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TWO-DIMENSIONAL DILUTED ISING ANTIFERROMAGNETS AT ZERO TEMPERATURE IN A UNIFORM FIELD: A GROWTH SIMULATION MODEL

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We search for the ground state of the square lattice diluted Ising antiferromagnet in a uniform field through computer simulations. In particular, the existence of long-range antiferromagnetic order is investigated. Traditional approaches consist of first constructing a random distribution of present and absent sites (the geometric configuration), and then trying to minimize the energy by conveniently setting the spin variable at each present site (the spin configuration). The search for the ground state spin configuration, however, is severely hampered due to the non-vanishing correlations between distant spins along the lattice. In this work we adopt an alternative approach where the geometric configuration is grown site by site, starting from the empty lattice, and simultaneously the spin configuration is re-examined at each step, trying to minimize the energy. Entire clusters of connected present spins are allowed to flip as a whole, giving rise to large-length-scale fluctuations; although the algorithm does not include *all* fluctuations, the sampling of length scales explored suffices to make it qualitatively distinct from the one-spin-flip approaches.

1. Introduction

In this paper we discuss the zero-temperature properties of two-dimensional diluted Ising antiferromagnets in a uniform magnetic field (DAFFs), and their relationship with those of Ising ferromagnets in a random field (RFIMs). The correspondence between the two models was first proposed by Fishman and Aharony [1], and opened the way to the experimental realization of the random field (RF) problem, since the parameters (dilution and field strength)

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which induce random-field-like behaviour in the DAFF can be easily controlled in the laboratory.

Theoretical analyses have usually been carried out with the RFIM in mind, particularly as regards the conditions for existence of long-range order; it is usually assumed that results thus obtained will be valid for DAFF as well, owing to the above-mentioned correspondence. The early domain-wall arguments of Imry and Ma [2], which gave the lower critical dimensionality $d_\ell = 2$ for the RFIM were criticized on grounds that interface roughening would push d_ℓ upwards to three [3]; however, it has since been shown that the borderline is indeed at $d = 2$. Specifically, Imbrie [4] showed that the ground state of the RFIM is ordered for $d > 2$; Bricmont and Kupiainen [5] proved that for $d > 2$ the RFIM can sustain order at (suitably low) non-zero temperatures; they could not draw definite conclusions about $d = 2$. Aizenman and Wehr [6] showed that for a $d = 2$ RFIM with a continuous distribution of the random fields, there is no order even at zero temperature. Discrete (e.g., double-delta) RF distributions seem to be out of reach of their proof.

Concerning DAFF itself, experiment indeed shows marked differences between two- and three-dimensional behaviour [7–9]; in the former the transition is rounded as soon as a field is turned on [8], whereas for the latter there is a finite threshold $H_c(T)$ below which the transition remains sharp. However, it is still possible to find an ordered state in two dimensions for finite fields, provided that the sample has been previously cooled in zero field (ZFC); such a state is unstable in the sense that after field heating above an irreversibility threshold T_{irr}, order will not be restored upon field cooling (FC) [7]. For moderate fields, T_{irr} is not much lower than the corresponding zero-field Néel temperature (see fig. 1 of ref. [7]). For a review of experiments on DAFF, see ref. [9].

Irreversibility is present in computer simulations of DAFF as well [10, 11]; when compared to the corresponding simulations of the RFIM [11, 12], the main distinguishing feature is the freezing of domain states in the DAFF when the field is turned off, as the domain walls are pinned preferentially along lines of vacant sites. Such persistence of zero-field randomness has no parallel for the (pure) RFIM (where configurations relax more easily towards an ordered state when the field is removed [11–13]). This makes the analysis of, e.g., low-temperature properties quite involved, especially as regards the ground state. For instance, although the authors of ref. [11] could establish unambiguously that at $T = 0$ for the RFIM in $d = 2$ the long-range ordered state has higher energy than the domain state in the limit of infinite sample size, no such clearcut result emerged from the analysis of two-dimensional DAFF.

Position-space renormalization-group (PSRG) methods give different results in either case: two-dimensional DAFFs with bond-[14] or site-[15] dilution are

predicted to have an ordered phase for suitably low amounts of temperature, impurity concentration *and* field, while the analysis of RFIMs in $d = 2$ shows no order at any non-zero field intensity [16] (for $d = 3$ a similar method predicts order for the RFIM [17], thus making it safe to say that the PSRG has no built-in bias against ordering in the random-field problem). The ordered phase found for DAFFs corresponds to the state with non-zero staggered magnetization experimentally seen [7] on field heating of ZFC samples; its existence and structure can be traced back to the internal structure of the PSRG [15], where essentially one equates exactly evaluated partition functions for finite (small) systems, whose ground state can be antiferromagnetic for finite fields. On the other hand, ferromagnetic ground states can also be found for finite RF intensities in the corresponding small systems used for the PSRG treatment of the $d = 2$ RFIM, without giving rise to a spurious ordered phase [16, 18]. The question then arises whether the two-dimensional DAFF does have an ordered ground state, however out of reach it is from the experimental or simulation viewpoint, owing to the irreversibility and domain-freezing effects mentioned. In order to obtain further information on this, we have carried out zero-temperature simulations of the DAFF, whose distinctive feature is that instead of varying, e.g., field values for a given dilution configuration, we scan throughout *impurity concentrations* for fixed fields; such a procedure, coupled with an algorithm (to be described below) which allows clusters of all sizes to flip simultaneously, ensures that domain-freezing effects are significantly reduced. The whole process corresponds to a growth simulation model where fluctuations on all length scales are taken into account. While our results cannot be regarded as definitely showing the existence of an ordered ground state for the two-dimensional DAFF, they nevertheless underline the rich nature of the interplay between dilution and uniform field, which has no parallel in the related RFIM problem.

2. The algorithm

We consider the problem of filling a two-dimensional square array, by randomly occupying its sites with magnetic (Ising spin-$\frac{1}{2}$) atoms; these interact antiferromagnetically with their (occupied) nearest neighbours, and with an external, spatially uniform, magnetic field. At zero temperature the only relevant parameter is the ratio H/J (H = field intensity; J = absolute value of the exchange interaction).

On an $L \times L$ lattice, as one randomly fills the L^2 sites at a given value of H/J and tries to minimize the overall (exchange and magnetic) energy each time a new site is added, one is scanning the zero-temperature section of the

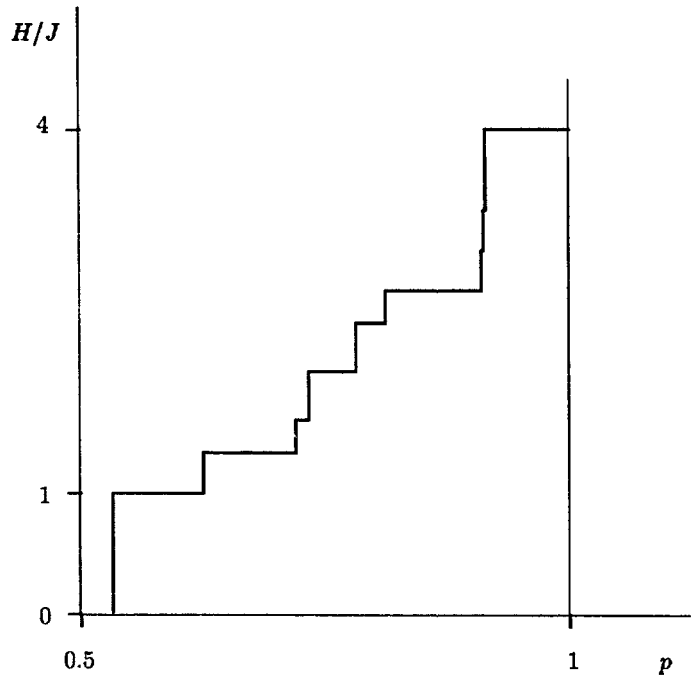

Fig. 1. Phase diagram at zero temperature, for a site-diluted square lattice Ising antiferromagnet in a field, as obtained by the PSRG in ref. [15].

phase diagram of a site-diluted antiferromagnet along the concentration (p-) axis, keeping the field constant. In the approximate PSRG calculation of ref. [15], the phase boundary between ordered and disordered regions in the p–H/J plane was found to have a staircase-like structure, the critical values of H/J remaining fixed at specific rational numbers (related to cluster structures) for finite intervals of p-variation (fig. 1); qualitatively similar results were found for the bond-diluted problem [14].

For each new site added, it may: (a) be isolated, which is the most usual situation while the concentration is still low; (b) have one occupied nearest neighbour, whereby it will join the cluster to which the occupied neighbour already belongs; (c) have two occupied nearest neighbours, in which case two possibilities arise: either (c1) both neighbours already belong to the same cluster, or (c2) each belongs to a different cluster, so the new atom will bring the two clusters together into a new, larger one; (d) have three, or (e) four occupied neighbours. For each of (d) and (e), several possibilities arise depending on whether the occupied sites belong to the same or distinct clusters.

Each time a site is added, for each of the two states of the new spin we consider the two possible orientations of (each of) the cluster(s) to which it has been joined (at most, we have 32 situations to consider, when the new site

brings together four distinct, previously mutually disconnected clusters; such situations are, however, quite rare). We then choose the combination with least overall energy. At the start of the simulation, we choose one of the two chessboard sublattices α and β of the square lattice to be the preferred one (say α), so if the final configuration of the new cluster recently formed happens to be insensitive to an overall field inversion, we put it into a state for which the sum of the number of α-spins parallel to the field plus the number of β-spins opposed to the field is maximum; this is equivalent to applying an infinitesimal symmetry-breaking staggered field. We note that Andelman et al. [19] used a similar (though finite) symmetry-breaking field in simulations of the RFIM.

This, however, is not enough: by allowing a given cluster, at a specified stage, only to flip as a whole we are disregarding possible internal rearrangements. Thus, after the energy minimization mentioned above, we check all the sites of the lattice which have already been occupied: for each of them we check whether its overall interaction energy (with neighbours and field) is reduced if its spin is overturned; we go over the lattice until no more spins can be overturned this way. We then overturn the field direction throughout the lattice and repeat the whole process. After many field overturnings, the system eventually converges to a stable state. It is to be noted that this part of the algorithm, when applied to an already full lattice, always reproduces the Néel state for $H/J < (H/J)_{\text{critical}} = 4$, for any initial spin configuration. On the other hand, when the lattice is randomly filled (i.e., "grown" in the sense described above) with a field $H/J < 4$ there are a few runs in which one ends up with two reversed domains, instead of a single Néel state. This is because specific dilution configurations may be grown in different sectors of the lattice, with mutually reversed Néel states, and they only coalesce together at the end of the growth process; by this time, the mechanisms built into our algorithm do not suffice to overturn the situation. We have chosen to disregard data coming from such runs (which anyway occur infrequently, and ever more so as the lattice size grows; thus it seems that by neglecting these data we are not introducing an undesired bias towards ordering in our calculations).

Our algorithm then incorporates the possibility of flipping clusters as a whole, in its first part, and single-spin updating in the second part. This is different from usual simulations for the DAFF, which rely only on single-spin updating [10, 11]. The need for simultaneous updating of large clusters, as a means to reduce trapping in local minimum configurations, has long been acknowledged; several multigrid schemes have been developed accordingly (see e.g., refs. [20–25], for a sampling of recent references). While general requirements exist for a multigrid algorithm to be efficient [24], the details of its implementation vary widely according to the specific features of the problem under discussion [21, 23]; see ref. [26] for dilute systems in zero field and ref.

[27] for a proposal of a generalization of Wolff's [22] algorithm for random-bond and random-field Ising models. In the present case we take advantage of the very structure of the diluted clusters, since they have been shown to be the main factor that singles out the DAFF from the RFIM. Note that by allowing different clusters to change their orientation when they are joined together, we are including fluctuations that reach all length scales (respectively, those of the sizes of the clusters being joined). We are not, however, including *all* fluctuations: our algorithm does not allow an already existing cluster to be broken into finite domains (except for the single-spin updating of the second part, which may have such an effect). Nevertheless we expect that the sampling of length scales explored by our algorithm will suffice to make it qualitatively distinct from, e.g., one based only on single-spin updating. Note also that, in the random lattice-filling process, each time a new site is added the existing clusters have just been optimized at the single-site level; we then proceed to optimization at the cluster level. This is in accordance with the general principle of multigrid algorithms, of considering large-scale moves only after the short-scale ones have been spanned [24].

3. Results

We have performed simulations on lattices of linear sizes $L = 20, 30$ and 40, with periodic boundary conditions. For fixed size and field intensity, we have computed averages over 10, 20 and 30 runs of the lattice-filling process. Averages over 10 runs usually seem to give as much information as we can extract, provided that the lattice size is large enough; in other words, the problem is self-averaging. We will return to this point later. We have computed the average staggered magnetization (m_s) normalized by L^2. Recall that an infinitesimal symmetry-breaking staggered field is present; also, we include all clusters (finite or "spanning"), so at $H = 0$ the m_s vs. p graph would be a straight line at 45 degrees.

The region of real interest to us is at and above the percolation threshold, $p \geq p_c \simeq 0.59$; from the approximate calculation of ref. [15] it is expected that, for fixed H/J, as p increases one will cross the boundary from paramagnetic to the antiferromagnetic phase. For $H/J < 1$, this ought to happen at p_c (in ref. [15] p_c is approximately given by 0.533, owing to small-cell PSRG effects). For higher H/J the boundary should be crossed at higher concentrations, see fig. 1. Going deeper into the ordered phase, the magnetization curve would approach the 45-degree line; of course, finite-size effects would round and smear out the results. However, this is not what happens for $H/J \lesssim 1$, where the order

parameter clearly goes to *zero* for all $p < 1$, as the lattice size increases (fig. 2). On the other hand, for $H/J > 1$ the overall picture is much as expected; a change in concavity of the m_s vs. p diagram is clearly noticeable and persists for the largest lattice sizes used (fig. 3): the magnetization curve indeed

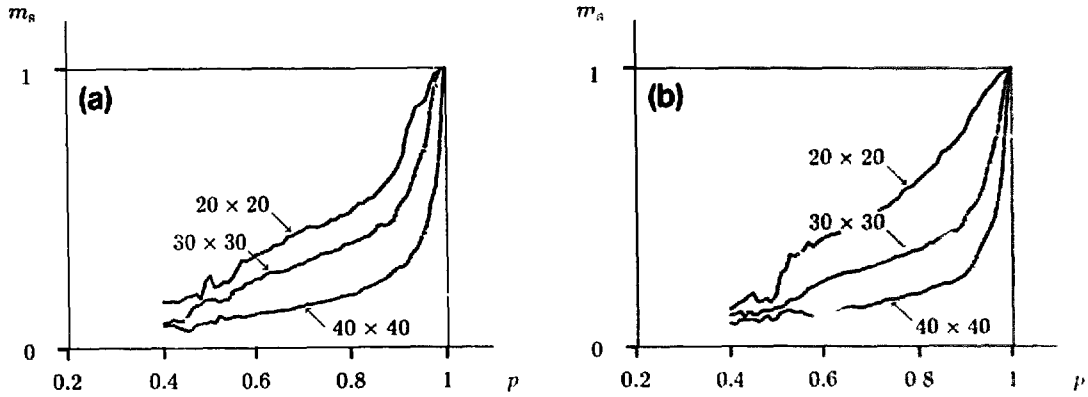

Fig. 2. m_s vs p graph for (a) $H/J = 0.5$ and (b) $H/J = 0.9$. Lattice sizes as indicated. All averages over 10 runs. Note that m_s clearly vanishes for increasing lattice sizes for both (a) and (b).

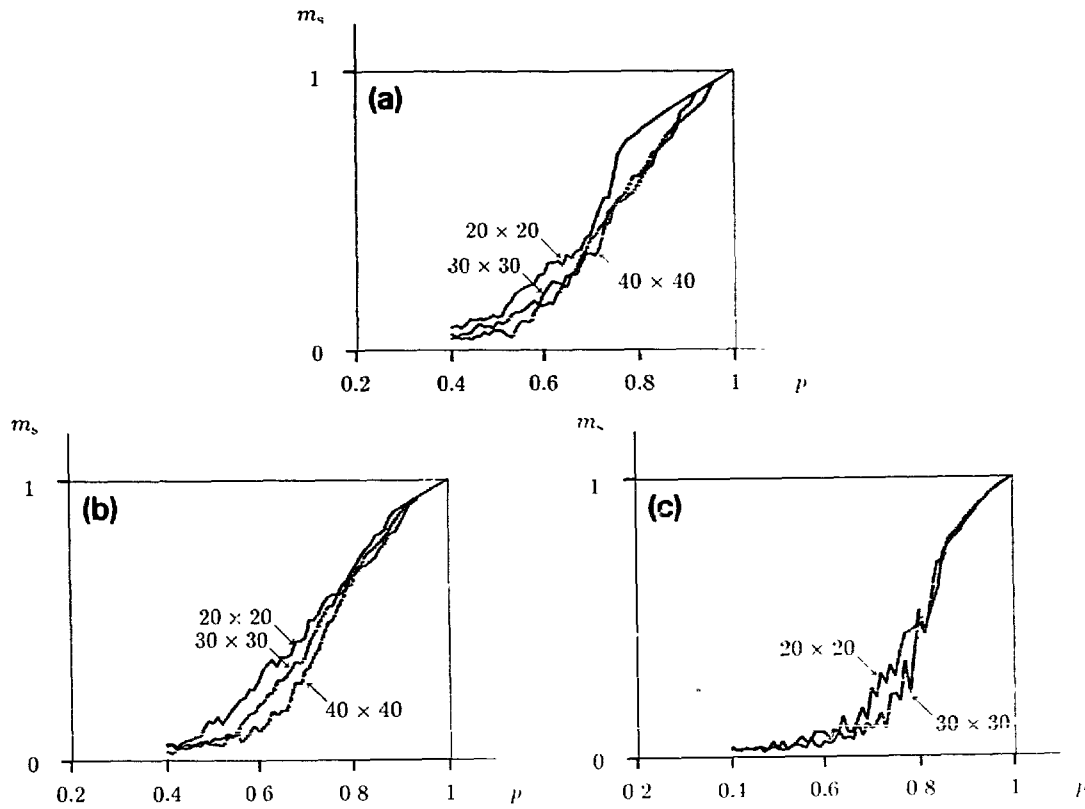

Fig. 3. m_s vs. p graph for (a) $H/J = 1.1$, (b) $H/J = 1.5$ and (c) $H/J = 2.9$. Lattice sizes are the same as in fig. 2, except for (c) where the largest size is missing. All averages over 10 runs. In contrast with fig. 2, the existence of long-range order is clearly shown.

approaches the 45-degree line. We have also performed simulations for several other values of the field strength (not shown); the general behaviour is the same both for $H/J<1$ and $H/J>1$.

The key to this difference in behaviour lies in that the phase boundary is expected to rise vertically at $p=p_c$, up to $H/J=1$ [15]; thus, for $H/J<1$ as the lattice is grown the percolation threshold is crossed simultaneously with the phase boundary. The strong concentration fluctuations at p_c are such that "mismatched" domains of all sizes coalesce just as (in our concentration-sweeping scheme) the system should be entering the ordered phase. The resulting energy barriers are distributed over so many scales that our algorithm cannot cope with it; as a result, the domain structure remains well into what ought to be the ordered phase. On the other hand, for $H/J>1$ the crossing into the ordered phase is expected to occur at p-values finitely different from p_c, owing to the staircase-like structure of the phase diagram. First, at and slightly above p_c the geometric clusters join each other; only at higher concentrations the system goes into the magnetically ordered phase, this time away from the concentration fluctuations at p_c; the drive towards magnetic order is not hampered by mismatched domains coming together. A marked difference in the overall behaviour of the DAFF for $H/J<1$ and $H/J>1$ was also obtained by Fernandez and Pytte [28] using a transfer matrix technique.

We have not been able to see the quantitative effect of the other steps predicted in ref. [15]; for instance, for $H/J\simeq 4/3$ the phase boundary is expected to be reached at a value of p considerably smaller than, e.g., for $H/J>8/3$ (see fig 1). Most probably, apart from finite-size effects the transition is second order, thus the build-up of magnetization is slow as p varies; this contrasts with the case for the pure system, where the staggered magnetization jumps from zero to one at $H/J=4$ as one decreases the field.

Finally, in fig. 4 we provide visual evidence to our earlier assertion that

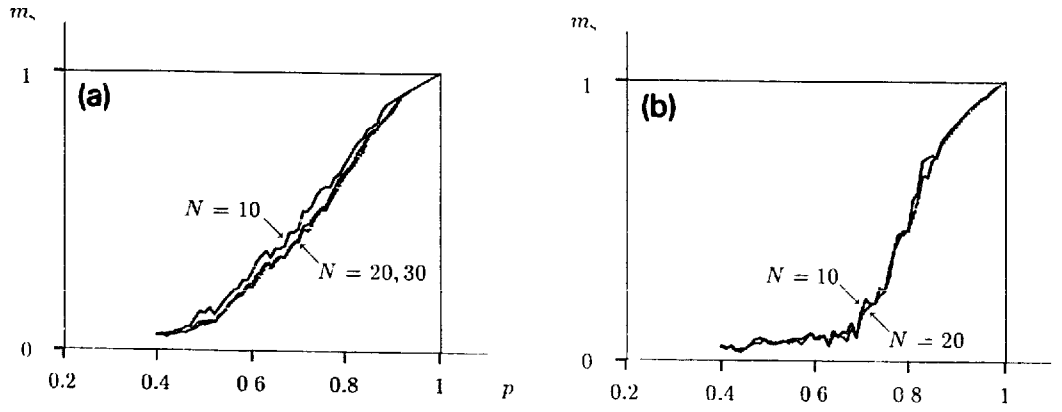

Fig. 4. m_∞ vs. p graph for (a) $H/J=1.5$, (b) $H/J=2.5$. Lattice size: 20×20. In (a), averages over $N=10$, 20 and 30 runs – the latter two are nearly indistinguishable; in (b), $N=10$ and 20.

averages over 10 runs seem to give as much information as averages over 20 or 30 runs. As discrepancies grow smaller with increasing lattice size, we have chosen the smallest lattices in order to underline the maximum distortion to be expected.

4. Conclusions

We have discussed the ground state properties of site-diluted Ising antiferromagnets in a uniform field on a square lattice, obtained by a growth simulation model which takes into account fluctuations on all length scales. Since our algorithm spans increasing concentrations of the magnetic species as the external field is kept constant, it is not expected to simulate experimental conditions (where not only the concentration is fixed, but a specific *geometric configuration* of magnetic atoms is frozen in a sample) literally. Nevertheless, we have been able to gain insight into the interplay between dilution and magnetic field, which is unique to the DAFF problem. Our results are consistent with the general belief that $d = 2$ is the marginal dimensionality for the DAFF problem, just as it is so for the RFIM. This statement, however, must be qualified: while the two-dimensional RFIM never sustains order for non-zero RF intensity, the DAFF seems to be able to exhibit order in certain circumstances (experimentally, this corresponds to field-heating of zero-field-cooled samples [7]), though this is of a complicated, probably even non-equilibrium nature, as far as actual experiments are concerned.

While we cannot say that our results amount to a definite evidence for ordering of the $T = 0$ two-dimensional DAFF, they certainly display features which are consistent with the findings of refs. [14, 15]. In particular, the striking difference between the m_s vs. p curves for $H/J < 1$ and $H/J > 1$ can be explained in terms of the interplay between geometric (percolation) and magnetic (ordering) transitions, in accordance with the shape of the phase diagram predicted in ref. [15]. Further, our findings indicate that the magnetic ordering transition is second order along the $T = 0$ phase boundary; this is in contrast to the first-order transition which takes place at zero temperature for the pure system, where there is a magnetization jump at $H/J = 4$.

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