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SITE PERCOLATION THRESHOLDS OF FCC LATTICE

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Percolation thresholds, p_c , for site diluted spin systems on the fcc lattice are determined for exchange interactions extending up to the shell of the fourth nearest neighbors. If the interactions include the nearest, second, third, and fourth neighbors, p_c is equal to 0.198, 0.136, 0.061, and 0.05 respectively. These results agree with the Roberts approximate formula for p_c . Estimation of p_c to even longer-ranged couplings is presented. For instance for $p_c = 0.01$ the range of the couplings should extend at least to the eight shell of neighbors.

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In many diluted magnetic semiconductors (DMS) [1] the magnetic ions occupy randomly selected sites on the fcc lattice. The properties of such systems are governed by the site occupational probability x of the magnetic ions. For large enough x one observes ordered magnetic structures, like antiferromagnetism of the III kind seen in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ [2]. For intermediate values of x the systems show features typical of spin glasses. The frustration here is due to an interplay between randomness and the fcc lattice geometry. Existence of any magnetic ordering, such as occurring in spin glasses, requires that the exchange interactions span the system in a percolating fashion. Otherwise the system would consist of isolated and thus paramagnetic magnetic clusters. The percolation threshold p_c is defined here as the lowest value of x such that one observes a cluster which spans an infinite system. The effective value of x depends on the range of interactions in the system. For instance, if only the nearest neighbor interactions are present, i.e. the coordination number $z = 12$, $p_c = 0.195$ [3]. Thus one would expect that for x

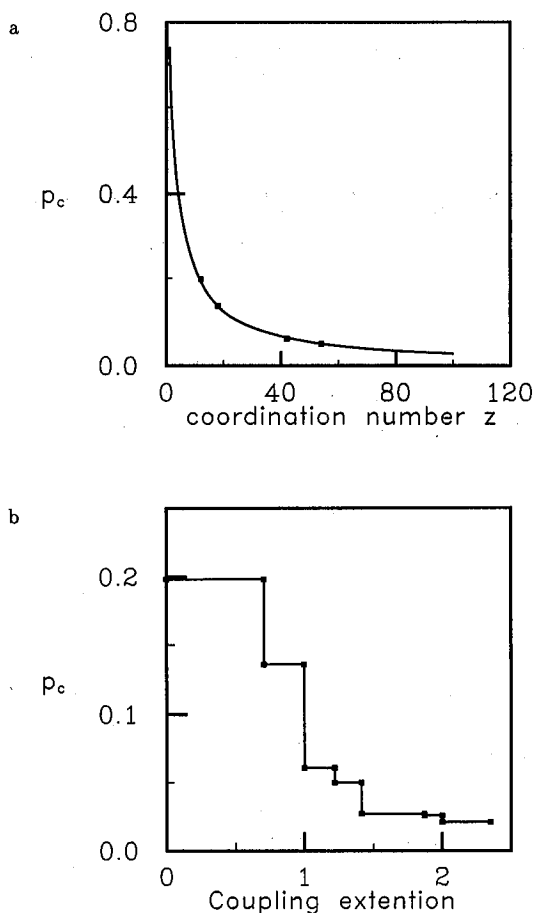


Fig. 1. The dependence of p_c on the coordination number z (a) and on the coupling range in units of the lattice constant (b), for the interaction extending to first, second, third, and fourth nearest neighbors, respectively.

less than this value there would be no spin glass phase allowed. There are many evidences, however, that the spin glass order exists at much lower values of x . This points to existence of longer ranged couplings. Giebultowicz, e.g., finds that in $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ the next nearest neighbor interaction is in absolute value equal to 0.1 of the nearest neighbor exchange coupling. Swagten et al. [4] even suggest existence of couplings which decay with distance as a power law $\sim R^{-6.8}$ even though the DMS systems studied were not metallic. Grabecki et al. [5] observe a cusp in the susceptibility of $\text{Hg}_y\text{Cd}_{1-y-x}\text{Mn}_x\text{Te}$ for $y = 0.80$ and $x = 0.01$ in the millikelvin range. This may or may not be an equilibrium effect but clearly points to longer ranged couplings. In this case these effects may be for instance due to the dipole-dipole interactions [6].

In this paper, we investigate the dependence of p_c on the connectivity as determined by the range of the exchange interactions. Our results are as follows:

$$\text{second nearest neighbors} \quad (z = 18), \quad p_c = 0.136, \quad (1)$$

$$\text{third nearest neighbors} \quad (z = 42), \quad p_c = 0.061 \pm 0.0005, \quad (2)$$

$$\text{fourth nearest neighbors} \quad (z = 54), \quad p_c = 0.050 \pm 0.0005, \quad (3)$$

where the corresponding coordination numbers are shown in the brackets. The plot of p_c 's vs. z is shown in Fig. 1a. Results (1), (2) agree with those obtained by the series expansion for the mean cluster size [7], but the couplings extending to the fourth nearest neighbors have not been considered. Roberts [8] has suggested that p_c of ordered, disordered, and random lattices can be approximately represented by the universal formula

$$p_c \approx (a_D z + b_L)^{-1}. \quad (4)$$

For ordered lattices, such as the fcc lattice considered here $b_L = 1$ and $a_D = 0.350$ (for the dimensionality $D = 3$). Our results agree with this formula very well as seen in Fig. 1a. The deviations are 3%, 2%, 4%, and 0.5% for the first, second, third and fourth nearest neighbor, respectively. In Fig. 1b the dependence of p_c on the coupling range (in lattice constant units) is presented. It is seen that for the coupling range extending to the seventh shell of neighbors ($z = 132$) $p_c = 2.1$. In order to obtain p_c close to 0.01, z of 283 is needed, which requires interaction extending beyond the eight shell of neighbors.

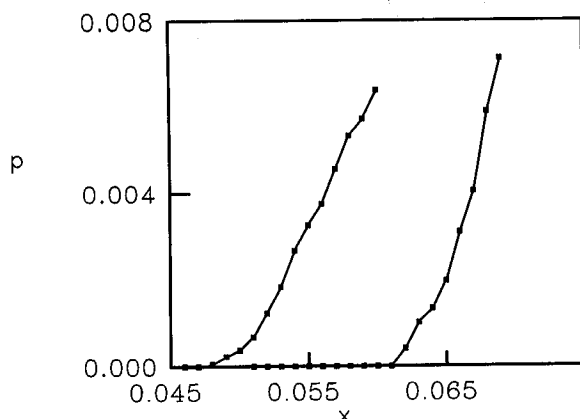


Fig. 2. The dependence of p_c vs. x for the interactions extending to third and fourth nearest neighbors (for the system with 4×45^3 lattice sites).

Our results were obtained in the following way. We used Hoshen and Kopelman's [9, 3] algorithm for percolation analysis on fcc lattice with the number of the lattice sites up to 4×45^3 . For each size of the system and for each occupation probability we made an average over 1000 different random realizations. Results (1), (2), (3) were obtained as extrapolation of results for different lattice sizes. In

Fig. 2 we show results for the largest size of the system and interactions including third and fourth neighbors.

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