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Entropy, specific heat, susceptibility, and Rushbrooke inequality in percolation

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We investigate percolation, a probabilistic model for continuous phase transition, on square and weighted planar stochastic lattices. In its thermal counterpart, entropy is minimally low where order parameter (OP) is maximally high and vice versa. In addition, specific heat, OP, and susceptibility exhibit power law when approaching the critical point and the corresponding critical exponents α,β,γ respectably obey the Rushbrooke inequality (RI) $\alpha + 2\beta + \gamma \geqslant 2$. Their analogs in percolation, however, remain elusive. We define entropy and specific heat and redefine susceptibility for percolation and show that they behave exactly in the same way as their thermal counterpart. We also show that RI holds for both the lattices albeit they belong to different universality classes.

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The emergence of a well-defined critical value accompanied by a dramatic change in the order parameter (OP) and entropy (S) without jump or discontinuity is an indication of second-order or continuous phase transition (CPT) which has acquired a central focus in condensed-matter and statistical physics [1]. In CPT, the numerical value of OP, which measures the extent of order, is always zero above T_c where entropy is significantly high and hence the high-T phase is the disordered phase. On the other hand, near T_c the numerical value of S, which measures the degree of disorder, drops significantly following a sigmoidal shape where OP grows with $\epsilon \sim T - T_c$ following a power law OP $\sim \epsilon^{\beta}$ and eventually $S \to 0$ while OP $\to 1$ revealing that the low T is the ordered phase. The CPT is further characterized by the power-law growth of the specific heat $C \sim \epsilon^{-\alpha}$ and susceptibility $\chi \sim \epsilon^{-\gamma}$ near T_c and by their divergences at T_c. Remarkably, one finds that a wide range of systems belong to one of a comparatively small number of universality classes where each class shares the same set of critical exponents. Besides this, the values of the critical exponents are bound by some scaling relations. One of the most interesting scaling relations is the Rushbrooke inequality (RI) $\alpha + 2\beta + \gamma \geqslant 2$ which reduces to equality under the static scaling hypothesis [2]. Many experiments and exactly solvable models too support equality.

Percolation is one of the simplest paradigmatic models for CPT. Besides this, its notion has also been used *in extenso* to study the spread of forest fires, the flow of fluid through porous media, the spread of biological and computer viruses, etc., where the extent of connectivity has a profound impact [3–5]. To define percolation one has to first choose a lattice or a graph. Then in random bond (site) percolation each bond (site) is occupied randomly with probability p independent of the state of its neighbors [3,6]. Clearly at $p = 0$ in bond percolation, each site is a cluster of its own size; whereas, at $p = 1$, there is just one cluster, contiguous sites connected by occupied bonds, of size coinciding with the size of the lattice. Interestingly, by tuning p from $p = 0$, one finds that clusters are continuously formed and grown on the average, and eventually arrive at a threshold value p_c at which there appears a spanning cluster for the first time that spans across the entire system. Such transition from isolated finite-sized clusters to a spanning cluster across p_c is found to be reminiscent of the CPT. This is why scientists, in general, and physicists, in particular, find it so interesting.

In order to make the percolation theory a successful model for CPT, it is necessary that we know how to relate its various observable quantities to the corresponding quantities of the thermal CPT. To this end, Kasteleyn and Fortuin (KF) mapped the q-state Potts model onto the percolation problem and established some useful connections [7]. Thanks to the KF mapping, we now know that the relative size of the spanning cluster is the order parameter P, mean cluster size is the susceptibility, the relation between $p - p_c$ with linear size L of the lattice is the equivalent counterpart of the relation between ϵ and the correlation length ξ, etc. However, we still do not know how to define entropy and specific heat, although they are the key parameters to characterize CPT. In addition, we regard the mean cluster size as the susceptibility but it exhibits the expected divergence only if the spanning cluster is excluded, and even then the corresponding exponent γ is too high to obey RI. Realizing these drawbacks, some authors already have proposed an alternative which, although it exhibits divergence without the exclusion of the spanning cluster, the problem of high γ still persists [8–11]. Finally, proving whether the Rushbrooke inequality holds in percolation or not, remains elusive.

Motivated by the issues outlined above, in this Rapid Communication, we investigate bond percolation on square and weighted planar stochastic (WPS) lattices. First, we propose a labeled cluster picking probability (CPP) that a site picked at random belongs to cluster i to measure Shannon entropy H. We show that the resulting entropy has the same expected features as that of its thermal counterpart. In one phase, where $P = 0$, we find that H is significantly high and in the other phase where $H \approx 0$ we find that P is significantly high, as expected. Note that H and P both cannot be extremely low or high at the same time since H measures the degree of disorder and P measures the extent of order. Second, we define specific heat and find positive critical exponent α for both the lattices, which is in sharp contrast to the existing value $\alpha = -2/3$ for square lattice. We also redefine susceptibility and show that it diverges at the critical point without having to exclude the spanning cluster. In addition, we also obtain its critical exponent γ and find that it is significantly smaller than the existing known value. The values of α and γ reaffirm our earlier findings that percolation on square and WPS lattices belong to two distinct universality classes, although they are embedded in the same spatial dimension [12]. Finally, we find

that the elusive RI holds in random percolation regardless of whether it is on square or on WPS lattices.

We find it worthwhile first to discuss the construction process of the WPS lattice which we proposed in 2010 [13]. It starts with a square of unit area which we call an initiator. Then, in the first step, we divide the initiator randomly into four smaller blocks. In the second step and thereafter, only one of the blocks at each step is picked from all the available blocks preferentially according to their respective areas and divide that randomly into four smaller blocks. The details of the algorithm and image of the lattice can be found in [13,14]. Percolation on such a lattice has already shown unique results [12]. For instance, it is well known that random percolation on all lattices, regardless of the type of percolation and the structural difference of the lattice, share the same set of critical exponents *vis-a-vis* belonging to the same universality class provided they share the same dimension. However, we have recently shown that percolation on the WPS lattice does not belong to the universality class of all the known two-dimensional lattices [12].

To study percolation, we use the Newman-Ziff (NZ) algorithm which, apart from being the most efficient one, has also many other advantages [15]. For instance, it helps in calculating various observable quantities over the entire range of p in every realization instead of measuring them for a fixed probability p in each realization. According to the NZ algorithm, all the labeled bonds $i = 1,2,3,\ldots,M$ are first randomized and then arranged in the order in which they will be occupied. Using the periodic boundary condition we get $M = 2L^2$ for the square lattice and $M \sim 8t$ for the WPS lattice where t is the time step. One advantage of using the NZ algorithm is that we can create percolation states consisting of $n+1$ occupied bonds simply by occupying one more bond to its immediate past state consisting of n occupied bonds. Initially, there are L^2 and $3t+1$ clusters of size one in the square and WPS lattices, respectively. Occupying the first bond means forming a cluster of size two. Each time thereafter, either the size of an existing cluster grows due to occupation of the intercluster bond or remains the same due to occupation of the intracluster bond. We calculate an observable, say X_n, as a function of n and use it in the convolution relation

$$X(p) = \sum_{n=1}^{M} \binom{M}{n} p^n (1-p)^{M-n} X_n \qquad (1)$$

to obtain X as a function of p that helps in obtaining a smooth curve for $X(p)$.

Phase transitions always entail a change in entropy in the system regardless of whether the transition is first or second order in character. Thus, a model for CPT is not complete without a proper definition of entropy. We find that the Shannon entropy is the most appropriate one for percolation as it is too probabilistic in nature. In general, it is defined as

$$H = -K \sum_{i}^{m} \mu_i \log \mu_i, \qquad (2)$$

where we set the constant $K = 1$ since it merely amounts to a choice of a unit of measure of entropy [16]. In information theory, it is a common practice to choose $K = 1/\log 2$. Although there is no explicit restriction *per se* on the choice of

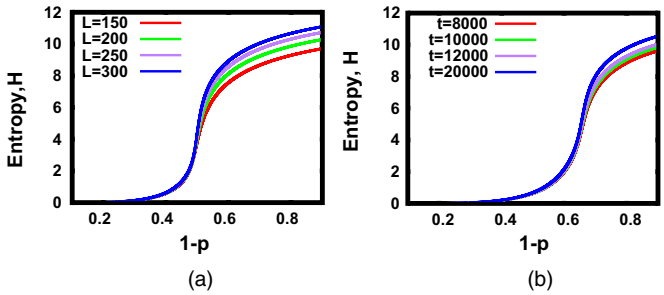

FIG. 1. Change in Shannon entropy H with $1-p$ for (a) square and (b) WPS lattices. The sharp rise in H occurs near $q_c = 0.5$ and $q_c = 0.6543$ for (a) and (b), respectively.

μ_i for Shannon entropy, when we use it to describe entropy for phase transition there ought to be some implicit restrictions. We all know from thermodynamics and statistical mechanics that G vs T should be a concave curve with negative slope to ensure that entropy $S \geqslant 0$. On the other hand, the slope of the S vs T plot must have a sigmoid shape with positive slope since $C \geqslant 0$ and according to the second law of thermodynamics $\Delta S \geqslant 0$ [2]. The entropy for percolation too must have the same generic features.

The key question in percolation is not whether we can measure Shannon entropy or not. Rather, faced with a number of different normalized probabilities, the question is, can we use them? Earlier, some authors used w_s, the probability that a site picked at random belongs to a cluster exactly of size s, to measure entropy using Eq. (2) and they both found a bell-shaped curve with peaks at around their respective critical points [17,18]. This implies that the system is in the most ordered state at $p = 0$ since entropy is minimally low there and at the same time it is in the most disordered state since the order parameter P is also zero there—hence we see a contradiction. The problem with using w_s is that the sum in Eq. (2) is not over cluster size s, rather it is over cluster label i so that it measures the amount of information conveyed by each cluster, not by a class or group of clusters of size s. Thus, we have to choose a probability that contains information about individual clusters. To find the appropriate probability for μ_i of Eq. (2), we assume that for a given p there are m distinct, disjoint, and indivisible labeled clusters $i = 1,2,\ldots,m$ of size $s_1,s_2,\ldots,s_m$, respectively. We then propose the labeled picking probability (CPP) μ_i, that a site picked at random belongs to cluster i. The most generic choice for CPP would be $\mu_i \propto s_i$ so that the probability $\mu_i(p) = s_i / \sum_{j=1}^{m} s_j$ where $\sum_{j=1}^{m} s_j = N$ is the normalization factor.

Substituting $\mu_i(p) = s_i/N$ in Eq. (2), we first find the microcanonical ensemble average of entropy H_n as a function of n from 10 000 independent realizations. Then we use it in Eq. (1) to get the canonical ensemble average of $H(p)$ as a function of p. In Figs. 1(a) and 1(b) we plot $H(p)$ versus $q = 1-p$ and find that the curve has the desired sigmoidal shape. We see that the entropy is maximum $H = \log(N)$ at $q = 1$ where $\mu_i = 1/N\ \forall i$ as there are N clusters of equal size (one). This is exactly like the state of an isolated ideal gas where all microstates are equally likely and hence $q = 1$ corresponds to the most disordered state and it is consistent with the fact that $P = 0$ there. As we lower the q value from

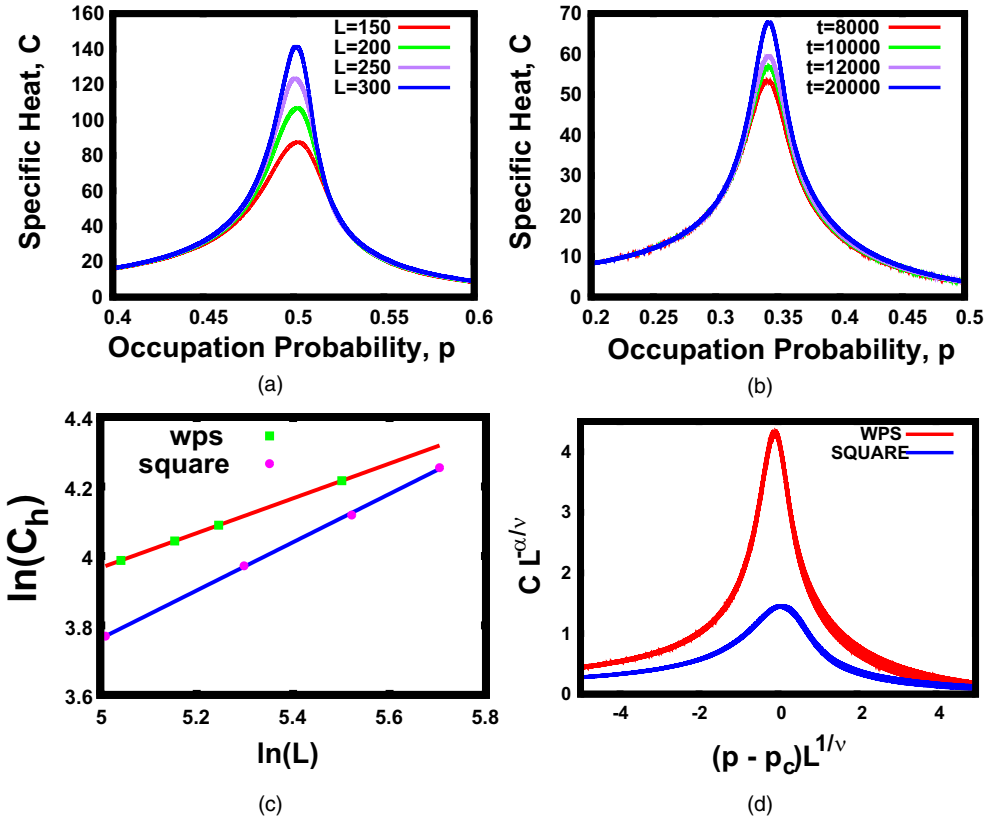

FIG. 2. Specific heat $C(p)$ vs p for (a) square and (b) WPS lattices. (c) Slope of the plots of $\log(C_{\rm h})$ versus $\log(L)$ gives $\alpha/\nu = 0.68(1)$ and $\alpha/\nu = 0.5007(3)$ for square and WPS lattices, respectively. (d) Plots of $C(p)L^{-\alpha/\nu}$ vs $(p - p_c)L^{1/\nu}$ of the same data as in (a) and (b) shows excellent data collapse (top curve for the WPS lattice and the bottom one for the square lattice).

$q = 1$ we see H decreases slowly; however, as q approaches q_c we observe a sudden drop in entropy. This is because in the vicinity of p_c, the coagulation of two moderately large clusters happens so frequently that we already see a sign of the emergence of a spanning cluster that causes a sharp rise of CPP which eventually becomes the spanning cluster. Already at q_c the incipient spanning cluster becomes so prevailing that it embodies almost all the sites. Lowering q further to below q_c, we see that the extent of uncertainty diminishes sharply. Exactly at $q = 0$, we have $\mu_1 = 1$ and hence entropy $H = 0$. This situation is like perfect crystal as the extent of uncertainty, which is synonymous to degree of disorder, completely ceases to exist. The term percolation thus refers to the transition across q_c from ordered phase at low q to disordered phase at high q exactly like ferromagnetic transition.

To find the specific heat $C(p)$ for percolation we just need to use its thermodynamic definition $C = T\frac{dS}{dT}$ and replace S by H and T by $1 - p$ to obtain

$$C(p) = (1 - p)\frac{dH}{d(1 - p)}. \tag{3}$$

In Figs. 2(a) and 2(b) we plot it for both the lattices as a function of p for different system sizes. Now following the finite-size scaling (FSS) hypothesis we can write

$$C(p,L) \sim L^{\alpha/\nu}\phi_C[(p - p_c)L^{1/\nu}], \tag{4}$$

where ϕ_C is the scaling function for specific heat. Note that we already know $1/\nu = 0.75$ for square latice and $1/\nu = 0.613$ for WPS lattice [12]. To find an estimate for the exponent α/ν, we measure the height of the peak $C_{\rm h}$ at p_c as a function of L. Plotting $\log(C_{\rm h})$ versus $\log(L)$ we get straight lines [see Fig. 2(c)], with slopes $\alpha/\nu = 0.68(1)$ for the square lattice and $\alpha/\nu = 0.5007(3)$ for the WPS lattice. Note that $CL^{-\alpha/\nu}$ and $(p - p_c)L^{1/\nu}$ are dimensionless quantities and hence if we now plot $CL^{-\alpha/\nu}$ as a function of $(p - p_c)L^{1/\nu}$, then the distinct plots of C vs p should collapse onto a single universal curve ϕ_c. Indeed, Fig. 2(d) shows that all the distinct plots of Figs. 2(a) and 2(b) collapse superbly into their own universal curve. Using the relation $L \sim (p - p_c)^{-\nu}$ in $C(p) \sim L^{\alpha/\nu}$ we find that the specific heat diverges:

$$C(p) \sim (p - p_c)^{-\alpha}, \tag{5}$$

with $\alpha = 0.906(13)$ for the square lattice and $\alpha = 0.816(4)$ for the WPS lattice. Our value of α for the square lattice is in sharp contrast to the existing value $\alpha = -2/3$ [19]. Note that the negative value of α means the specific heat does not diverge at the critical point; rather it behaves more like an order parameter.

Recall that the order parameter P of percolation is defined as the the ratio of the size of the largest cluster $s_{\rm max}$ to the lattice size N. We then keep a record of the successive jump size in P, i.e., ΔP within the successive interval $\Delta p = \frac{1}{M}$ where M is the total number of bonds. The idea of successive jump size in P was first studied by Manna in the context of explosive percolation [20]. We, however, here consider the ratio $\frac{\Delta P}{\Delta p}$ and define it as the susceptibility $\chi(p)$. In Figs. 3(a) and 3(b) we

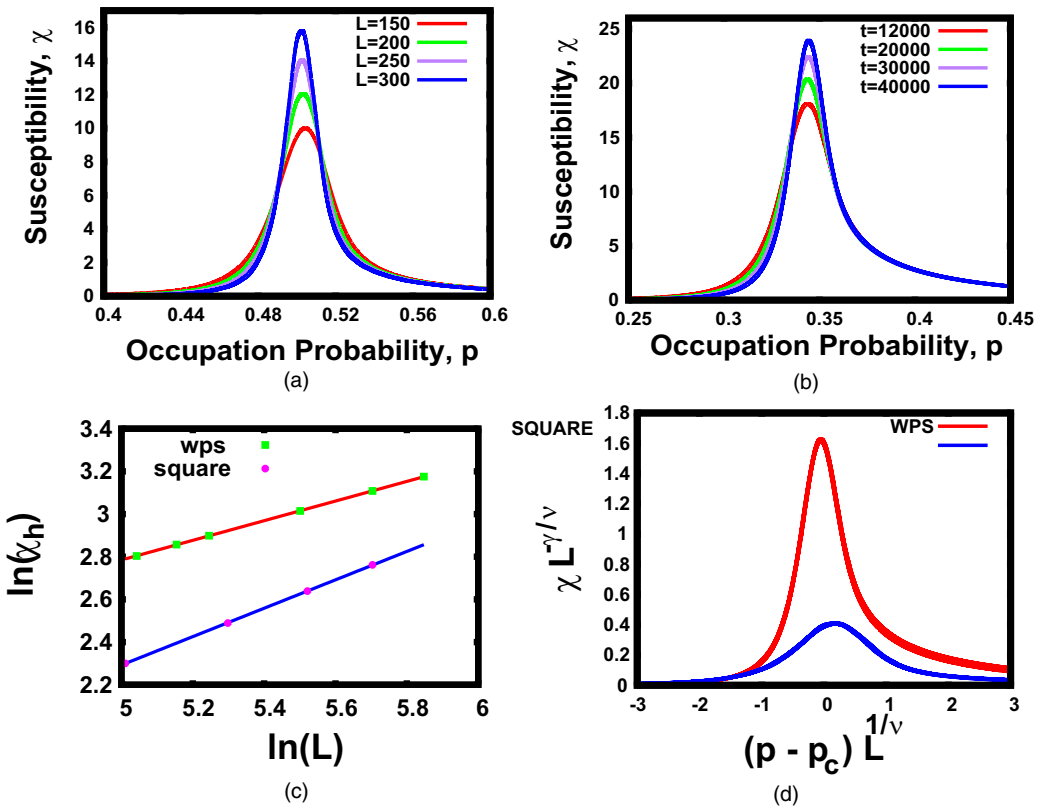

FIG. 3. Plots of χ vs p for (a) square and (b) WPS lattices where data represents the convolution of ensemble average of 10 000 independent realizations. (c) The slopes of the plots of $\log(\chi_h)$ vs $\log(L)$ give $\gamma/\nu = 0.635(2)$ and $\gamma/\nu = 0.460(1)$ for square and WPS lattices, respectively. In (d) we plot $\chi L^{-\gamma/\nu}$ vs $(p - p_c)L^{1/\nu}$ and find the same data as in (a) and (b) collapse into their respective universal curves. The top curve is the scaling function for WPS lattice and the bottom one is that of the square lattice.

plot $\chi(p)$ as a function of p for both types of lattice and find that $\chi(p)$ grows as we increase p and as we approach p_c the growth is quite steep. However, beyond p_c it decreases sharply without excluding the size of the spanning cluster. This is in sharp contrast to the existing definition of susceptibility as we know that the mean cluster size decreases beyond p_c only if the spanning cluster size is excluded. To find the exponent γ, we apply the FSS hypothesis. Following the same procedure done for $C(p)$, we find $\gamma/\nu = 0.635(2)$ for the square lattice and $\gamma/\nu = 0.460(1)$ for the WPS lattice [see Fig. 3(c)]. Plotting $\chi L^{-\gamma/\nu}$ versus $(p - p_c)L^{1/\nu}$ we find that all the distinct plots of Figs. 3(a) and 3(b) collapse into their own distinct universal curve as shown in Fig. 3(d). It implies that

$$\chi(p) \sim (p - p_c)^{-\gamma}, \tag{6}$$

where $\gamma = 0.846(2)$ and $\gamma = 0.750(6)$ for square and WPS lattices, respectively. It suggests two important developments. First, we find that the susceptibility diverges at the critical point without having to exclude the spanning cluster. Second, the value of the critical exponent γ is far less than what we find from the mean cluster size.

Note that we already know the critical exponent β for both the lattices [12]. We now substitute the values of α, β, and γ in the Rushbrooke relation and the results are shown in Table I. It clearly suggests that Rushbrooke inequality holds in percolation. However, the point to emphasize is that it obeys rather more as an equality, within the limits of error, than as an inequality. Many experiments and exactly solvable models of thermal CPT too suggest that the Rushbrooke inequality actually holds as an equality [21]. Through this work we show that the entropy and the order parameter complement each other exactly like in the thermal counterpart. For instance, we find that the order parameter P, which quantifies the degree of order, is equal to zero for $q \geqslant q_c$ but entropy, which measures the degree of order, is significantly high revealing the high q is the disordered phase exactly like the high-T phase in the ferromagnetic transition. On the other hand, at $q < q_c$ we find that the entropy H is negligibly small where P increases with decreasing q to its maximum value at $q = 0$ revealing that low q is the ordered phase which is once again like the low-T phase in the ferromagnetic transition. It all implies that percolation is indeed an order-disorder transition.

To summarize, in this Rapid Communication we proposed the equivalent counterpart of entropy and specific heat and redefined the susceptibility for percolation model. To measure entropy for percolation we proposed cluster picking probability (CPP) and show that the Shannon entropy for CPP has

TABLE I. The critical exponents and Rushbrooke inequality for random percolation on square and WPS lattices.

Lattice	α	β	γ	$\alpha + 2\beta + \gamma$
Square	0.906	0.1388	0.846	2.029
WPS	0.816	0.222	0.750	2.01

the same generic feature as the thermal entropy. Until now, we could only quantify the extent order of the ordered phase by measuring P and we could say nothing about the other phase since $P = 0$ there. Now, having known entropy, we can also quantify the other phase and regard it as the disordered phase as entropy is high and always keep increasing with $1 - p$. We have also shown that specific heat diverges with positive slope and susceptibility exhibits both power law near p_c and divergence at p_c without having to exclude the spanning cluster from their calculations. Using the FSS hypothesis and the idea of data collapse, we numerically obtained the critical exponents α and γ for both the lattices. Their distinct values for the two lattices once again confirm that they belong to two different universality classes. Finally, we showed that the Rushbrooke inequality holds in percolation on both the lattices albeit they belong to two distinct universality classes.

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