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Monte Carlo study of percolation on disordered triangular lattices

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ABSTRACT

A simple model for amorphous solids, consisting of a mixed bond triangular lattice with a fraction of attenuated bonds randomly distributed (which simulate the presence of defects in the surface), is studied here by using computational simulation. The degree of disorder of the surface is tunable by selecting the values of (1) the fraction of regular [attenuated] bonds ρ $[1-\rho]$ $(0 \leq \rho \leq 1)$ and (2) the factor r, which is defined as the ratio between the value of the conductivity associated to an attenuated bond and that corresponding to a regular bond $(0 \leq r \leq 1)$. The results obtained show how the percolation properties of the disordered system are modified with respect to the standard random bond percolation problem $(r = 0)$.

1. Introduction

The percolation problem has been a focal point of statistical mechanics research for several decades and the activity in this field is still growing [1–11]. Some aspects of the percolation process like the geometrical phase transitions occurring in the system have gained a particular impetus due to the introduction of techniques like Monte Carlo (MC) simulations and series expansions [12–21]. Despite the number of contributions to this problem, the problem is far from being exhausted.

The central idea of the pure percolation theory is based on finding the minimum concentration of elements (sites or bonds) for which a cluster [a group of occupied sites (bonds) in such a way that each site (bond) has at least one occupied nearest neighbor site (bond)] extends from one side to the opposite one of the system. This particular value of the concentration rate is named *critical concentration or percolation* threshold and determines a phase transition in the system [2]. Thus, in the random percolation model, a single site (or a bond connecting two sites) is occupied with probability ρ. For the precise value $\rho = \rho_c$, the percolation threshold of sites (bonds), at least one spanning cluster connects the borders of the system (indeed, there exists a finite probability of finding n (>1) spanning clusters [22–26]). In that case, a second order phase transition appears at ρ_c which is characterized by well-defined critical exponents.

More general percolation problems can be formulated by introducing a sort of correlation between the occupation probabilities of adjacent sites and bonds which are usually grouped by the named *correlated percolation*. Among them, one of the most studied is the so-called directed percolation, or percolation with a special direction along which the activity can only propagate one way but not the other [27].

Percolation also represents a standard model for a structurally disordered system with a wide range of applications [2–5]. Generalizations of the pure percolation model include surface geometric heterogeneity (like variable distance among neighboring sites or variable connectivity). In this sense, several contributions have been devoted to the analysis of bond disordered lattices [28,29]. Most of these results are compiled in the excellent review paper by Tsallis and de Magalhaes [30]. More recently, the effects of geometric quenched disorder of the substrate on the percolation properties of monomer and dimer adsorbed layers have been studied [31]. In Ref. [31] the disorder was represented by a variable connectivity, as inspired by the problem of percolation on the surface of amorphous solids.

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Nomenclature

r	Ratio between the value of the conductivity associated to an attenuated bond and that corresponding to a regular bond
n	Number of spanning clusters
z	Lattice connectivity
L	Lattice side
M	Total number of lattice sites
B	Total number of lattice bonds
C_i	ith cluster of regular bonds
C_{ij}	Cluster formed by connecting the ith and jth clusters of regular bonds
l_i	ith attenuated bond connecting two clusters of regular bonds
n_a	Number of attenuated bonds interconnecting two clusters of regular bonds
R_L^R	Probability of finding a rightward percolating cluster
R_L^D	Probability of finding a downward percolating cluster
R_L^I	Probability of finding a cluster which percolates both in a rightward and in a downward direction
R_L^U	Probability of finding either a rightward or a downward percolating cluster
R_L^A	Average of R_L^R and R_L^D given by the relation, $R_L^A \equiv \frac{1}{2}\left(R_L^R + R_L^D\right)$
R^{X*}	Intersection point of the curves R_L^X, $(X = I, U,$ and $A)$
m	Total number of simulated samples
m^X	Number of simulated samples for which a percolating cluster of the desired criterion X is found
d	Space dimension
a	Parameter introduced in Eq. (1)
b	Parameter introduced in Eq. (1)
z_{eff}	Effective lattice connectivity

Greek symbols

ρ	Fraction of regular bonds
ρ_c	Percolation threshold or critical concentration of regular bonds
σ	Conductivity of a regular bond
ρ_0	Parameter introduced in Eq. (1)

Other interesting application of the percolation theory is concerned with the study of dispersed ionic conductors [32–34] and micro- and nanocrystalline materials [35–37]. In the first case, a substantial amount of research has concentrated after the discovery by Liang [32] that insulating fine particles with sizes of the order of 1 μm, dispersed in a conductive medium (e.g. Al_2O_3 in LiI), can lead to a conductivity enhancement. This effect has been found to arise from the formation of a defective, highly conducting layer following the boundaries between the conducting and the insulating phase. Effectively, the system thus contains three phases. In the case of micro- and nanocrystalline materials, which are prepared by mixing two different powders and pressing them together to a pellet, the grain size of both ionic conductor and insulator can be varied over several orders of magnitude and the system contains two phases.

From the theoretical point of view, amorphous i-phase solids as described above (dispersed ionic conductors $i = 3$, and diphase micro- and nanocrystalline materials $i = 2$) can be represented by i-component impedance network models. In this line of thought, a simplified statistical model for amorphous solids is presented in this contribution. Here, a mixed bond triangular lattice with a fraction of attenuated bonds randomly distributed (which simulate the presence of defects in the surface) is studied by using computational simulation. It is quite obvious that the present model is highly idealized and is not meant to reproduce a particular experimental system such as those mentioned above. However, the intention of this work is (1) to identify and characterize the most prominent features of this particular process, (2) to draw general conclusions concerning how the percolation properties of the disordered system are modified with respect to the standard random bond percolation problem and (3) to stimulate the development of more sophisticated models which can be able to reproduce real experimental situations.

The paper is organized as follows. The basis of the model is described in Section 2. Results are presented and discussed in Section 3. Finally, conclusions are drawn in Section 4.

2. The model

We consider a triangular lattice (connectivity $z = 6$) with $M = L \times L$ sites, $B = 3M$ bonds, and periodic boundary conditions. Each bond can be either a regular bond, characterized by a conductivity σ, or an attenuated bond, characterized

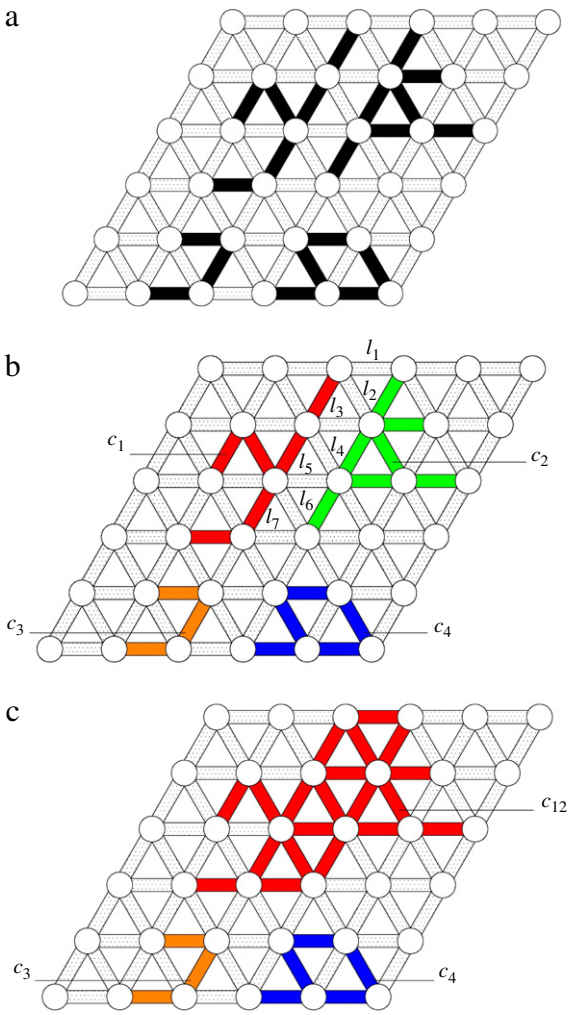

Fig. 1. (a) Schematic representation of a disordered triangular lattice modeled as an array of regular (solid lines) and attenuated (dotted lines) bonds, which are randomly distributed with concentration ρ and $1-\rho$. In this case we set $\rho = 0.5$ and $r = 1/3$. (b) Clusters of regular bonds, denoted as C_i's, constructed on the basis of the standard percolation criterion. Different colors indicate different clusters. (c) State obtained after the application of the criterion of connectivity of two regular clusters. As can be observed, C_1 and C_2 are interconnected by four attenuated bonds (denoted as $l_1 - l_7$). Then, $n_a = 7$, $n_a r > 1$, and consequently, C_1 and C_2 are merged into a bigger cluster (denoted as C_{12}). The rest of the clusters remain invariant.

by a conductivity $r\sigma$, where the factor r varies between 0 and 1. Regular and attenuated bonds are randomly distributed with concentration ρ and $1-\rho$, respectively [see Fig. 1(a)]. In this way, the degree of disorder of the surface is tunable by selecting the values of ρ and r. In the extreme limit where $r = 0$, the standard random bond percolation problem is recovered. On the other hand, a fully connected network is obtained for $r = 1$ and any value of ρ, thus making the problem meaningless.

As mentioned in Section 1, the central idea of the percolation theory is based on finding the minimum concentration of elements for which a cluster extends from one side to the opposite one of the system. In the present model, the standard percolation picture is modified in order to include the effect of the attenuated bonds. The new scheme is built on the basis of three major stages:

(1) The number and size of clusters of regular bonds are determined [see Fig. 1(b)].
(2) Now, the connectivity of two clusters of regular bonds is defined in terms of the weight of the attenuated bonds. The criterion is the following: if two clusters of regular bonds [as for instance C_1 and C_2 in Fig. 1(c)] are interconnected by a number of attenuated bonds, n_a, such that $n_a r \geq 1$, they are merged into a bigger cluster.[1] This procedure is repeated for all the pairs of clusters of regular bonds.

[1] The criterion is based on a simple principle: if the conductivity of the attenuated bonds is decreased n_a times ($r = 1/n_a$), one needs n_a attenuated bonds to reproduce the conduction properties of a regular bond.

(3) The existence of an infinite percolation cluster (cluster connecting the opposite sides of the lattice) is verified on the lattice obtained in step (2).

As was already mentioned, the main goal of this paper is to determine how the percolation properties are modified when a geometric disorder is introduced in the lattice. For this purpose, long scale numerical simulations are required in order to predict the behavior of the system in the thermodynamic limit. A study of the finite-size effects allows us to make a reliable extrapolation to the $L \to \infty$ limit. Details of this study will be given in the next section.

3. Results and discussion

As the scaling theory predicts [12], the larger the system size to study, the more accurate the values of the threshold obtained therefrom. Thus, the finite-size scaling (FSS) theory gives us the basis to achieve the percolation threshold and the critical exponents of a system with a reasonable accuracy. For this purpose, the probability $R = R_L^X(\rho)$ that a lattice composed of B bonds percolates at a concentration ρ of regular bonds can be defined [2]. Here, as in Refs. [13,14], the following definitions can be given according to the meaning of X: (a) $R_L^{R(D)}(\rho)$ = the probability of finding a rightward (downward) percolating cluster, (b) $R_L^I(\rho)$ = the probability that cluster which percolates both in a rightward and in a downward direction, (c) $R_L^U(\rho)$ = the probability of finding either a rightward or a downward percolating cluster, and (d) $R_L^A(\rho) \equiv \frac{1}{2}[R_L^R(\rho) + R_L^D(\rho)] \equiv \frac{1}{2}[R_L^I(\rho) + R_L^U(\rho)]$ [13–18].

The FSS theory allows for various efficient routes to estimate the percolation threshold ρ_c from computational data. One of these methods, which will be used in this case, is from the coverage dependence of $R_L^X(\rho)$, which is independent of the system size for $\rho = \rho_c$. In other words, ρ_c is found from the intersection of the curves $R_L^X(\rho)$ for different values of L, since $R_L^X(\rho_c) = \text{const}$.

These considerations allow us to establish a strategy for determining the percolation threshold. Thus, each simulation run consists of the following steps: (a) the construction of the lattice for a given coverage ρ of regular bonds and $1 - \rho$ of attenuated bonds and (b) the cluster analysis by using the Hoshen and Kopelman algorithm [19] and the criterion of connectivity between clusters of regular bonds described in previous section. The spanning cluster could be determined by using the criteria R, D, I or U. m runs of such two steps are carried out for obtaining the number m^X of them for which a percolating cluster of the desired criterion X is found. Then, $R_L^X(\rho) = m^X/m$ is defined and the procedure is repeated for different values of both ρ and lattice sizes. A set of $m = 5 \times 10^4$ independent samples are numerically prepared for each value of ρ and L ($L = 48, 60, 72, 90$).

In Fig. 2, the probabilities $R_L^I(\rho)$ (filled symbols), $R_L^U(\rho)$ (cross symbols) and $R_L^A(\rho)$ (open symbols) are presented for $r = 0$ [standard random bond percolation, Fig. 2(a)], $r = 1/2$ [Fig. 2(b)] and different lattice sizes as indicated. From a first inspection of the figure (and from data do not shown here for the sake of clarity) it is observed that: (a) curves cross each other in a unique universal point, R^{X^*}, which depends on the criterion X used and allows us to make a preliminary identification of the universality class of the transition [38]; (b) the numerical values of R^{X^*} change for different values of r used; (c) those points are located at very well-defined values in the ρ-axes determining the critical percolation threshold ρ_c for each r; and (d) ρ_c shifts to the left upon increasing r.

Several conclusions can be drawn from Fig. 2. On the one hand, the value obtained for the percolation threshold in the case of $r = 0$, $\rho_c(r = 0) = 0.347(1)$, coincides, within the statistical uncertainty, with the exact estimate of the percolation threshold for the standard random bond percolation in a triangular lattice, $\rho_c = 2\sin(\pi/18) \approx 0.347296$ [2,39]. This result allows us to validate the computational scheme.

On the other hand, the percolation threshold $\rho_c(r)$ decreases as r is increased, indicating that the region percolating, or a range of values of ρ for which the system percolates, increases with the increase of r. In the limit of r close to 1, the percolation threshold takes the value $\rho_c(r \approx 1) = 0.159(1)$.

Finally, the change observed in the fixed point of the curves of $R_L^X(\rho)$ for different values of r used may be taken as a first indication that the universality class of the phase transition is not conserved for disordered lattices. However, as recently pointed out by Selke and Shchur [40,41], the value of the cumulant intersection (or its equivalent R^{X^*}) may depend on various details of the model, which do not affect the universality class (boundary condition, shape of the lattice, etc.). Consequently, more research is required to determine the universality class of a phase transition. An exhaustive study on this subject will be the object of future work.

The procedure of Fig. 2 was repeated for different values of r in the range $0 \le r \le 1/2$, showing that ρ_c decreases monotonically with r. This situation is reflected in Fig. 3 where, for the sake of clarity, only one curve (that corresponding to $L = 90$) of R_L^A vs. ρ is shown for each r. The values obtained for $\rho_c(r)$ are plotted in the inset of Fig. 4 and collected in the second column of Table 1. In all cases, the error in the determination of $\rho_c(r)$ is of the order of 0.001.[2]

[2] For each criterion, one looks for the highest ρ below the intersection point(s) at which the error bars of R_L^X do not overlap, and for the lowest ρ above the intersection point(s) at which they also do not overlap. The critical concentration is then the mean of these two, and their difference (divided by 2) gives the error in the measurement. This procedure is done for $X = I$, U, and A. Combining the three estimates, we obtain the final value of $\rho_c(r)$ (and its error).

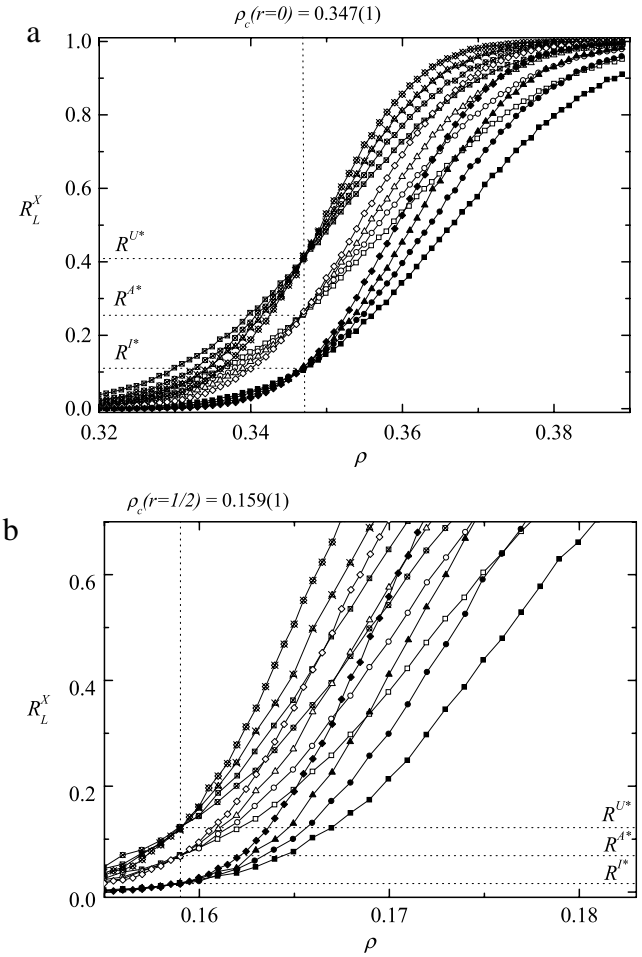

Fig. 2. Fraction of percolating lattices R_L^X, as a function of the concentration ρ of regular bonds for (a) $r = 0$ (standard random bond percolation) and (b) $r = 1/2$. Squares, circles, triangles and diamonds correspond to lattice sizes $L = 48, L = 60, L = 72$ and $L = 90$, respectively. Different criteria are used for establishing the spanning cluster, namely, $R_L^U(\rho) =$ the probability of finding either a rightward or a downward percolating cluster (cross symbols); $R_L^I(\rho)$ the probability that we find a cluster which percolates both in a rightward and in a downward direction (filled symbols); $R_L^A(\rho) \equiv \frac{1}{2}[R_L^R(\rho) + R_L^D(\rho)] \equiv \frac{1}{2}[R_L^I(\rho) + R_L^U(\rho)]$ (open symbols). Horizontal dashed line shows the R^{X*} universal point. Vertical dashed line denotes the percolation threshold in the thermodynamic limit $L \to \infty$.

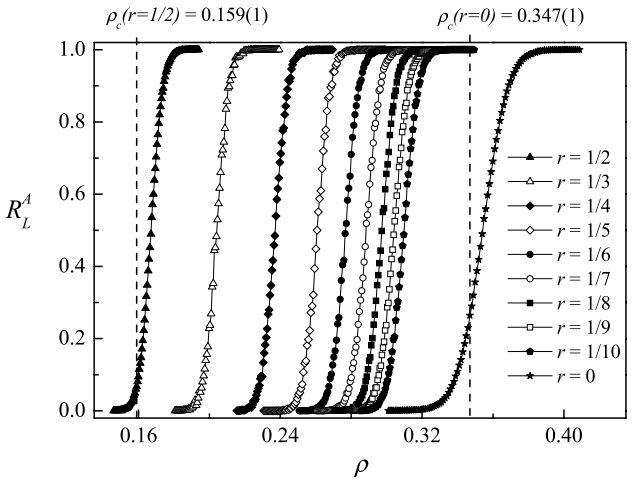

Fig. 3. Fraction of percolating lattices R_L^A, as a function of the concentration ρ of regular bonds for $L = 90$ and different values of r as indicated.

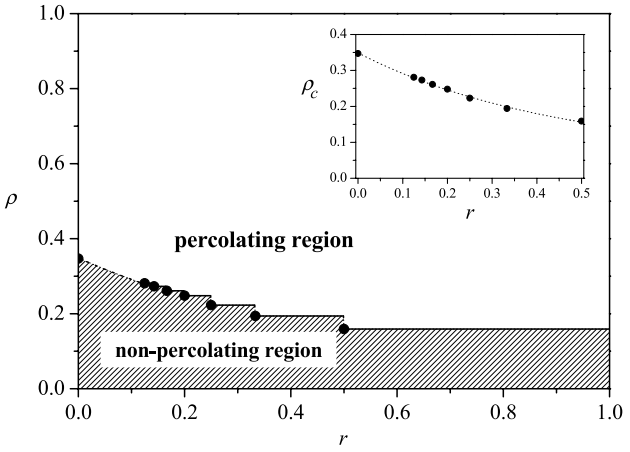

Fig. 4. Phase diagram, ρ vs. r, which shows the curve separating the percolating and non-percolating regions. Inset: Critical percolation threshold ρ_c as a function of the factor r. The dotted line is drawn as a guide for the eye. The error bars are smaller than the symbol size.

Table 1
Values of z_{eff} obtained for different values of r studied in the present paper.

r	Percolation threshold ρ_c	Effective connectivity z_{eff}
0	0.347(1)	6.03
1/8	0.281(1)	7.83
1/7	0.273(1)	8.13
1/6	0.261(1)	8.61
1/5	0.248(1)	9.19
1/4	0.223(1)	10.56
1/3	0.194(1)	12.69
1/2	0.159(1)	16.60

Given that n_a (number of attenuated bonds for interconnecting two clusters) is a discrete variable ($n_a = 2, 3, 4, \ldots$), the connectivity criterion $n_a r \geq 1$ leads to a unique value of ρ_c for all r in the interval $\left(\frac{1}{i} \leq r < \frac{1}{i-1}\right)$ with $i = 2, 3, 4, \ldots$. Thus, the critical line separating the percolating and non-percolating regions is a stepped line as shown in Fig. 4, where the $(\rho - r)$ phase diagram is presented.

Fig. 4 also shows that the percolation threshold $\rho_c(r)$ decreases upon increasing r. The curve varies between $\rho_c = 0.347(1)$ for $r = 0$ and $\rho_c = 0.159(1)$ for $r \to 1$. This finding indicates that the region percolating, or a range of coverage of regular bonds at which the transition occurs increases as r is increased.

As is well known [42,43], percolation thresholds are found to depend on both the space dimension d and the lattice connectivity z. In Ref. [42], the authors found one unique power law to yield, within an excellent accuracy, both site and bond percolation thresholds for all regular lattices at all dimensions.[3] The power law is:

$$\rho_c = \rho_0[(d-1)(z-1)]^{-a} d^b, \tag{1}$$

where $b = 0$ for site percolation and $b = a$ for bond percolation. From a log–log plot all data were found to fit on two straight lines. One line includes two-dimensional honeycomb, square and triangular lattices, which constitute the first class, characterized by $\{\rho_0 = 0.8889;\ a = 0.3601\}$ for site percolation and $\{\rho_0 = 0.6558;\ a = 0.6897\}$ for bond percolation. Two-dimensional Kagomé and all other regular lattices (for $d \geq 3$) align on the other unique line and constitute the second class, characterized by $\{\rho_0 = 1.2868;\ a = 0.6160\}$ and $\{\rho_0 = 0.7541;\ a = 0.9346\}$ for sites and bonds, respectively.

From this perspective, it is possible to interpret the effect of the attenuated bonds in terms of effective connectivity. For this purpose, we start from Eq. (1), for the case of bond percolation on triangular lattices (first class), and write z as a function of ρ_c:

$$z = 2\left(\frac{0.6558}{\rho_c}\right)^{1/0.6897} + 1. \tag{2}$$

We can now think of a mapping from an original disordered lattice, characterized by a factor r and a percolation threshold $\rho_c(r)$, to an effective regular lattice, whose connectivity, denoted as z_{eff}, is consistent with a percolation threshold equal to $\rho_c(r)$. Thus, introducing different values of ρ_c obtained for each r in Eq. (2), the corresponding values of z_{eff} can be calculated.

[3] Later, in Ref. [43], the study was extended to non-regular lattices.

The results are collected in Table 1. As is possible to observe, small changes in r produce a dramatic increase in the effective lattice connectivity, showing the importance of including the attenuated bonds in the system.

4. Conclusions

In this work, we have used computational simulations and FSS theory to study the percolation properties of disordered triangular lattices with a fraction of attenuated bonds randomly distributed (which simulate the presence of defects in the surface). The degree of disorder of the surface is tunable by selecting the values of (1) the fraction of regular [attenuated] bonds ρ $[1-\rho]$ and (2) the ratio r between the value of the conductivity associated to an attenuated bond and that corresponding to a regular bond.

According to the present analysis, the critical behavior of the system is characterized by the following properties:

(1) As $r = 0$, the standard random bond percolation problem is recovered, being $\rho_c(r=0) = 0.347(1)$.
(2) The percolation threshold $\rho_c(r)$ decreases upon increasing r. This finding indicates that the region percolating, or a range of values of ρ for which the system percolates, increases with the increase of r. In the limit of r close to 1, the percolation threshold takes the value $\rho_c(r \approx 1) = 0.159(1)$.
(3) The numerical values of the fixed point of the curves of $R_L^X(\rho)$ change for different values of r used as the first indication that the universality class of the phase transition is not conserved for disordered lattices.
(4) Finally, the analysis of the behavior of the system in terms of connectivity shows that small changes in r produce a dramatic increase in the effective lattice connectivity. The results show the importance of including the attenuated bonds in the system.

Future efforts will be directed to develop an exhaustive study on critical exponents and universality in all ranges of values of r.

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