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Correlation Function and Misfit in a Computer-Simulated Two-Dimensional Amorphous Ising Antiferromagnet

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Amorphous systems with antiferromagnetic interactions (e.g. glasses containing high concentrations of transition elements (1, 2) and ferrimagnetic rare earth-transition metal amorphous films for bubble devices (3, 4)) have been the subject of several investigations. Nevertheless up to now the existence of amorphous antiferromagnetism is a controversial point (5, 6) because of the high degree of misfit: Due to the structural disorder it is not possible to surround a plus spin by minus spins only or vice versa. By artificially suppressing the misfit the simple sublattice model of amorphous antiferromagnets (7 to 9) favours an antiferromagnetic order in an inadmissible way.

We have simulated a kind of hard sphere gas. Hard disks, positions of which are chosen as random numbers, are put into a two-dimensional box. Periodical boundary conditions are used (Fig. 1). Within the Ising model with the Hamiltonian

$$H = -\sum_{i<j} I_{ij}(r) S_i^z S_j^z$$

we have calculated that spin configuration which belongs to the lowest energy (ground state) for the case $S = 1/2$ and $I_{ij}(r) < 0$.

The result is shown in Fig. 1 for 23 spins and a distance dependend exchange interaction as given in Fig. 2b.

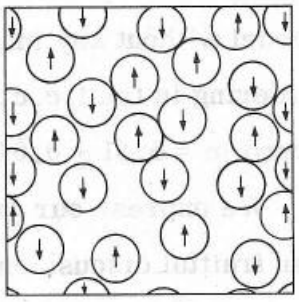

Fig. 1. Ground state of a computer-simulated amorphous antiferromagnetic Ising system

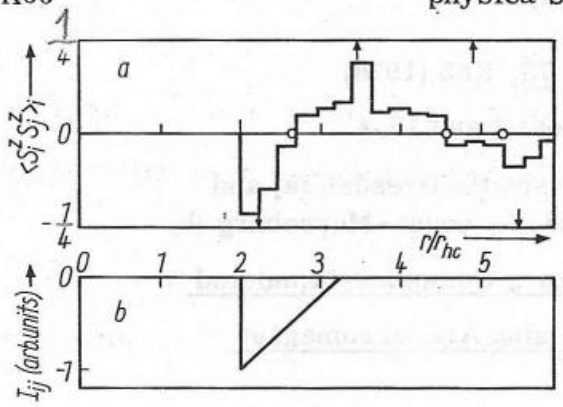

Fig. 2. Distance dependence of a) the structural correlation function $\langle S_i^z S_j^z \rangle_i$; the circles and arrows belong to the triangular and square lattices, respectively; b) the exchange integral $I_{ij}(r)$

The structural correlation function $\langle S_i^z S_j^z \rangle_i$ (see (10) and the recent paper by Sadoc (11)) as function of r is shown in Fig. 2a. Here $\langle \ldots \rangle_i$ denotes the structure averaged value under the condition that the spin i has a fixed direction (central spin). To calculate the average value we have chosen successively all spins of a given system as the central spin and beyond it we have regarded an ensemble of 7 systems with the same structural and magnetic interaction, but with other random numbers for the positions of spins.

For total missing of antiferromagnetic order we would obtain for the structural correlation function $\langle S_i^z S_j^z \rangle_i = 0$ for all r (total misfit, e.g. triangular lattice (12)). The other limit case (without misfit) is realized by a system with $\langle S_i^z S_j^z \rangle_i = 1/4$ or -1/4 at the discrete positions of spins. For a square lattice this is marked by arrows in Fig. 2a. Our curve lies between these both cases. The maxima are smeared out for higher distances.

Beside the correlation function we have determined the quantity

$$m = \frac{E_{max} - |E_o|}{E_{max}} ,$$

where E_o is the ground state energy and E_{max} the energy for that configuration, at which all spins are aligned parallel. This quantity can be considered as a measure of this misfit of the whole system and as a number between 0.0 (b.c.c. two-sublattice model without any misfit) and 1.0 (total misfit). For the first type of antiferromagnetic ordering in the f.c.c. lattice one gets m = 2/3, and for our amorphous system we found $m = 0.31 \pm 0.04$.

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