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# PERSISTENCY OF THE SPACIALLY MODULATED ORDERED PHASES IN A DILUTED ISING MODEL

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Monte Carlo simulation was carried out to confirm persistency of the spacially modulated ordered phases against dilution of magnetic ions. The critical concentration is predicted below which the modulated structure may no longer be recognized.

## 1. Introduction

Recently the anisotropic next-nearest-neighbor Ising model has been studied extensively, because of the simplest model which shows spacially modulated magnetic structures [1]. A three dimensional simple cubic system with competing interactions between nearest layers and next-nearest layers ( perpendicular to the z axis ) exhibits the sinusoidal structures in space with the associated wave-vector q ( z-component ). The model Hamiltoian is defined by

$$H = -\sum_{NN} J_1 S_i S_j - \sum_{\substack{NNN \\ \text{in z}}} J_2 S_i S_j \quad ,$$

where NN and NNN indicate summations over nearest- and next-nearest-neighbor spins respectively. ( In the following discussion $J_1$ is set positive. ) The results obtained so far on the basis of the Hamiltonian are summarized as follows [1]: i) As a function of ratio $J_2/J_1 (\equiv \lambda)$ the Lifshitz point is determined, which separates the paramagnetic, ferromagnetic and a modulated phases. ii) The ground state is ferromagnetic for $J_1 + 2J_2 > 0$ and "two-up and two-down" antiferromagnetic for $J_1 + 2J_2 < 0$ [2]. iii) The modulated order changes stepwise in the wave-vector q as temperature varies [3,4,5]. Since the periodic structures exhibit hysteresis (metastable behavior) which is a result of subtle balance between competing interactions as well as thermal fluctuations, introduction of disorder into the magnetic structure will disturb this balance to modify the above-mentioned properties.

In the previous note [6], this point was studied on the basis of molecular field theory and high-temperature series expansion method. Within the molecular field approximation, the essential part of the results remains unchanged in the diluted system, and discussion can be done completely parallel, if the temperature T is replaced by T/p , to that of the pure system. This replacement is effective even in the higher order approximation in that the wave-vector q charactizing the modulated phases is expressed as a function of T/p in the wider range of concentration as shown in Fig.1. From the Pade approximation on poles of the susceptibility, a threshold value of the ratio $\lambda$ in the diluted system, below which the ferromagnetic state becomes unstable, is found to be the same as in the pure system, as is seen in Fig.2. And it was concluded that the essential profile of the modulated phases was kept unchanged by di-

lution. It also means that the chaotic phase is detectable if it could be seen in the pure system [7].

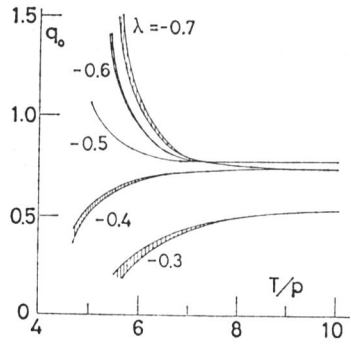


Fig. 1 Wave-vector q(p,T;λ) versus T/p. Curves [ $0.6 \leq p \leq 1$ ] are in each shaded area. [6]

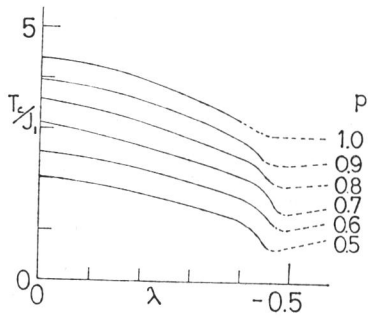


Fig. 2 Transition temperature of the mode (q=0) versus λ. Dotted curves indicate real parts of complex solutions where the ferromagnetic state becomes unstable. [6]

## 2. Results and Discussions

In this paper to confirm these properties the Monte Carlo simulation is carried out on the same Hamiltonian. A simple cubic lattice with 10 10 40 is used and periodic boundary condition is invoked. The ratio λ is fixed at 0.6 for the convenience of comparison with the previous results [2,3]. Then the temperature is normalized by the critical temperature $T_c$ ($=3.63J_1$) of the pure system [2]. Results shown below have been obtained, starting the simulation from the "two-up and two-down" configuration at a fixed concentration and temperature, by runs of at least 2000 MCS/spin ; for some points near the apparent jumps in q, as many as 4000 or 8000 MCS/spin were used. The diluted model is prepared by random deletion of magnetic ions and their sites are fixed thereafter; a quenched model is used. As a reference a lattice with 6 6 40 was also used, results on which are not reported here.

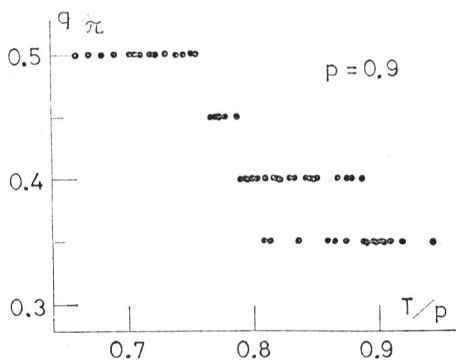


Fig. 3 Temperature dependence of wave-vector q. Temperature is scaled by T/p . Each point represents the average of several runs.

The periodicity is doublly checked by using the structure factor defined by

$$S(q) = \sum_r \langle S_0 S_r \rangle e^{iqz} \quad ,$$

and Fourier amplitude of M(z)(averaged magnetization of a layer at z) defined by

$$C(q) = \sum M(z) \exp(i\pi qz/20.).$$

Temperature dependence of the wave-vector q(T) is studied at a magnetic concentration p=0.9. It is apparent from Fig. 3 that in the wider range of temperature the wave-vector locks in at a constant value and the staircase-like behavior remains unchanged though the system is diluted. It is however found that transition temperatures of jumps in q do not necessarily obey the scaled relation T/p

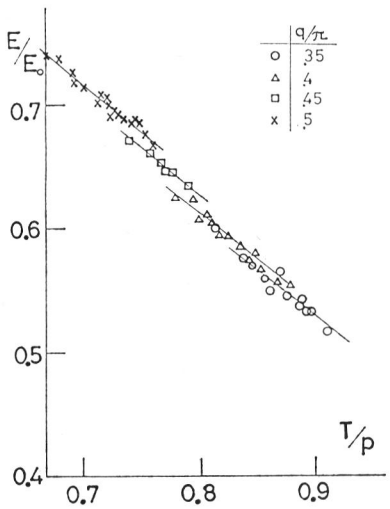


Fig. 4 Temperature dependence of the internal energy. Eo is the gound state energy of the pure system. The jumps between two neighboring phases are not clear. Lines on marks serve merely as a guide to the eye.

when compared with the pure system. In Fig. 4 temperature variation of the internal energy is shown for phases. The jumps in the energy between two neighboring phases are not clear in the diluted system as in the pure one. It may be attributed to the randomness, which broadens specturm of the structure factor and Fourier amplitued defined above. In Fig. 5 concentration dependence of the

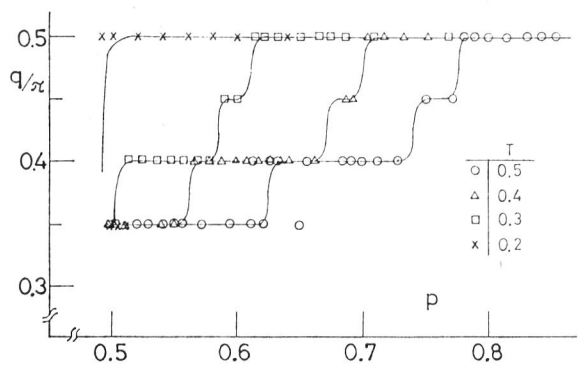


Fig. 5 Concentration dependence of wave-vector q at temperatures T=0.5, 0.4, 0.3 and 0.2. Staircase-like behavior is clearly seen. Below p=0.5 definite periodicity is hardly recognized even in the long runs.

wave-vector is shown at several lower temperatures. As the dilution proceeds, the wave-vector behaves also stepwise as a function of concentration; the lock= in phenomena appear in the concentration space, too. In addition there seems to be a critical concentration below which the periodicity may no longer be re-

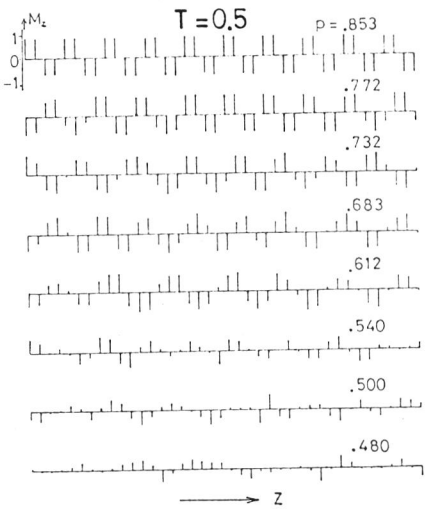


Fig. 6 Sequence of spin configurations of layers. Full length of spin in each layer is normalized unity at each concentration.

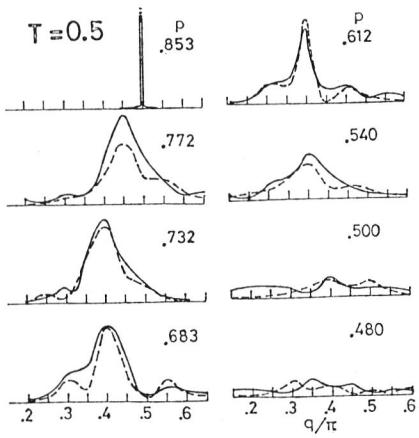


Fig. 7 Profiles of structure factor and Fourier amplitudes at concentrations corresponding to Fig. 3.

cognized. This threshold concentration is apparently higher than the percolation concentration in a three dimensional lattice with an anisotropic next= neighbor correlation, and is rather comparable to the usual threshold of the two dimensional lattice. It may suggest that formation of the periodic structer is mainly governed by the existence of the two dimensional long range order in each layer. The averaged magnetization at each layer is plotted in Fig. 6 where effect of unlinked spin cluster becoms significant below p=0.5. As a reference the corresponding profiles of the structure factor and the Fourier amplitude versus q are shown in Fig. 7. See the profiles below p=0.5.

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