 0.7. We consider the $q$-intercepts of these lines, and plot them against $1/L$. This is shown in Fig. 5.3. The extrapolated value of this intercept, as $1/L \to 0$, yields $q_c$. We denote these estimates by $q_c^1$, and list them in the fifth column of Table 5.1. These values are sufficiently close to the earlier estimates (shown in the fourth column of the same table). However, the accuracy of this graphical method is limited.

Figure 5.2: Plot of scaled function $L^bF^{(2)}$ against scaled variable $L^a(q-q_c)$, for the graphs of Fig. 5.1. Range of scaled abscissa corresponds to $q \in [0, .23]$. 
Table 5.2: The scaling exponents $a$, $b$, and the threshold $q_c$, for different $r$ in two dimensional square lattice. Error margins for $a$, $b$ and $q_c$ are $\pm 0.02$, $\pm 0.02$ and $\pm 0.0001$ respectively.

<table>
<thead>
<tr>
<th>Type</th>
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<th>$F^{(2)}$</th>
<th>$F^{(2)}_\infty$</th>
<th>$S^{(2)}$</th>
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<td></td>
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<td>0.1153</td>
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</tr>
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<td>$b$</td>
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<tr>
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<td></td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td>$q_c$</td>
<td>0.0358</td>
<td>0.0358</td>
<td>0.0358</td>
</tr>
</tbody>
</table>

In the spirit of the point object percolation problem one can calculate the probability $p$ that an arbitrary lattice site is allowed to be the center of a percolating object. For an object of radius $r$ containing $n(r)$ allowed sites, two factors contribute to this probability: $(1 - q)$ for the central site itself, and $(1 - q)^{n-1}$ for the symmetrically placed $(n - 1)$ neighbors. Thus, the required probability is

$$p(q, r) = (1 - q)^{n(r)}. \tag{5.3}$$

Using the values of $n(r)$ and $q_c$ as shown in Table 5.1, we calculate $p(q_c, r)$ at the threshold $q_c$ for various object types, and list them in the sixth column of the same table. For $r = 0$ (point percolation case) we have $p(q_c, 0) \equiv p_c = 0.5927$ (obtained from Table 4.1).
5.3.2 Critical exponents $\beta$ and $\gamma$

Exponent $\beta$

As in the standard point object percolation problem, we find clusters of all possible sizes for our system. We have introduced the strength $P_\infty$ of the infinite cluster in Chapter 4. This is defined as the number of occupied sites constituting the infinite cluster, normalized by the total number of lattice sites. In a similar vein, we study the distribution of the sizes of the largest clusters, averaged over many lattice realizations, as $q$ is varied gradually. We denote this quantity as $P_\infty^{(2)}$. Fig. 5.4 plots the variation of $P_\infty^{(2)}$ with $q$ for different lattice sizes and with radius $r = 1$. As expected, the plot exhibits a sharp fall at the threshold $q_c$ for large $L$. Similar behavior has been observed for all the other object types.
Figure 5.4: Plot of maximum size $P_\infty^{(2)}(q)$ versus $q$, for different $L$ as in Fig. 5.1 and with $r = 1$.

We have observed a finite-size scaling behavior similar to (5.2), given by

$$P_\infty^{(2)}(q, L) \to L^{-b} P_\infty(L^a |q - q_c|),$$  \hspace{1cm} (5.4)$$

where $P_\infty$ is the scale-independent function. Fig. 5.5 shows that the decay profiles of the graphs of Fig. 5.4, when properly scaled, coincide onto each other near $q_c$. The fifth column of Table 5.2 shows the values of the scaling exponents $a, b$, and also the threshold $q_c$ of (5.4), for all types of objects as obtained by this scaling scheme. It is seen that the estimates of $a$ and $q_c$ yield the same values as those obtained earlier. However, $b$ is now nonzero and is independent of $r$.

The critical exponent $\beta$ has been defined for point object percolation in (4.15). It has been shown there that $[\sum_s s n_s]_{\text{sing}} \propto P_\infty$. In order to obtain $\beta$ for our system,
we have studied the nature of the decay of the graphs of Fig. 5.4 near $q_c$. We see that this obeys a power law of the form

$$P_{\infty}^{(2)}(q) \propto (q_c - q)^{\beta}.$$  

(5.5)

We have estimated the exponent $\beta$ of (5.5) for different radii $r$. In the seventh column of Table 5.1 we list these $\beta$ values. The associated error margin is ±0.01. We see that an accurate estimation of $\beta$ depends on the factor $(q_c - q)$, and is thus sensitive to reliable determination of the threshold $q_c$. Therefore $q_c$ must be determined as accurately as the largest lattice size $L$ permits. We have also included the value of $\beta$ for the point object (taken from Table 4.2) for the sake of comparison.
Exponent $\gamma$

In Chapter 4 we have defined the average size $S$ of the clusters, excluding the infinite cluster, through the Eq. (4.7). We have studied the distribution of this quantity, normalized by the total number of lattice sites and denoted by $S^{(2)}$, with $q$ for all values of $r$. Fig. 5.6 shows the variation of $S^{(2)}(q)$ with $q$ for the same set of values of $L$ as in the earlier figures, and with $r = 1$.

$L$ as in the earlier figures, and with $r = 1$. $S^{(2)}$ clearly exhibits a diverging trend near $q_c$ from both sides for large $L$. The same divergence has also been observed with the other object types.

This function exhibits a similar finite-size scaling as seen in the earlier two cases.
with a form

\[ S^{(2)}(q, L) \rightarrow L^{-b} S(L^a|q-q_c|), \quad (5.6) \]

\( S \) being the scale-independent function. This is evident in Fig. 5.7 which shows a

Figure 5.7: Plot of scaled function \( L^b S^{(2)} \) against scaled variable \( L^a(q-q_c) \), for the graphs of Fig. 5.6. Range of scaled abscissa corresponds to \( q \in [0,.23] \).

collapse of all the graphs of Fig. 5.6 onto one another for the proper combination of the parameters \( a, b \) and \( q_c \) in (5.6). We list these values for all \( r \) in the sixth column of Table 5.2. The values of \( a \) and \( q_c \) are found to be the same as those in the previous two columns, whereas \( b \) takes a different value from the other estimates and is also independent of \( r \).

We have estimated the critical exponent \( \gamma \), as defined for the point object percolation case in the relation (4.16). From Eq. (4.7) we know that, near \( q_c \), \( \sum_s s^2 n_s \text{sing} \propto \)
We study the divergence of $S^{(2)}$ near the threshold $q_c$. This is a power law:

$$S^{(2)}(q) \propto |q - q_c|^{-\gamma}.$$  
(5.7)

The exponent $\gamma$ of (5.7) has been estimated for all the radii $r$ under consideration. We show these estimates in the eighth column of Table 5.1. The error is ±0.1. Like in the case of $\beta$, the accurate determination of $\gamma$ depends on the accuracy with which $q_c$ is obtained. We also show the corresponding value for the point object case (taken from Table 5.2) for comparison.

This brings us back to the important question of the dependence, if any, of the critical exponents, and hence the universality class, on the size $r$ of the percolating objects. We shall see later that for a simple one dimensional infinite lattice the exact calculations show that $\gamma$ does not depend on $r$. As for the two dimensional lattice, Table 5.1 shows that the estimated values of both $\beta$ and $\gamma$ for different radii $r$ are the same within their respective errors. This, of course, does not automatically rule out any such dependence. In order to make any definitive statement one must estimate these exponents with a much higher degree of accuracy. It has already been pointed out that this accuracy depends on the precision of $q_c$ measurement, which in turn depends crucially on the size $L$ of the lattice itself and increases with larger $L$. However, the computer runtime also increases drastically with $L$, in addition to the fact that larger $L$ occupies bigger memory blocks. We have carried out the entire set of calculations that are reported in this chapter on a Silicon Graphics workstation with a 64-bit R8000 microprocessor and 64 megabytes of RAM (random access memory). Any further reduction of the error margin will require the use of much bigger and faster machines than that available at our disposal. We do hope that with the access to improved computational facilities this issue will be settled soon.
5.4 Fractality of the percolating cluster

We have seen in Chapter 4 that at the threshold \( p_c \) the largest cluster takes on a fractal shape, and has an associated fractal dimension \( D \) given by the relation (4.3), which is rewritten here:

\[
 s_l \propto L^D, \quad (L \to \infty).
\]

We have studied the variation of the size \( s_l \) of the largest cluster at the threshold \( q_c \), averaged over many lattice realizations, with the lattice size \( L \). Fig. 5.8 shows the plot of \( s_l \) versus \( L \) on a log-log scale, for all the five different radii \( r \) of the objects. We see a clear straight line extending for the entire range of \( L \), thereby validating the
relation (4.3) for our system also. Moreover, all the graphs corresponding to different object types are parallel to each other and they almost coincide. This indicates that within the limit of accuracy the fractal dimension $D$ is same for all $r$. Values of $D$ are listed in the ninth column of Table 5.1. The associated error margin is ±0.01. We have also shown $D$ for the point object case [1] for comparison. It is observed that within the prescribed error limits the value of $D$ is independent of $r$. Like in the cases of the exponents, better computational facilities are needed to make a more precise measurement of $D$ and investigate its possible dependence on $r$.

5.5 Fisher exponent $\tau$

We have introduced the Fisher exponent $\tau$ in the relation (4.12), as the exponent for the asymptotic power law decay of the number $n_s(p_c)$ of clusters with their size $s$ at the threshold $p_c$. In a similar manner we investigate the distribution of the number $n_s(q_c)$ with $s$ at the threshold $q_c$, for all the radii $r$ and with a large enough lattice (we have taken $L = 50000$ for this study). As suggested in Ref. [1], we combine different neighboring cluster sizes into bins corresponding to the intervals $[2^n, 2^{n+1}-1]$ (with $n = 0, 1, 2, \ldots$), the bin size increasing exponentially with $n$. We then plot the result against the geometric mean $s$ of the two border sizes of this bin. Thus the data size is manageable even with a very large $L$.

Fig. 5.9 shows the variation of $n_s(q_c)$ with the size $s$ of the clusters at the threshold $q_c$, on a log–log scale, for different radii $r$. The plot exhibits a power law for a range of values of $s$, with the form:

$$n_s(p_c) \propto s^{-\tau}.$$  \hfill (5.8)

For large $s$ all the graphs for different object types merge onto each other, thereby implying that the exponent $\tau$ is independent of $r$ within the obtainable accuracy limit. We list the values of $\tau$ in the last column of Table 5.1. The error margin for these
estimates is ±0.05. We have also shown the value for $r = 0$. Within the error the exponent appears to be independent of $r$. As in the earlier cases, one has to work with better computers to find any possible dependence of $r$ on $r$.

With this we conclude the discussion of our percolation problem on the two dimensional square lattice. Let us now turn to the other lattice: A three dimensional simple cubic lattice. We shall soon see an interesting application for this model.

### 5.6 Three dimensional simple cubic lattice

For a three dimensional simple cubic lattice we have considered seven different types of spherical percolating objects, with their respective radii $r$ and the number $n(r)$ of
Table 5.3: The quantities $n(r)$, $q_c$, $q_{c_1}$, $p(q_c, r)$, $\beta$ and $\gamma$, for different $r$ in three dimensional simple cubic lattice. With $r > 0$ the error margins for $q_c$, $\beta$, and $\gamma$ are $\pm 0.0001$, $\pm 0.05$ and $\pm 0.5$ respectively.

<table>
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<tr>
<th>Type</th>
<th>$r$</th>
<th>$n(r)$</th>
<th>$q_c$</th>
<th>$q_{c_1}$</th>
<th>$p(q_c, r)$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
</tr>
</thead>
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<td>1.90</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>33</td>
<td>0.0591</td>
<td>0.059</td>
<td>0.1340</td>
<td>0.32</td>
<td>2.00</td>
</tr>
<tr>
<td>5</td>
<td>$\sqrt{5}$</td>
<td>57</td>
<td>0.0355</td>
<td>0.036</td>
<td>0.1247</td>
<td>0.31</td>
<td>1.95</td>
</tr>
<tr>
<td>6</td>
<td>$\sqrt{6}$</td>
<td>81</td>
<td>0.0285</td>
<td>0.029</td>
<td>0.0961</td>
<td>0.38</td>
<td>1.80</td>
</tr>
<tr>
<td>7</td>
<td>$\sqrt{8}$</td>
<td>93</td>
<td>0.0242</td>
<td>0.024</td>
<td>0.1025</td>
<td>0.33</td>
<td>1.82</td>
</tr>
</tbody>
</table>

allowed sites as shown in Table 5.3. The ‘type 0’ object ($r = 0$) is also mentioned for comparison. The lattice sizes that we have studied are $L = 10, 20, 40, 80, 160$ and 250. For each value of the probability $q$ the data are averaged over 100000, 30000, 10000, 2000, 200, and 10 realizations for the corresponding values of $L$. We have employed periodic boundary conditions for this lattice due to the reasons stated earlier.

As in the case of a two dimensional lattice, we define the fraction $F_3^{(3)}(q)$ of percolating realizations (the superscript ‘3’ reminds us that the lattice is three dimensional) and study its variation with $q$ for different values of $L$ and for all $r$. Fig. 5.10 shows the results of our observation for different $L$ and for the ‘type 1’ object ($r = 1$). We see, quite similar to Fig. 5.1, an approach towards a step function of the form (5.1) for larger $L$. The same behavior is seen for all the other radii $r$, with the only difference that $q_c$ decreases with increasing $r$ as shown in the fourth column of Table 5.3.

The graphs of Fig. 5.10 satisfy the finite (lattice) size scaling relation (5.2). The fourth column of Table 5.4 shows the values of the scaling exponents $a, b$ and the threshold $q_c$ for the function $F_3^{(3)}$. The associated error margins are also mentioned. Like in the case of a two dimensional lattice, $a$ decreases steadily with increasing $r$, so
Figure 5.10: Plot of percolating fraction $F^{(3)}(q)$ versus $q$, for different lattice sizes $L$ and with $r = 1$ (type 1).

does $q_c$, whereas $b$ remains zero throughout. The same $q_c$ values are quoted again in the fourth column of Table 5.3. Table 5.3 also lists the $q_c^1$ values, obtained by plotting the $q$–intercepts against $1/L$ which yields a graph very similar to Fig. 5.3. These two sets of estimates for $q_c$ agree fairly well.

In the sixth column of Table 5.3 we list the values of $p(q_c, r)$, obtained by using Eq. (5.3). For $r = 0$ (point object) we have $p(q_c, 0) \equiv p_c = 0.3116$ (taken from Table 4.1). One interesting point to be noted from both Table 5.1 and Table 5.3 is that the objects with finite $r$ are percolating at lower values of $p$ than the point objects, irrespective of the lattice dimensionality. The reason for this becomes clear if we look at the equivalent problem of obstacles. Here the sites are disallowed in clumps rather than in a homogeneous manner (which is the case with point percolation) throughout
Table 5.4: The scaling exponents \( a, b, \) and the threshold \( q_c, \) for different \( r \) in three dimensional simple cubic lattice. Error margins for \( a, b \) and \( q_c \) are \( \pm 0.02, \pm 0.02 \) and \( \pm 0.0001 \) respectively.

<table>
<thead>
<tr>
<th>Type</th>
<th>( r )</th>
<th>((a, b, q_c))</th>
<th>( F^{(3)} )</th>
<th>( P^{(3)}_{\infty} )</th>
<th>( S^{(3)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>( a ) \qquad 1.17</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.1921</td>
<td>( a ) \qquad 1.17</td>
</tr>
<tr>
<td>2</td>
<td>( \sqrt{2} )</td>
<td>( a ) \qquad 1.10</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0912</td>
<td>( a ) \qquad 1.10</td>
</tr>
<tr>
<td>3</td>
<td>( \sqrt{3} )</td>
<td>( a ) \qquad 1.05</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0752</td>
<td>( a ) \qquad 1.05</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>( a ) \qquad 1.00</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0591</td>
<td>( a ) \qquad 1.00</td>
</tr>
<tr>
<td>5</td>
<td>( \sqrt{5} )</td>
<td>( a ) \qquad 0.99</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0355</td>
<td>( a ) \qquad 0.99</td>
</tr>
<tr>
<td>6</td>
<td>( \sqrt{6} )</td>
<td>( a ) \qquad 0.98</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0285</td>
<td>( a ) \qquad 0.98</td>
</tr>
<tr>
<td>7</td>
<td>( \sqrt{8} )</td>
<td>( a ) \qquad 0.97</td>
<td>( b ) \qquad 0.50</td>
<td>( q_c ) \qquad 0.0242</td>
<td>( a ) \qquad 0.97</td>
</tr>
</tbody>
</table>

the lattice, thereby leaving more channels open for percolation. This effect becomes more pronounced with increasing radius. As an example, Table 5.3 shows that in three dimension, for \( r = \sqrt{6}, \) the lattice percolates even with the removal of more than 90% of its sites \( (p(q_c, r) = 0.0961 \text{ for } r = \sqrt{6}) \) ! This also brings out another feature. The dependence of \( p(q_c, r) \) on \( r \) is not monotonous; it exhibits occasional peaks (in Table 5.1 one peak is at \( r = 2 \) and in Table 5.3 two peaks can be seen at \( r = 2 \) and \( \sqrt{8} \)). This feature is clearly seen in Fig. 5.11, which shows \( p(q_c, r) \) against \( r \) for both
Figure 5.11: Plot of the probability \( p(q, r) \) versus radius \( r \), for both two (\( d = 2 \)) and three (\( d = 3 \)) dimension.

two and three dimensional lattices.

Fig. 5.12 shows the variation of the size \( P_{\infty}^{(2)}(q) \) of the largest cluster with \( q \), for different \( L \) and with \( r = 1 \). The plot is similar to Fig. 5.4. This plot also obeys finite size scaling. We show the scaling parameters \((a, b, q_c)\) in the fifth column of Table 5.4. We see that \( a \) and \( q_c \) remain the same as in the earlier estimate, whereas \( b \) takes on a nonzero value independent of \( r \).

Close to \( q_c \), \( P_{\infty}^{(3)} \) scales with \( q \) in a manner similar to that in (5.4):

\[
P_{\infty}^{(3)}(q) \propto (q_c - q)^\beta.
\]  

(5.9)

We have estimated the critical exponent \( \beta \), which we show in the seventh column of Table 5.3. We also mention the value corresponding to the point object case for
Figure 5.12: Plot of maximum size $P^{(3)}_\infty(q)$ versus $q$, for different lattice sizes $L$ as in Fig. 5.10 and with $r = 1$ (type 1).

comparison. The error margin of our estimate is ±0.05 which is appreciably larger than that for the two dimensional lattice. This is because the highest $L$ that we could consider, given the limitation of computational resources, is just 250. A much larger lattice must be taken for better accuracy.

In Fig. 5.13 we plot the average size $S^{(3)}(q)$ of the finite clusters, normalized by the total number of lattice sites, against $q$ for different $L$ and the 'type 1' object. We observe the same behavior for all other radii $r$. As in Fig. 5.6, we see a similar divergence of $S^{(3)}$ at $q_c$ from either side for large $L$. We observe finite size scaling for this plot similar to (5.6), and show the scaling parameters $(a, b, q_c)$ in the last column of Table 5.4. Values of $a$ and $q_c$ remain the same as that of the other two estimates, but $b$ is different and does not depend on $r$.  

98
Figure 5.13: Plot of average size $S^{(3)}(q)$ versus $q$, for various $L$ as in Fig. 5.10 and with $r = 1$ (type 1).

$S^{(3)}$ diverges near $q_c$ in a manner similar to that in (5.7): 

$$S^{(3)}(q) \propto |q_c - q|^{-\gamma}.$$  \hspace{1cm} (5.10)

We have estimated the exponent $\gamma$ and show the values in the last column of Table 5.3. The value for $r = 0$ is also listed for comparison. The error associated with these estimates is $\pm 0.5$ which is much higher than that for the two dimensional estimates for reasons stated earlier.

As for the two dimensional lattice, here also we could not ascertain any possible dependence of the exponents on $r$ because of the appreciable error margins. Much better computational facilities are necessary to carry out more precise measurements.

We now come to an interesting experimental situation in which one can make a
possible application of our model on the three dimensional lattice.

5.7 Transport in impurity–doped ceramic

5.7.1 The experiment

In a recent experiment [16], Ogale and his associates have studied the effect of Fe–impurity on the transport properties of the ceramic $\text{La}_{0.75}\text{Cao.25Mn}_3\text{O}_3$. The concentration $x$ of the dopant Fe in $\text{La}_{0.75}\text{Cao.25Mn}_{1-x}\text{Fe}_x\text{O}_3$ has been varied between 0.0 and 0.05, and the resistivity $\frac{\rho_x}{\rho(x=0)}$ of the material measured at room temperature for each value of $x$. Fig. 5.14 reveals an interesting dependence of $\frac{\rho_x}{\rho_0}$ on $x$. We see

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.14}
\caption{Plot of resistivity $\frac{\rho_x}{\rho_0}$ versus concentration $x$ of Fe–impurity at room temperature, on a log–linear scale.}
\end{figure}

that for a small change of concentration $x$ from $x = 0.0425$ to 0.045, the resistivity
jumps by a factor of about 22, as against a factor of only about 6 for large increase of x from 0.01 to 0.0425. It has been emphasized that the x-ray analyses of the samples do not show any structural phase transition over the entire range of x values.

The following observations are significant in understanding the underlying physical aspect of the abovementioned resistivity profile: Firstly, the isomer shift measurement shows that the Fe ions are present in the 3+ state only. The most favorable sites for these Fe ions to occupy in the perovskite (Mn–O–Mn) matrix is that of Mn because of their compatible ionic radii and characteristic d–shell chemistry. It is known [23] that Fe$^{3+}$ cannot act as a double exchange partner for Mn$^{4+}$ since their energy bands have only a slight overlap. Secondly, for x = 0.0425 and 0.045 the measurement of the magnetization data (M versus H) shows a close agreement, whereas Fig. 5.14 exhibits a dramatic difference of their transport data. This, along with the previous observation, suggests that Fe atoms do not directly participate in transport process which occurs primarily through the Mn$^{3+}$–O–Mn$^{4+}$ network. Finally, the average Fe–Fe separation is found to decrease to below 3 lattice units for x > 0.04 where the jump in the resistivity occurs. This observation implies that a quasiparticle excitation, presumably a magnetic polaron, with a finite spread of its wave function of this order must be associated with the double exchange process (it may be noted that experimental as well as theoretical findings have already suggested the role of polarons as possible carrier of transport in the oxide perovskite systems [17, 18, 19, 22]).

5.7.2 Percolation as a model

The emerging physical picture that for x > 0.04 the Fe ions prevent the transport of polarons, which are finite–sized quasiparticles, and thus cause the jump in the resistivity has inspired us to interpret this phenomenon as a percolation transition for the polarons. We use our percolation problem on the three dimensional simple cubic lattice as a model for this phenomenon, where the finite–sized objects simulate the
polarons.

Our model offers an estimate of the size of the polarons in the following way. Identifying the concentration $x$ of the impurity Fe ions with the probability $q$, we see from the fourth column of Table 5.3 that $x \approx 0.0425$, which falls between the $q_c$ values 0.0355 and 0.0591, should correspond to a radius $r$ between 2 and $\sqrt{5}$ lattice unit for the polaron. This is somewhat higher than the abovementioned experimental estimate of the average Fe–Fe separation of about 3 lattice units, which suggests a radius of one and a half lattice units or less (assuming the polarons to be spherical in shape). This difference may result because of the fact that the Fe ions are more likely to be distributed randomly, rather than in a homogeneous manner, in the lattice. This leaves many channels open for transport and thereby allows objects with bigger radii to pass through. At the same time we appreciate that ours is essentially a classical model and therefore corrections due to quantum effects are expected. However, we note that for this experiment the model that we propose is exact in geometrical sense because of the underlying lattice structure of the ceramic solid, unlike a continuum percolation model (as discussed in the previous chapter) which can only be approximate (in geometrical sense) and cannot yield interesting information such as the radius of the polarons.

There is another way in which our model can be used. If the size of the polarons is already established independently from other measurements, this may be used in our estimates to obtain a bound on the concentration $x$ of the impurity which can be added to the sample without changing its physical properties significantly.

5.8 Some exact results

In this section we try to obtain [21] some exact results for our model on the same two lattices as used in Chapter 4: A one dimensional infinite linear chain, and the Bethe lattice.
5.8.1 One dimensional infinite lattice

In this lattice one can consider a percolating object of any size \( r \) with suitably chosen center on a site. For an object with odd \( n(r) \) the natural choice for the center is the middle site and we get

\[
n(r) = 2r + 1.
\]  

(5.11)

Three factors contribute to the number \( n_s \) of \( s \)-clusters: The probability \( (1 - q)^s \) that \( s \) sites are allowed; the probability \( (1 - q)^{n(r)-1} \) that sufficiently close sites on its either side are also allowed; and the probability \( q^2 \) that denotes the boundary of the cluster. Thus we get the normalized cluster number as:

\[
n_s(q, r) = q^2 (1 - q)^{s+n(r)-1}.
\]  

(5.12)

For \( q = 0 \) all sites in the lattice are allowed. For every \( q > 0 \) the number of disallowed sites in a lattice of size \( L \) varies as \( qL \) which goes to infinity as \( L \to \infty \). In other words, there is no percolating cluster (in this case the entire chain with all allowed sites) for \( q > 0 \). Thus the threshold is

\[
q_c = 0.
\]  

(5.13)

The total number of finite clusters, \( \sum_s s n_s \), can be obtained by using Eq. (5.12) as follows:

\[
\sum_s s n_s = q^2 (1 - q)^{n(r)-1} \sum_s s(1 - q)^s
\]

\[
= q^2 (1 - q)^{n(r)} \sum_s [\frac{d}{dq}((1 - q)^s)]
\]

\[
= q^2 (1 - q)^{n(r)} [\frac{d}{dq}(\sum_s (1 - q)^s)]
\]

\[
= q^2 (1 - q)^{n(r)} [\frac{d((1 - q)/q)}{dq}].
\]
This yields the expression

\[ \sum_s s \, n_s = (1 - q)^{n(r)}, \quad (q > q_c). \]  

(5.14)

One can also get this relation in a more direct way. Clearly this sum is just equal to the probability that an arbitrary site is allowed: \( \sum_s s \, n_s = p(q, r) \). Using Eqs. (5.3) we get back (5.14).

The average size \( S^{(1)} \) can also be obtained similarly. The numerator of Eq. (4.7) takes the form:

\[ \sum_s s^2 \, n_s = q^2 (1 - q)^{n(r) - 1} \sum_s s^2 (1 - q)^s \]

\[ = q^2 (1 - q)^{n(r) + 1} \left( \frac{d}{dq} \right)^2 \sum_s (1 - q)^s \]

\[ = 2(1 - q)^{n(r) + 1}/q. \]

Along with the denominator of (4.7), given by Eq. (5.14), we get

\[ S^{(1)} = 2 \left( \frac{1 - q}{q} \right), \quad (q > q_c). \]

(5.15)

We note that Eq. (5.15) signifies a divergence of \( S \) near \( q_c = 0 \) as \( S^{(1)} \propto |q_c - q|^{-\gamma} \), with \( \gamma = 1 \), as in the case of point object percolation. This shows that in a one dimensional infinite lattice the critical exponent \( \gamma \) does not depend on \( r \).

It can be seen that for \( r = 0 \), \( n(r) = 1 \), which along with Eq. (5.3) reduces Eqs. (5.12), (5.14) and (5.15) to their point object counterparts (4.4), (4.6) and (4.8).

5.8.2 The Bethe lattice

We have seen in Chapter 4 that in a Bethe lattice with \( z \) neighbors, each bond leads to a new site from which \( z - 1 \) new bonds emanate. Thus the number of connected allowed sites constituting a percolating object of radius \( r \) can be given as

\[ n(r) = 1 + z + z(z - 1) + \cdots + z(z - 1)^{r-1} \]
\[ r - 1 = l + z \left[(z - l)^r - 1\right] = (z - 1)\left[z(z - 1)^{r-1} - 1\right]. \] (5.16)

In order to calculate the percolating threshold and other quantities for the Bethe lattice, it is more convenient to formulate the problem of obstacles. Starting from an allowed site, we find \( z - 1 \) new bonds emanating from it, leading to as many new neighbors. Each of these neighbors is allowed if none of the sites distance \( r \) apart from it, except along the original direction, contains the center of an obstacle (the sites within this distance must not have contained obstacle center in order for the starting site to be allowed). There are \( (z - 1)^r \) such sites, each of which contains an obstacle center with a probability \( q \). So for the continuity along the infinite path we have the relation

\[ (z - 1)(1 - q)^{(z-1)^r} = 1, \]

which gives us the expression for the threshold

\[ q_c = 1 - \frac{1}{(z - 1)^{1/(z-1)^r}}. \] (5.17)

The number \( n_s(q, r) \) of \( s \)-clusters can be calculated by the same logic as used for the one dimensional lattice. It can be seen that \( s(z - 2) + 2 \) outward branches emanate from an \( s \)-cluster of any shape (to prove this: We note that for \( s = 1 \), the number of branches is just \( z \); for \( s = 2 \) it is \( z + z - 2 \); for \( s = 3 \) it is \( z + 2(z - 2) \), and likewise for a cluster with \( s \) sites we have the number \( z + (s - 1)(z - 2) = s(z - 2) + 2 \). It is easy to see that adding a single allowed site anywhere in a cluster increases the number by \( z - 2 \). Now, \( s \) sites and all the sites up to the distance \( r \) along each of these \( s(z - 2) + 2 \) branches must not contain an obstacle center. Each branch has \( (n(r) - 1)/z \) sites up to a distance \( r \). So the total number of these sites is \( S_i = s + (s(z - 2) + 2)(n(r) - 1)/z, \)
and the probability is \( (1 - q)^{St} \). This should be multiplied by the probability that along each branch there is at least one obstacle center at a distance \( r + 1 \). Each branch has \((z - 1)^r\) sites at a distance \( r + 1 \), and they will not have obstacle centers with a probability \( (1 - q)^{(z-1)r} \). So the probability that there is at least one such obstacle center is \( 1 - (1 - q)^{(z-1)r} \). There are \( s(z - 2) + 2 \) such branches. Therefore, the total probability for a cluster of size \( s \), \( n_s \), is given by

\[
 n_s(q,r) = (1 - q)^{St} \left[ 1 - (1 - q)^{(z-1)r} \right]^{s(z-2)+2} \\
= (1 - q)^{s(s(z-2)+2)} (n(r)-1)^s \left[ 1 - (1 - q)^{(z-1)r} \right]^{s(z-2)+2}. \quad (5.18)
\]

### 5.9 Summary

In this chapter we have discussed a new percolation phenomenon – percolation of finite-sized objects – on a two dimensional square lattice and a three dimensional simple cubic lattice. We observe a well-defined percolating threshold for our model, the threshold depending on the radius of the percolating objects. There exists a scaling due to the finite size of the lattice, thereby allowing us to obtain important quantities for infinite systems from finite samples. We have estimated the critical exponents \( \beta \) and \( \gamma \) for our system. The presence of an appreciable error margin does not allow us to conclude about any possible dependence of these exponents on the size \( r \) of the percolating objects. We have discussed an experiment on transport properties of an impurity-doped ceramic, and applied our percolation problem on the three dimensional lattice as a viable model for this experiment. This application allows us to offer an estimate for the size of the magnetic polarons, which are believed to be the carriers for the abovementioned transport. We have also derived some exact relations for a one dimensional infinite lattice and for the Bethe lattice.

This brings us to the end of this chapter. The following chapter, which is also the last chapter of the thesis, summarizes and concludes the entire thesis.
Bibliography


