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Ground State of an Ising Antiferromagnet with a Dense Random Packing Structure

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Although the existence of ferromagnetism in amorphous materials is well confirmed both from the theoretical and the experimental point of view the appearance of antiferromagnetism in such substances is dubious. First a simple theory of amorphous antiferromagnetism was given using the molecular field theory.[1,2] The structural disorder was simulated by a sublattice model, i.e., the spins were arranged on lattice points with the antiferromagnetic exchange interactions between them fluctuating randomly. However, in this model all nearest neighbors of a given spin belong to the other sublattice. This assumption is an inadmissable restriction, since in real amorphous systems it is impossible to surround a plus spin by minus spins only or vice versa. Amorphous antiferromagnetism can be disfavored by having the so-called misfit structure, which also occurs in some crystalline antiferromagnets (e.g., fcc lattice with nearest neighbor interaction).[3-5] For an improved description random packing of hard spheres, which succeededs in interpreting the radial distribution functions of amorphous systems, are more suitable structure models. Recently there are first attempts to investigate magnetic properties using these models.[6-8]

Several methods have been given to construct random packings by computer. We follow the procedure proposed by Finney[9] to obtain very dense packings by an algorithm which involves the possibility of local rearrangements of spheres: The coordinates of the centres of the spheres are chosen by a pseudo-random number generator. In the case of overlaps the spheres are moved along the connecting lines between the centres until they just touch, irrespective of other overlaps that may be created. After removing successively all overlaps the sphere diameter is increased by a small amount

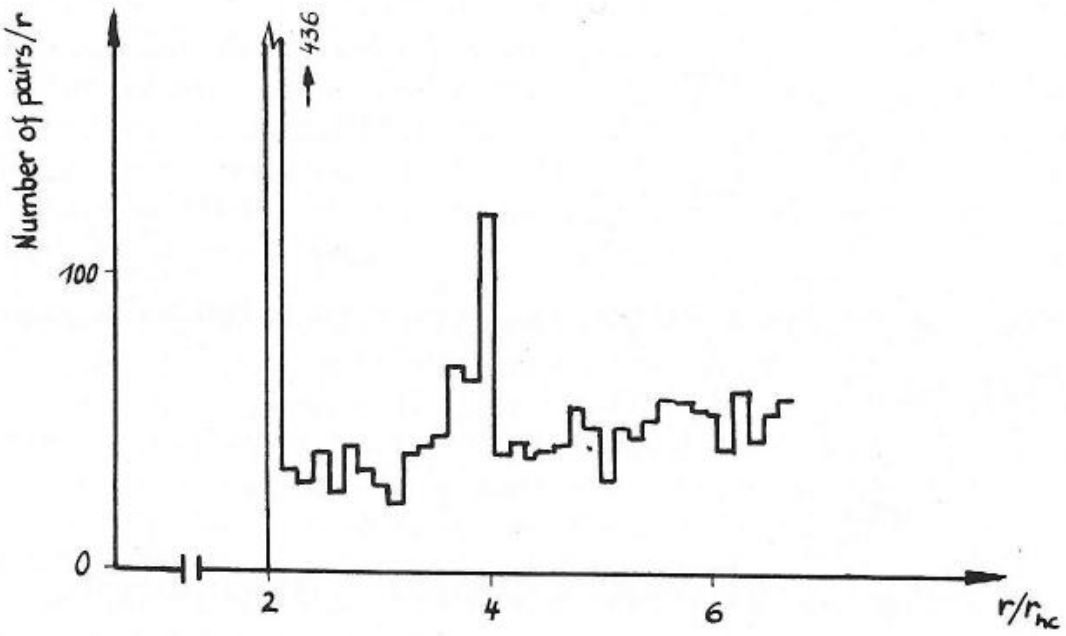

Fig. 1. a. Radial distribution function.

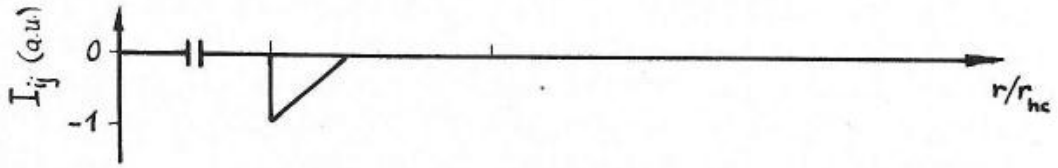

Fig. 1. b. Exchange interaction.

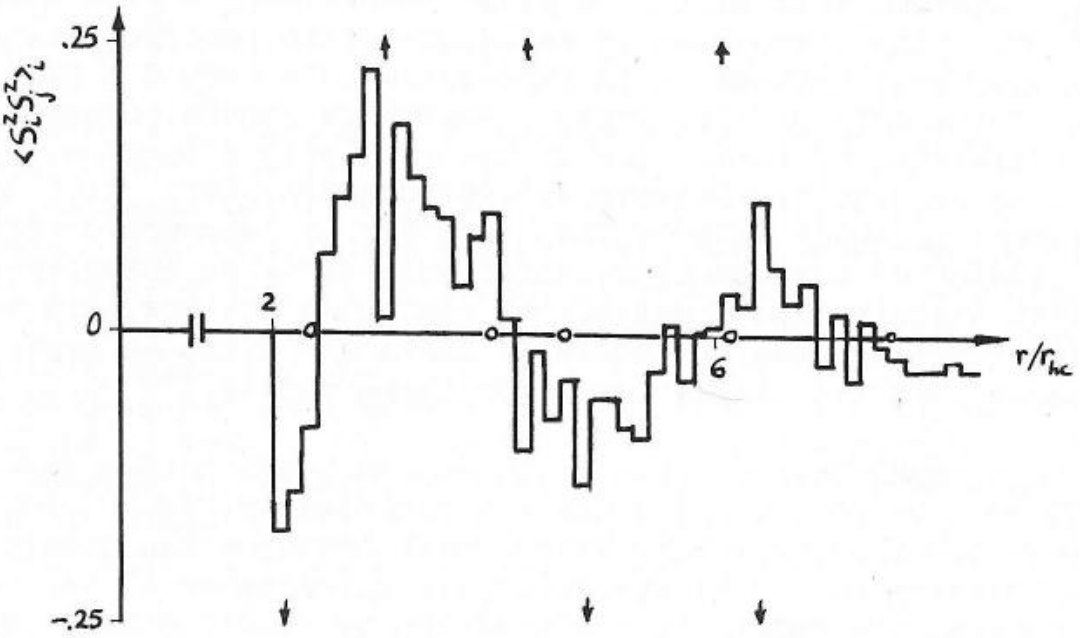

Fig. 1. c. Correlation function $\langle S_i^z S_j^z \rangle_i$; the circles and arrows belong to the triangular and square lattices, respectively, with the same density.

and the procedure is repeated. We have used a two-dimensional version of this algorithm with N = 40 disks in a square box. As opposed to Finney's original work, in which a cluster of 500 spheres with free boundary is considered, we have chosen periodic boundary conditions because of the great portion of surface disks in our small system. In the example of Fig. 2 the density is ρ = 0.68, i.e., 68% of the full square is occupied by disks. The histogram of the radial distribution function is shown in Fig. 1a. For the averaging procedure all disks are successively chosen as centres. An ensemble of 3 systems is constructed with the same density, but with another set of starting coordinates.

Considering the random structure obtained as a fixed one we start with the Ising Hamiltonian in the absence of an external field,

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

for S = 1/2; and we calculate the exact magnetic ground state, where a simple distance dependent antiferromagnetic exchange interaction $I_{ij}(r)$ with limited range is assumed (Fig. 1b). The result is shown in Fig. 2. If we identify as neighbors all spins within the magnetic interaction range of each other and we find that the average number of neighbors is 4.5. Figure 3 shows the distribution of the effective fields H_{eff} discussed by Simpson[1,5].

A more quantitative representation can be given by plotting the "magnetic radial distribution function". In analogy to the structure description by the radial distribution function we consider the probability of magnetic ordering of a spin having a certain distance from a central spin. Such information is involved in the correlation function $\langle S_i^z S_j^z \rangle_i$, where $\langle \ldots \rangle_i$ is the structure average value under the condition that the central spin i has a fixed direction[7,10,11]. A histogram of the distance dependence of this function in Fig. 1c shows a short-range antiferromagnetic order with more and more smeared out extrema at higher distances. (For the average procedure again all spins of the 3 equivalent systems are successively chosen as central spins.) For an amorphous ferrimagnet a corresponding correlation function was obtained by Rhyne et al.[12] with neutron diffraction measurements on $TbFe_2$.

Except for the first one, the extrema in the magnetic and the structural radial distribution functions seem not to be correlated. For a loose 23 spin system the magnetic curve is related to the values for the triangular and the square lattices with the same density[7]. This correspondence is well confirmed in our case.

Since every spin, which is aligned parallel to its neighbor due to misfit, increases the ground state energy E_o compared to

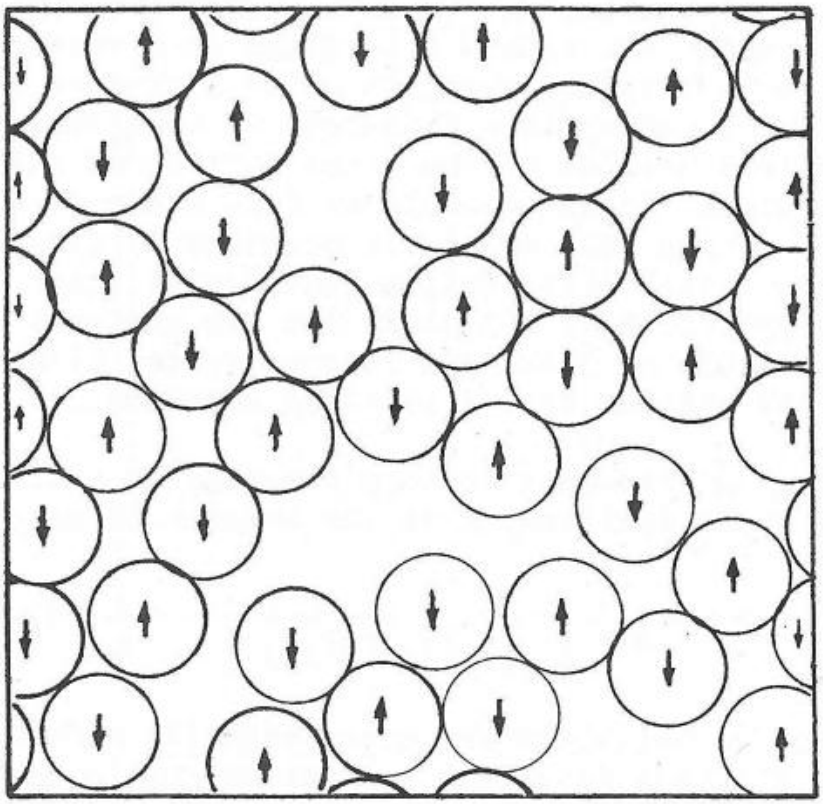

Fig. 2. Ground state of a computer-simulated amorphous antiferromagnetic Ising system with periodical boundary conditions.

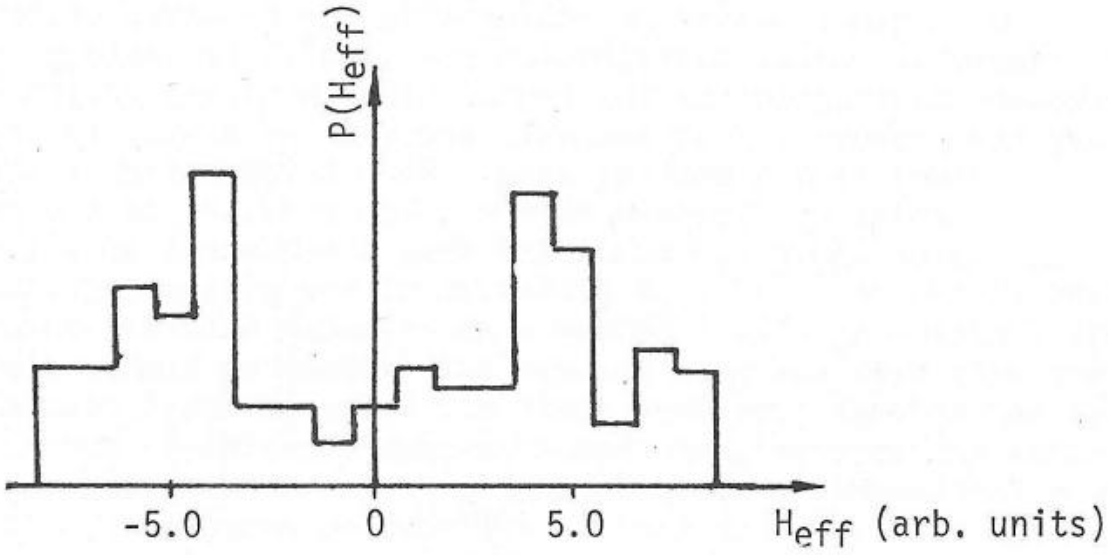

Fig. 3. Distribution of the effective fields H_{eff}.

that of an ideal system without any misfit (E_{id}), a global misfit parameter

$$m = 1 - \frac{E_o}{E_{id}}$$

is proposed[7]. This parameter m is summarized in Table 1 for various crystalline lattices with nearest neighbor antiferromagnetic inter action and computer-simulated amorphous (csa) systems, where

$$\alpha = \frac{\text{range of magnetic interaction}}{\text{hard core diameter}} .$$

Table 1

Dimension	System	m
2	square	0.0
3	body-centered cubic	0.0
2	csa[7], N = 23, ρ = 0.49, α = 1,39	0.31 ± 0.04
2	csa, N = 40, ρ = 0.68, α = 1,36	0.39 ± 0.02
3	csa, N = 30, ρ = 0.58, α = 1,17	0.56
3	face-centered cubic (1^{st} type)	0.67
2	triangular	1.0

Despite the simplifications of our model and the smallness of the investigated computer-simulated random packing clusters, we have found information on amorphous systems with antiferromagnetic interactions and suggested possible descriptions. However, we cannot directly predict the existence of "long-range ordered" amorphous antiferromagnetism and transition temperatures.

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