

## Concentration Transitions on the Crystalline Lattices

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Results of numerical modeling of dilute 2D and 3D crystalline lattices are presented. The percolation thresholds for face-centered cubic (fcc), body-centered cubic (bcc) and the simple cubic (sc) lattices for the first, second and third coordination spheres are obtained by means of Monte Carlo (MC) method. It is shown, that the mean value of the percolation cluster density has a minimum value at the percolation threshold.

**Keywords:** Condensed matter physics, Phase transitions, Monte Carlo simulation, Lattice gauge theory.

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### 1. INTRODUCTION

Active studies of magnetic properties of 2D and 3D crystalline and amorphous systems with controlled degree of disorder has a place due to the wide use of magnetic materials in the manufacture of non-volatile memory devices [1, 2]. In addition, the development of nanotechnology supposes the using of the finite size systems, while most of the theoretical results obtained for the case of infinite systems [3-9]. Therefore, considerable interest in the research of a concentration of transitions for 2D and 3D systems of finite sizes.

In [10, 11] formulated the approach, which allows us to calculate the distribution function of the random fields of the exchange interaction. Interesting conclusion of this approach is an analytical expression for the critical concentration (percolation threshold).

In this paper we present the numerical Monte Carlo simulation of 2D and 3D systems, which are randomly distributed magnetic atoms, in order to study the features of the concentration transitions.

### 2. CALCULATION OF THE CRITICAL CONCENTRATION OF MAGNETIC IMPURITIES

As it was shown in [10, 12], the critical concentration  $p_c$  magnetic atoms interacting through direct exchange interaction

$$p_c = 2/z \quad (1)$$

The expression (1) allows calculate the critical concentration for lattices with coordination number  $z$ . It is possible to see, these critical concentration are very close to the percolation threshold. Comparison of the

critical concentration  $p_c$  with the results of percolation theory allows indirectly estimate the range of applicability of the approximations and the accuracy of the method of random fields of the exchange interaction.

Table 1 presents the critical concentration for comparison  $p_c^1$ , obtained for bulk lattices of random fields of the exchange interaction by the formula (1) and  $p_c^2$  [13]. Figures 1, 2, 3 denote the number of coordination spheres. Observations show that up to  $p_c \sim 0.08$  difference between  $p_c^1$  and  $p_c^2$  does not exceed 20 %.

### 3. MONTE CARLO SIMULATION OF DILUTED CRYSTAL LATTICE

In addition to the determining the percolation thresholds by means of the numerical simulation we obtained the information on such important characteristics of partially disordered media as the average cluster size, the maximum density of the cluster, the proportion of particles in the clusters of a given size. Results of calculations of the cluster size distribution depending on the concentration of atoms  $p$  near the percolation threshold for the fcc lattice of  $100 \times 100 \times 100$  shown in Fig. 1.

Histograms in Fig. 1 clearly show the distribution law for the occupied sites  $N_s / N$ , located in clusters of a given size  $N_s$  approaching the percolation point for small concentrations ( $p < p_c$ ) at percolation point ( $p = p_c$ ) and above ( $p > p_c$ ).

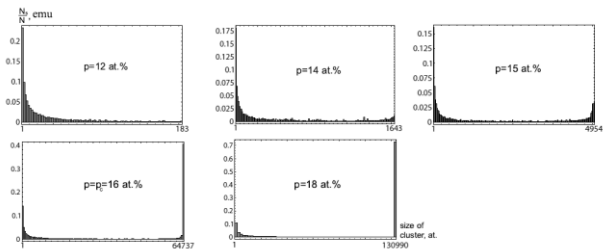
Percolation, or the formation of a maximal cluster, characterized by a sharp increasing of the proportion of occupied sites in the percolation cluster. With changing concentration on 6 % (from 12 % to 18 %) for the fcc lattice to a total amount of  $10^6$  sites maximal cluster

**Table 1** – Percolation threshold of the site problem with connections between remote neighbors in comparison with the calculated values of the critical concentrations by means of MC

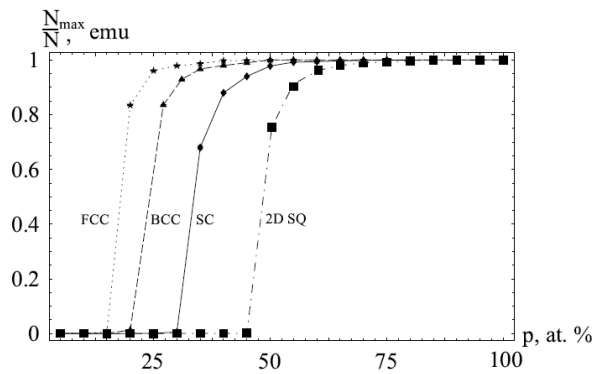
The lattice type	FCC 1	FCC 2	FCC 3	BCC 1	BCC 2	BCC 3	SC 1	SC 2	SC 3
$Z$	12	18	42	8	14	26	6	18	26
$p_c^1$	0.167	0.111	0.047	0.250	0.143	0.077	0.333	0.111	0.077
$p_c^2$ [14]	0.195	0.136	0.061	0.253	0.175	0.095	0.307	0.137	0.097

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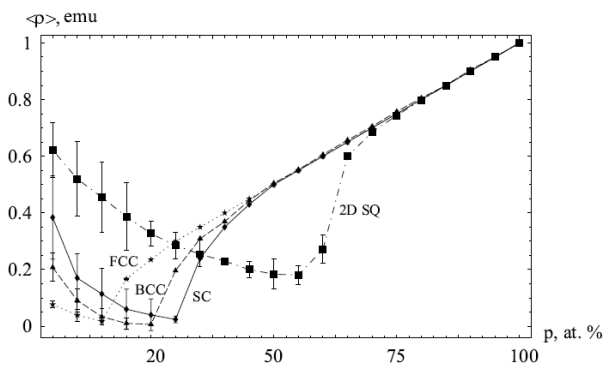
size increased on the 3 orders of the magnitude, in this case from  $10^2$  to  $10^5$ . Fig. 2 shows the density of lattice's cites in the maximal cluster in dependence of total concentration. Figure Notes: FCC – face-centered cubic lattice ( $p_c = 16\%$ ), BCC – volume centering cubic lattice ( $p_c = 25\%$ ), SC – a simple cubic lattice ( $p_c = 33\%$ ), 2D SC – just a flat square lattice ( $p_c = 50\%$ ).



**Fig. 1** – Distribution of atoms in clusters for different concentrations of  $p$  near the percolation threshold for the fcc lattice with  $10^6$  cites



**Fig. 2** – The maximum proportion of atoms in the cluster according to the impurity concentration of  $p$ . For all lattices – fcc, bcc, sc and 2D sc 106 the number of nodes



**Fig. 3** – The mean value of the density of the maximal cluster, depending on the concentration of lattice sites occupied

As can be seen from Fig. 2 the relative size of the largest cluster increases sharply. Results of numerical experiments for lattices with the number  $10^6$  indicate good repeatability – error interval for the values of the

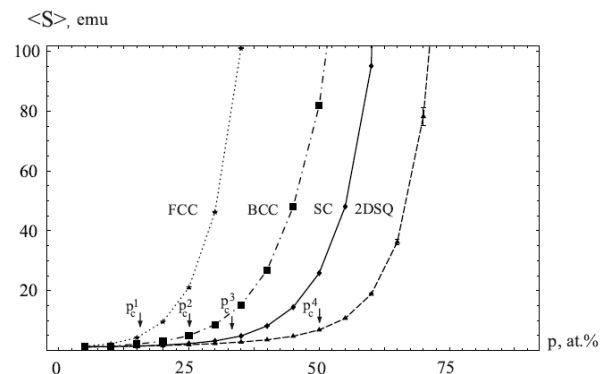
maximum size of the cluster obtained in the experiment is too small (smaller than the size of the points, which shown in the illustration). As the ferromagnetism is a manifestation of quantum properties in macro scale (a phenomenon of the correlated behavior of the spin system combined into a very large cluster) calculated percolation thresholds allow to make conclusions about the critical concentration necessary for the occurrence of ferromagnetism. Thus, the formula (1) allows us to calculate fairly accurately the critical concentration required for ferromagnetic ordering in the particle containing  $\sim 10^6$  cites.

The average density of the maximal cluster  $\langle p \rangle$  with increasing impurity concentration decreases, reaching the minimum in percolation point, see Fig. 3. In this point the percolation cluster has very "porous" structure, and accordingly, a very low density.

Average cluster size is calculated by the formula

$$\langle S \rangle = \frac{\sum_i N_i S_i}{\sum_i N_i} . \quad (2)$$

For finite lattices, particularly for lattices  $10^6$  dimensions, the average cluster size increases linearly with increasing concentration, and the growth rate increases considerably cluster after percolation threshold crossing (Fig. 4.).



**Fig. 4** – Dependence of the mean value cluster size on the concentration of occupied cites. - Critical concentration limits obtained in percolation theory for FCC, BCC, SC and 2D SC lattices, respectively

From the results of that analytically obtained by the method of random fields of the exchange interaction expression for the critical concentration, makes it simple to estimate the magnitude of percolation thresholds  $p_c$ , necessary for the existence of the concentration of different types of transitions in lattices. It is observed good agreement of theory and numerical experiments.

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