ON SITE PERCOLATION
ON THE CORRELATED SIMPLE CUBIC LATTICE

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We consider site percolation on a correlated bi-colored simple cubic lattice. The correlated medium is constructed from a strongly alternating bi-colored simple cubic lattice due to anti-site disordering. The percolation threshold is estimated. The cluster size distribution is obtained. A possible application to the double 1:1 perovskites is discussed.

Keywords: Correlated percolation; Percolation threshold; Simple cubic lattice; Double perovskites.

1. Introduction

In percolation theory one aims to model random (disordered) media to evaluate their typical properties. The simplest example is called Bernoulli percolation, where all sites have the same probability to be occupied independent of each other. The assumption of stochastic independence is too strong for consider many natural systems. For such systems a medium is not Bernoulli rather then correlated. Recently, a particular lattice topology and a particular constraint were investigated. We will deal with another particular correlated medium.

Let us consider a strongly alternating bi-colored simple cubic lattice (Fig. 1). Each ‘white’ site is surrounded by ‘black’ ones and vice versa, i.e. each of the sites is isolated and forms a cluster of unit size. The medium is fully ordered. One can divide the lattice into two sublattices: ‘black’ and ‘white’. The probability that a ‘white’ site belongs to the ‘white’ sublattice is unity. Let us assume that alternating order is partially destroyed. We will denote $p$ the probability to find a ‘white’ site in the ‘black’ sublattice. If $p > 0$, then one can find a ‘white’ cluster of size more than the unity. If $p = 0.5$ (fully disordered system) then there is an infinity cluster indeed, because the site percolation threshold for the simple cubic lattice and Bernoulli percolation is 0.311608. We will look for a critical disturbance $p_c$ where an infinity cluster is formed, for the first time.

2. Cluster size distribution
The probabilities per cluster site $n_s$ that a randomly chosen lattice site belongs to a cluster of $s$ sites are

\begin{align*}
n_1 &= \frac{1}{2} \left( (1-p)^7 + p^7 \right), \\
n_2 &= 3p^6(1-p)^6, \\
n_3 &= \frac{3}{2} p^5(1-p)^5 \left( p^7 + (1-p)^7 + 4p^6 + 4(1-p)^6 \right), \\
n_4 &= 3p^{11}(1-p)^{11} + 51p^{10}(1-p)^{10} \\
&\quad + 6p^4(1-p)^4 \left( (1-p)^{12} + (1-p)^{12} \right) + 4p^4(1-p)^4 \left( (1-p)^{11} + (1-p)^{11} \right), \\
n_5 &= \frac{3}{2} p^{10}(1-p)^{10} \left( (1-p)^7 + 8p^6 + 8(1-p)^6 \right) \\
&\quad + 32p^5 + 32(1-p)^5 + 8p^4 + 8(1-p)^4) \\
&\quad + 12p^9(1-p)^9 (p^8 + (1-p)^6 + 3(1-p)^7 + 8 (p^6 + (1-p)^6)) \\
&\quad + \frac{15}{2} p^3(1-p)^3 \left( (1-p)^{17} + (1-p)^{17} \right).
\end{align*}

The numerical results were obtained using Hoshen–Kopelman algorithm. We investigated a number of sample lattices with linear size $L$ up to 128 sites. The theoretical results and the computer simulations are in the reasonable agreement (see Fig. 2–6).

Cluster size distribution is surprising. In contrast with Bernoulli percolation one can see the oscillations (see Fig. 7–8). If $p = 0.5$ (disordered medium) then the
distribution demonstrates classical behavior (Fig. 9). In Section 4 we will discuss a possible connection such oscillations with the experiments and the real world systems.

3. Numerical estimation of percolation probabilities

Estimates for $p_c$ have been obtained by means of percolation frequencies. Simulations give the percolation frequencies, which serve as an approximation of the percolation probability. Critical percolation have been estimated by not-linear fit functions defined by

$$p = \frac{1}{2}(1 + \text{erf}((p - p_c)/a))$$

(6)

and

$$p = (1 + \exp(-(p - p_c)a))^{-1}.$$  
(7)

The first function converges to a step function as $a \to 0$ and the second one as $a \to \infty$. Moreover we used a polynomial of 3-th degree. The fits gave almost the same results for the places (the values of $p$) where the spanning probability curve reaches a value of $1/2$. The similar approach to estimate the critical probabilities was performed in works.\textsuperscript{2,6} Numerical estimation suggests that $p_c \approx 0.147$ for $L = 128$ (Fig. 10).

The percolation threshold was calculated for three values of the linear lattice size $L = 32, 64, 128$. The percolation threshold $p_c(\infty)$ for infinite lattices can be
Fig. 3. The probability that an arbitrary site belongs to cluster of size $s = 2$. Solid line — from Eq. 2, crosses — numerical data. Here and below one can see a visible deviation from the theoretical curve because of well known finite size effect for the large clusters.¹

Fig. 4. The probability that an arbitrary site belongs to cluster of size $s = 3$. Solid line — from Eq. 3, crosses — numerical data.
Fig. 5. The probability that an arbitrary site belongs to cluster of size $s = 4$. Solid line — from Eq. 4, crosses — numerical data.

Fig. 6. The probability that an arbitrary site belongs to cluster of size $s = 5$. Solid line — from Eq. 5, crosses — numerical data.
Fig. 7. Cluster size distribution for $p = 0.05$. Here and below cluster of unit size is omitted because of very large magnitude.

Fig. 8. Cluster size distribution for $p = 0.1465$. 
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Fig. 9. Cluster size distribution for $p = 0.5$.

Fig. 10. Percolation frequency as a function of $p$ ($L = 128$) (high resolution).
found by fitting these results for different lattice sizes to the scaling relation

$$|p_c(L) - p_c(\infty)| \propto L^{-1/\nu},$$

where the critical exponent $\nu$ has the value 0.875 in three dimensions. This method leads to an estimate $p_c(\infty) \approx 0.1454$ (Fig. 11).

We observed some infinity clusters at percolation threshold, nevertheless we cannot assert there is not a finite size effect.  

4. Possible applications to the double 1:1 perovskites

In last decades, much attention has been paid to ABO$_3$ perovskite-type oxides due to their unique dielectric, electrooptic, and other properties. Complex perovskite-like oxides of the AB$_2$B'O$_3$ type, in particularly double 1:1 perovskites AB$_{1/2}$B'O$_3$,* e.g. (Ba, Sr)Fe$_{1/2}$Mo$_{1/2}$O$_3$ and PbFe$_{1/2}$Nb$_{1/2}$O$_3$, have much more surprising and useful properties. Examples of their applications are piezoelectric transducers and actuators, non-volatile ferroelectric memories, and microelectronic devices. The structure is built up by ordering perovskite blocks in a rock salt superlattice (Fig. 12) and the properties of the material are thought to critically depend on this ordering. The double perovskite Sr$_2$FeMoO$_6$ and related materials are good candidates for magnetic devices, as they combine a high Curie temperature and a fully polarized (half metallic) conduction band. For more detailed overview and a large collection of references see e.g.  

*Such the alloys are denoted as A$_2$BB'O$_6$, too.
Fig. 12. An example of ordered 1:1 double perovskite: PbFe\(_{1/2}\)Nb\(_{1/2}\)O\(_3\). Atoms of Fe and Nb form an alternating simple cubic lattice.

Little thing is known and understood about the microscopic mechanisms responsible for their very convenient properties. At the present, these materials are being extensively studied. One particular aspect that seems very promising is the effect of atomic ordering on the properties of these alloys. Anti-site disordering in Sr\(_2\)FeMoO\(_6\) double perovskites (containing B atoms at B\(_\prime\) positions, and vice versa) has recently been shown to have a dramatic influence in their magnetic and magnetotransport properties. Experiments suggest that, in many samples, the saturation magnetization is less than the expected value. This effect is usually ascribed to the presence of antisite defects, where, due to the similarity of their atomic radii, Mo ions are randomly placed on the Fe sublattice and conversely.

A model described above seems very promising to understand some features of the double perovskites. In particularly, the oscillations of the hyperfine magnetic fields distribution in the PbFe\(_{1/2}\)Nb\(_{1/2}\)O\(_3\) samples\(^{11}\) may be related with the oscillations of the cluster size distribution (Fig. 7,8).

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