Protected percolation: a new universality class pertaining to heavily-doped quantum critical systems

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Abstract

We present computer simulations on a class of percolative systems that forms a new universality class. We determine the universal critical exponents for this new class from simulations on lattices consisting of up to one billion sites. These new percolative systems differ from standard systems in that once a cluster breaks off the lattice spanning cluster, its sites become protected and cannot be removed. We demonstrate that despite this restriction on the evolution of isolated clusters, the scaling relationships between the critical exponents remain valid. Protected percolation closely mimics the situation in heavily-doped quantum critical systems where isolated magnetic clusters are protected from Kondo screening. We show that protected percolation in three dimensions violates the Harris criterion, explaining why universal exponents for quantum phase transitions have been elusive.

1. Introduction

Percolation is a phenomenon that applies to many physical systems whose critical behavior falls into known universality classes [1–3]. Percolation describes how a system responds to the removal of its elements or the connections between them. When enough of the connections are broken, the percolation threshold—the point where the system spanning connection fractures—is reached; the dimensionality and connectivity of the system determines when this happens. However, as a system approaches this threshold, universal behavior is displayed: behavior characterized by critical exponents that only depend on the dimensionality of the system and order parameter.

We describe a new type of percolation—inspired by observations on heavily-doped quantum critical systems [4] whose critical behavior falls in a new universality class. This new percolative system, dubbed protected percolation, has the restriction that upon emptying a lattice only sites attached to the lattice spanning cluster can be removed (see figure 1). The isolated clusters that form become ‘protected’ from further removal. This procedure is inspired by heavily-doped quantum critical systems that harbor a magnetic lattice whose moments are effectively removed through Kondo shielding as the system is cooled [5]. However, when magnetic clusters break off the lattice spanning cluster, the moments of the magnetic ions align with their neighbors because of quantum mechanical finite-size effects [6]; since ordered moments are not likely to be Kondo shielded because of the spin–flip interaction at the heart of this shielding [4, 7], such clusters are protected from further degradation. Therefore, this new percolation model is relevant to (heavily-doped) quantum critical systems.

A pilot study [6] indicated that protected percolation would fall in its own universality class. However, the computer simulations in that study lacked sufficient accuracy to confirm this, and the derivation for most of the critical exponents was incorrect. In this paper we present simulations on lattices larger by a factor of 10,000, and we provide the correct derivations of the critical exponents, linking them to those of standard percolation. In addition, we simulated both 2-dimensional and 3-dimensional systems for various lattice types in order to prove universality and to investigate whether the Harris criterion would be violated, or not.

The three-dimensional manifestation of protected percolation violates the Harris criterion [8] whereas the two-dimensional manifestation satisfies this criterion, as we will show. The Harris criterion states that impurities do not alter how a system transitions from a disordered to an ordered phase. This critical behavior is

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captured by a universal set of critical exponents that describe how, for instance, the order parameter (exponent $\beta$) or the mean cluster size (exponent $\gamma$) depend on the distance to the critical point. When the Harris criterion is satisfied,

$$\gamma + 2\beta > 2,$$

then impurities can shift the critical point, but they do not alter the values of the critical exponents [8]; when the criterion is violated ($\gamma + 2\beta < 2$), then the critical exponents become system dependent and universal behavior disappears. We show that in protected percolation the criterion is violated for three-dimensional lattices, but it is satisfied for two-dimensional lattices.

The outline of this paper is as follows. We first review the standard definitions pertaining to percolation theory. Then we discuss our Monte Carlo (MC) computer simulations we performed to obtain the critical exponents. Next we show the results for various lattice types and demonstrate that protected percolation falls in a new universality class. We end with a discussion on the Harris criterion and its implications for the low-temperature behavior of strongly correlated electron systems that have been doped to be at the quantum critical point.

In percolation theory [1], the point where (upon emptying a lattice) the lattice spanning connection fractures is called the percolation threshold, denoted by $p_c$. The fractional occupation of the lattice is denoted by $p$ ($0 \leq p \leq 1$). This threshold depends on the dimensionality of the lattice and the number of neighbors. As the system approaches the percolation threshold from above, the strength of the lattice spanning cluster, $P(p)$, decreases non-analytically and the second moment of the cluster size distribution diverges. The $k^{th}$ moment of the cluster size distribution is defined as

$$M_k(p) = \sum_s s^k n_s(p),$$

where $s$ is the number of sites in a cluster and $n_s$ is the number of clusters per lattice site containing $s$ sites [1]. The zeroth moment ($k = 0$) represents the mean number of clusters per lattice site and its second derivative shows non-analytical critical behavior [1]. The first moment ($k = 1$) represents the probability that an arbitrary site belongs to an isolated cluster, and it relates to $P(p)$ which is defined by:

$$P(p) = p - \sum_s s n_s(p).$$

The strength of the lattice spanning cluster exhibits power-law behavior near the percolation threshold. Finally, the second moment ($k = 2$) is used to calculate the mean cluster size, $S(p)$, as

$$S(p) = \frac{\sum s^2 n_s(p)}{\sum s n_s(p)} \approx \frac{\sum s^2 n_s(p)}{P},$$

where we have used that $S(p)$ becomes approximately equal to the second moment close to the percolation threshold since $P(p_c) = 0$. The results of simulations for equations (2)–(4) are shown in figure 2.
The strength of the lattice spanning cluster and the second moment of the cluster size distribution display power law dependences when measured as a function of how far the system is from the percolation threshold $p - p_c$ [1]. The distribution of cluster numbers at the percolation threshold $n_s(p_c)$ also shows a power law dependence [1]. All this is expressed as

$$P(p) = P_0(p - p_c)^\beta + (p - p_c)$$

$$S(p) = S_0(p - p_c)^\gamma$$

$$n_s(p_c) \sim s^{-\tau}$$

where $\beta$, $\gamma$, and $\tau$ are the critical exponents. We will distinguish between the critical exponents for standard and protected percolation by putting a prime on the latter.

2. Methods

Protected percolation requires a different MC algorithm than standard percolation. In particular, it is no longer possible to simulate a lattice at a particular occupancy, rather the lattice needs to be emptied one site at a time. In standard percolation a single instance of a lattice is randomly generated for a given occupancy after which the lattice is analyzed to determine its connectivity. However, in protected percolation sites cannot be removed from isolated clusters and hence, the prior history of when clusters become isolated needs to be taken into account. As such, protected percolation requires a lattice to be emptied step by step rather than to be analyzed at a single occupation. This greatly increases the computational overhead for carrying out the MC computer simulations.

In order to get around the computational overhead of determining cluster connectivity at every occupancy, we opted for filling the lattice one site at a time and use bookkeeping to correct for forbidden site removal from isolated clusters. Upon filling, it is easy to check whether a newly occupied site attaches to an existing cluster, connects existing clusters, or forms a new isolated cluster. We have opted to use a disjoint-set data structure [9] developed by Newman and Ziff [10, 11] to analyze the connectivity of the lattice. Bookkeeping is needed upon filling because some events that are included are forbidden in protected percolation, such as the merging of two isolated clusters as this would correspond to the breaking up of an isolated cluster upon emptying. We must retroactively correct our data as a function of occupancy. Whenever such a forbidden event happens, we add this to the calculated shift in threshold between standard and protected percolation. We verified this procedure by comparing the percolation threshold and the moments of the cluster distribution for a particular set of random numbers using our method with a Hoshen–Kopelman algorithm [12] while emptying a lattice and found identical results.\footnote{More than one lattice spanning cluster may appear and we have chosen to only use simulations containing a single percolating cluster for equations (2)–(4).} We also note that protected percolation terminates at $p_c$ when the lattice spanning cluster breaks up as this leaves the remainder of the occupied sites protected.

Figure 2. The results of MC simulations for a body-centered cubic lattice of size $1000^3$ averaged over 100 iterations. Standard and protected percolation are shown in red (light gray) and blue (dark gray), respectively. (a) The zeroth moment (equation (2) with $k = 0$), being the mean cluster number. (b) The strength of the lattice spanning cluster (equation (3)). (c) The average size of the clusters (equation (4)).
3. Results

3.1. Percolation threshold

We show our results for the percolation thresholds for various lattice sizes in figure 3 and for various lattice types in table 1. We used an identical set of random numbers for both protected and standard percolation. Our results for standard percolation match those in the literature; we used the Levinshtein method \([13]\) to calculate the thresholds. We ran separate simulations in order to determine the percolation threshold for 1000 iterations of varying lattice sizes (ranging from \(40^3\) to \(800^3\) sites).

Using the extrapolated thresholds shown in table 1, we plot the critical behavior of the second moment and \(P(p)\) for protected percolation in figure 4 for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) lattices. Since each of the data sets have identical slopes we conclude that protected percolation displays universal critical behavior. Given that the slopes are substantially different from standard percolation, we conclude that protected percolation represents a new universality class (see table 2).

| Lattice | Literature \(p_c\) | Standard \(p_c\) | Protected \(p_c\) |
|---------|---------------------|-----------------|-----------------|
| Square  | 0.592 746 01(2)\([14]\) | 0.592 758(18)   | 0.602 752(11)   |
| Triangular | 0.5 \([1]\)        | 0.500 009(20)   | 0.508 691(13)   |
| Honeycomb | 0.697 040 230(5)\([14]\) | 0.697 056(28)   | 0.707 168(17)   |
| SC      | 0.311 608 1(13)\([5]\)  | 0.311 593(7)    | 0.342 315 6(14) |
| BCC     | 0.245 961 3(10)\([16]\) | 0.245 966(7)    | 0.271 393 3(15) |
| FCC     | 0.199 236 3(10)\([16]\) | 0.199 239(4)    | 0.218 266 7(11) |

Figure 3. The inset shows the distribution of thresholds for protected percolation from 1000 iterations for three body-centered (BC) lattice sizes. The distribution is characterized by \(p_c\) average and the standard deviation \(\sigma\). With increasing system size, the distribution becomes more narrow while approaching the threshold for an infinite lattice. Using the relationship between \(p_c\) average and \(\sigma\), we obtain \(p_c\) by extrapolating to \(\sigma \to 0\). The fits for standard and protected percolation are shown by the red (lower) and blue (upper) lines, respectively. The error bars are given by \(\sigma\).

3.2. Critical exponents in protected percolation

There exists an analytical relation between the critical exponents of standard and protected percolation \([6]\). Heitmann et al. deduced the correct derivation for \(\beta\) (which we reproduce below), but the derivation of the other critical exponents was based on an assumption that we found to be incorrect, resulting in incorrect values. The main assumption was that when clusters breaks off the infinite cluster, the dominant occurrence would be only single clusters peeling off. However, we found that multiple clusters peeling off at the same time occurred with sufficient frequency to render this assumption invalid. Here we use scaling laws to determine the correct critical exponents, and use our simulation results to verify that these scaling laws do indeed hold.

The exponents \(\beta\) and \(\beta'\) are related as follows. In both scenarios, the strength of the lattice spanning cluster follows the same trajectory as sites are removed. When the percolation threshold is reached, the lattice spanning cluster will be identical in both cases. In the standard case, a site will be removed from the lattice spanning cluster (on average) every \(p/P(p)\) removal steps. In the protected case, only sites from the lattice spanning cluster can be removed, so the strength of the lattice spanning cluster decreases at each step in \(p\). As such, the lattice spanning
Thus, we will always be able to find a solution to the following equation for any value of \( p \) with \( p > p_c \):

\[
P(p) = P'(p').
\]

Since the equation holds, we can then equate the slope of \( P(p) \) to the slope of \( P'(p') \) using the fact that the slope for the protected case will be steeper by a factor of \( p/p_0 \) than the standard case (with \( x = p - p_c \), and \( x' = p' - p'_c \)):

\[
\frac{dP'(x')}{dx'} = \frac{dP(x)}{dx} \frac{P}{P(x)}.
\]

Using equation (5) to describe critical behavior, we rewrite equation (9) as

\[
\beta' P'_0 x'^{\beta-1} = \beta P_0 x^{\beta-1} \frac{P}{P(x)} \approx \frac{\beta (x + p_c)}{x} \approx \frac{\beta p_c}{x},
\]

where we have left out \((p - p_c)\) and \((p' - p'_c)\) terms close to the percolation threshold because the power law term dominates. The solution to equation (8) is found in a similar manner, yielding

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**Figure 4.** Simulation results for 1000 iterations for 3D lattices of size 400³. Lattice types consist of SC (top), BCC (middle), and FCC (bottom). (a) The strength of the lattice spanning cluster. (b) The second moment of the cluster size distribution. In both cases, the lines appear parallel demonstrating the universality of protected percolation. The dashed-dotted lines represent the literature values for the slopes in standard percolation.

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**Table 2.** The critical exponents for both standard and protected percolation as determined from fits. The value for the Harris criterion in each case is also included. All 2D critical exponents are exact values provided scaling relations hold.

| Critical exponent | 2D  | 3D Fit | 3D Literature |
|-------------------|-----|--------|---------------|
| \( \beta \)       | 5/36 | 0.4053(5) | 0.405(25) [17] |
| \( \gamma \)      | 43/18 | 1.819(3) | 1.805(20) [17] |
| \( \tau \)        | 187/91 | 2.1753(11) | 2.1892(18) |
| \( \gamma + 2; \beta(=\nu) \) | 2.667 | 2.6296(32) | 2.62(5) |
| \( \beta' \)      | 5/41 | 0.2887(15) | |
| \( \gamma' \)     | 86/41 | 1.3066(19) | |
| \( \tau' \)       | 187/91 | 2.1659(21) | |
| \( \gamma' + 2; \beta'(=\nu') \) | 2.3415 | 1.8811(19) | |
| \( \beta' - \beta/\beta + 1 \) | 0.0003(29) | |
| \( \gamma' - \gamma/\beta + 1 \) | 0.0122(29) | |
| \( \tau' - \tau \) | 0.0094(24) | |
Assuming scaling relationships to hold \[\text{as well as equation (5), (6), and (7), respectively, we obtain satisfactory fits (dashed lines in figure 5). The critical exponents obtained from the fits are given in table 2.}

In standard percolation, scaling relationships [1–3] relate the values of the critical exponents. Once two exponents are known, the remainder can be determined through (hyper-)scaling relationships such as \(d_\ell = d - \beta/\nu\), with \(d_\ell\) the fractal dimension of the lattice spanning cluster at the threshold. We show that these relations also hold for protected percolation. We note that it was not clear from the outset whether the same set of scaling relations would hold for protected percolation since the evolution of isolated clusters is different from that of the lattice spanning cluster while the scaling relations relate the critical exponents belonging to both sets of clusters. Also note that the fractal dimension of the lattice spanning cluster at the threshold is necessarily identical between standard and protected percolation: upon emptying the lattice (using an identical sequence of random numbers), identical sites will be removed from the lattice spanning cluster until it breaks up. Only the morphology of the finite-sized clusters differs between protected and standard percolation.

Assuming scaling relationships to hold [1–3], and using that the fractal dimension of the lattice spanning cluster is identical for both protected and standard percolation \(d_\ell = d_\ell\), we obtain the following relationships between the critical exponents for standard and protected percolation (as well as equation (13)): 

\[
\begin{align*}
\gamma' &= \frac{\gamma}{1 + \beta}, \\
\tau' &= \tau, \\
\nu' &= \frac{\nu}{1 + \beta}
\end{align*}
\]

where \(\nu\) is the critical exponent for the correlation length. We show in figure 5 and table 2 that these relationships are indeed borne out by our data and thus the scaling assumption appears to be justified for protected percolation as well; in particular, it is evident from figure 5(c) that \(\tau' = \tau\) independent of any fitting procedure.

The Harris criterion (equation (1))) is violated in three-dimensions for protected percolation, but not in two-dimensions. We list the value of the Harris criterion for each case in table 2, demonstrating that it is violated for

\[
x = \left(\frac{P'_0}{P_0}\right)^{1/\beta} (x')^{\beta'/\beta}.
\]

Substituting equation (11) into equation (10), we find [6]

\[
\beta P'_0 (x')^{\beta - 1} = \frac{\beta P}{x} = \frac{\beta P}{\left(\frac{P_0}{P_0}\right)^{1/\beta} (x')^{\beta'/\beta}}.
\]

Since this equality holds for all values of \(x'\), we must have that the prefactors as well as the powers of \(x'\) match on both sides. Solving this, we find

\[
\beta' = \frac{\beta}{1 + \beta}
\]

\[
P'_0 = (P_0)^{1/(\beta + 1)} ((1 + \beta)P_0)^{\beta/(\beta + 1)}.
\]
three-dimensional protected percolation ($1.8811 < 2$). As such, any three-dimensional protected percolation system should display unique critical exponents that depend on the details of the impurities in each system.

4. Discussion

Our results are relevant to heavily-doped quantum critical systems such as Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$ [4] and UCu$_4$Pd [19, 20]. Based on neutron scattering experiments it was found that, upon cooling, isolated clusters form in Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$ [21] and that they are protected from further degradation, as we detail next. As such, our protected percolation model captures the essence of the physics in doped quantum critical systems.

In systems such as Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$, Kondo shielding removes magnetic ions from the lattice, but because of the distribution of Kondo shielding temperatures that is inherent to doped systems, not all moments disappear at the same temperature and a percolation scenario ensues upon cooling. Whereas the clusters appear as short-range magnetic order in scattering experiments, they can actually be identified as random clusters through their correlation lengths: these clusters, when observed in such neutron scattering experiments [21], span identical numbers of moments along disparate crystallographic directions; also, they were observed to persist down to the lowest temperatures [21]. Given that the order is short-ranged and that the magnetic Ce-ions are separated by much larger distances along the c-axis than along the a-axis in this tetragonal compound ($c/a = 2.5$), one would not have expected identical numbers of moments to be correlated along all directions.

After all, the strength of the ordering interaction depends on the separation between Ce-ions. However, fully ordered, randomly formed clusters do come with the prediction of identical numbers of moments ordering, independent of the interaction strength [21]. In this particular system, the distribution of interatomic separations originating from Fe/Ru doping resulted in a distribution of Kondo screening temperatures as these are exponentially sensitive to interatomic separations [5, 22]. Therefore, each of the Ce-ions will be Kondo shielded at a unique temperature, thereby creating a percolation network upon cooling.

Once clusters of magnetic ions become separated from the infinite cluster, the moments on these clusters will align with their neighbors. This is a straightforward quantum mechanical finite-size effect [4, 6]. The magnon dispersion that dictates how much energy it would cost to misalign neighboring moments is no longer a continuous dispersion when it pertains to finite clusters. Rather the dispersion becomes a set of discrete points where the wavelength of the disordering fluctuation has to match the size of the cluster, or be related to it through an integer. This results in the lowest possible energy for a disordering fluctuation to end up having a finite cost in energy. Given the steepness of magnon dispersions and the low temperatures of quantum critical systems in regions of interest, such energies or not available as thermal fluctuations. Therefore, the moments on isolated clusters must line up as soon as they become isolated, shedding entropy in the process [23].

In addition, this percolation network must be a protected percolation network: isolated clusters are protected from further moment removal as the Kondo screening mechanism involves a spin-flip process [5, 7]. Such a process is highly unlikely in a magnetically ordered environment. Therefore, isolated clusters are protected from further degradation, as in our protected percolation model. The persistence of such isolated clusters in Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$ was demonstrated in an extensive series of polarized neutron scattering experiments [4]. In all, our percolation results should be directly applicable to (heavily-doped) quantum critical systems.

Given that the Harris criterion is violated, this would offer natural explanation as to why universal critical exponents for quantum phase transitions have not been obtained despite such systems having been widely studied [24, 25]. If, in fact, heavily-doped quantum critical systems follow a three-dimensional protected percolation model that violates the Harris criterion, we would not expect universal behavior because of the intrinsic disorder in these systems. We are currently performing MC simulations with added impurities in order to assess what level of impurity would lead to an experimentally observable change in critical behavior.

In conclusion, protected percolation represents a new universality class with critical exponents that analytically relate to those of standard percolation [6] and that violate the Harris criterion in three-dimensions. As such, impurities (should) lead to system dependent critical exponents causing universal behavior to disappear. Protected percolation models heavily-doped quantum critical systems whose isolated magnetic clusters become ‘protected’ from Kondo screening. We have found quantum critical compounds that follow this model, such as Ce(Fe$_{0.76}$Ru$_{0.24}$)$_2$Ge$_2$ [4]. Our work leads to a natural explanation as to why universal critical exponents have not been found for quantum critical systems.

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