REVIEW ARTICLE

Monte Carlo simulation of random magnets

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Significant progress has been made over the last few years in our understanding of the physics of random magnets using novel techniques of Monte Carlo simulation. In this work I summarize some of the recent results and compare these with corresponding experimental data as well as the theoretical predictions.

Random magnetic materials and models

The atoms/ions constituting a solid material sometimes possess non-zero magnetic moment due to unpaired spins and orbital angular momenta. Various kinds of magnetic ordering, e.g. ferromagnetic, antiferromagetic, ferrimagnetic, are possible in such materials at sufficiently low temperatures. The nature of the ordering, however, depends not only on the temperature but also on the particular material under consideration. For example, Euo orders ferromagnetically below the so-called Curie temperature whereas MnF_2 and Rb_2CoF_4 exhibit antiferromagnetic order below the corresponding Neel temperatures.

More than fifty years ago Heisenberg showed that the (exchange-) interaction between spins responsible for the magnetic ordering arises from a proper quantum mechanical treatment of the Coulomb interaction between charges and that the effective Hamiltonian for interacting spins, assumed located on lattice sites, is given by

$$\mathcal{H} = -\sum_{<ij>} J_{ij} \vec{S}_i . \vec{S}_j \qquad (1)$$

The spin $\vec{S}_i$ at the ith lattice site on a d-dimensional lattice interacts with the Z nearest neighbours $\vec{S}_j$ ($j = 1, \ldots, Z$) where the strength of the nearest-neighbour exchange interaction is J_{ij}. The summation on the right hand side of equation (1) is to be carried over all the nearest-neighbour pairs $<ij>$.

Fortunately, the Hamiltonian for several real magnetic materials is well approximated by the simpler expression, the so-called Ising Hamiltonian.

$$\mathcal{H} = -\sum J_{ij} S_i S_j, \qquad (2)$$

where each of the Ising spins can take only one of the two allowed values $S_i = \pm 1$. In the presence of an external magnetic field the Hamiltonian for the Ising model is given by

$$\mathcal{H} = -\sum J_{ij} S_i S_j + \sum H_i S_i \qquad (3)$$

where H_i is the strength of the external magnetic field at the ith site. My discussion here will be based entirely on the Ising model.

By 'randomness' and 'disorder' I mean *frozen* disorder rather than *thermal* disorder. Frozen randomness can arise either from strong structural disorder (e.g. glasses that are amorphous) or from random arrangement of atoms/ions on a lattice (e.g. random binary alloys). A magnetic material with 'frozen' disorder can be prepared in the laboratory by randomly substituting magnetic ions/atoms by non-magnetic impurities, for example, (i) Co by Mg in Rb_2CoF_4, (ii) Fe by Zn in FeF_2, (iii) Mn by Zn in MnF_2, and (iv) dysprosium by Yttrium in dysprosium aluminium garnet. So far as the theoretical models are concerned, (quenched-) randomness can be introduced into the Ising model (3) in several ways: (i) Random exchange Ising models (REIM): Suppose, each of the lattice sites is occupied by an Ising spin with probability p and occupied by a non-magnetic impurity with probability $1 - p$. This is one of the several possible ways of randomizing the exchange interaction J_{ij}. Note that H_i is non-random in the REIM: usually, one assumes $H_i = H$ for all i. (ii) Random-field Ising model (RFIM). The exchange interaction is assumed to be non-random, but the field H_i is random. In the RFIM one usually assumes $J_{ij} = J$ for all the nearest-neighbour pairs $< ij >$. In the laboratory it is, however, not possible to vary the external field randomly at the length scale of atomic distances. But, random *anti-ferromagnets* in a *uniform* external magnetic field are known to be physical realizations of the (ferromagnetic) RFIM.

Competing ferro- and antiferro-magnetic interactions can lead to a different type of magnetic ordering, namely, the spin glass. However, I shall not discuss spin glass ordering here and the reader is referred to a recent book[1] and review articles.[2,3] In this paper I shall mainly review the recent progress in the understanding of the physics of the REIM. I shall also briefly mention some of the recent interesting results obtained in the case of RFIM.

A brief introduction to the critical phenomena

Consider, for example, the paramagnet-to-ferromagnet phase transition in the pure Ising model. The spontaneous magnetization (i.e. magnetization in the absence of external magnetic field), which is non-zero in the ferromagnetic phase, vanishes continuously as the transition temperature T_c is approached from below. Therefore, so far as the ferromagnetic ordering is concerned, spontaneous magnetization is treated as the 'order parameter', a measure of the (long-range-) order in the system. It is possible to define a 'correlation length', that diverges at the critical point T_c. Theory of critical phenomena puts emphasis on a few universal aspects of such phase transitions. Most of the attention is focused on the 'critical exponents' that describe how specific thermodynamic quantities, e.g. the order parameter, the susceptibility, vanish or diverge at the critical point. This behaviour is captured in terms of certain critical exponents that characterize the power law dependence of these quantities on $(T - T_c)$. The standard symbols used in the literature for the exponents associated with the specific heat, order parameter, susceptibility and the correlation length are α, β, γ and ν respectively. These exponents associated with the static properties are universal in the sense that they depend on the spatial dimensionality, dimensionality of the order parameter (one in the Ising case and three in the Heisenberg case) and the range of the interaction but are independent of the other specific details of the system under consideration. Thus, the numerical values of the corresponding critical exponents for the *d*-dimensional Ising ferro- and antiferromagnets with nearest neighbour exchange interactions are the same.

Pure Rb_2CoF_4 is a tetragonal compound where nearest-neighbour CO^{2+} ions are arranged on square lattices in the basal planes. The planes of the spins are separated by two layers of RbF ions. Therefore, the interplanar exchange coupling is much weaker than the intraplanar coupling. Indeed, pure Rb_2CoF_4 is one of the best realizations of the two-dimensional Ising model[4]. The experimentally measured values of the static critical exponents for pure Rb_2CoF_4 are in good agreement with the corresponding theoretical values for the *two*-dimensional pure Ising model whereas those for pure FeF_2, MnF_2 and dysprosium aluminium garnet, for example, are consistent with the corresponding ones for the *three*-dimensional pure Ising model. Thus, $Rb_2Co_{1-x}Mg_xF_4$ is expected to be a physical realization of the *two*-dimensional REIM whereas $Fe_{1-x}Zn_xF_2$ and $Mn_{1-x}Zn_xF_2$ should behave like the *three*-dimensional REIM.

According to the theory of dynamical scaling the characteristic relaxation time τ near the critical point is given by $\tau \sim \xi^z$, where z is the (temperature-independent) dynamic critical exponent. The divergence of τ as $T \rightarrow T_c$ is known as the phenomenon of 'critical slowing down'. The exponent z can be predicted by the theory of critical dynamics and for real materials it can be measured, for example, by neutron scattering. For example, the experimentally measured value $z \approx 1.67$ for Rb_2CoF_4 is in good agreement with the corresponding theoretical prediction.

In conventional Monte Carlo (MC) simulations of Ising models consisting of N spins, one MC step consists of the following operations: (i) a spin is selected randomly for deciding whether or not to flip it; (ii) the energy change ΔE associated with that flip is computed; (iii) the transition probability $W = \exp(-\Delta E/k_BT) / [1+\exp(-\Delta E/k_BT)]$ for that flip is then computed; (iv) a random fraction f ($0 \le f \le 1$) is generated by the computer and if $f < W$ the spin is flipped ($S_i \rightarrow -S_i$), otherwise it is not flipped; (v) the whole process (i)–(iv) is repeated N times. The resulting spin configurations are used to compute the required thermodynamic properties.

Let us now summarize some of the common difficulties encountered in computing the critical properties of a system using MC simulation. The most appropriate definition of the exponent e for an arbitrary thermodynamic quantity X in a system undergoing a thermal phase transition is $e = \lim_{t' \rightarrow 0} (\ln X / \ln t')$ where $t' = (T - T_c)/T_c$ is called the reduced temperature. The actual dependence of X on t', however, can be expressed as

$$X = A t'^{e}(1 + b t^{c} + \ldots),$$

where the terms other than unity within the bracket give rise to 'corrections to scaling'. Unless such corrections are very small the effective exponents observed in computer simulations will be far from the true exponents if the simulation cannot be performed very close to T_c. But the closer is T to T_c, the larger is the correlation length and the stronger are the finite-size effects. Finite-size effects can be minimized by simulating systems as large as possible, albeit at the cost of enormously large CPU time. Very large systems of Ising spins (even in the presence of random exchange and/or random field) can be simulated using a recent technique called multi-spin coding where the orientations of several spins are stored in each of the computer words[5, 6]. Moreover, the closer is T to T_c, the slower is the simulation because of the phenomenon of critical slowing down. The latter difficulty, however, can be bypassed using an efficient algorithm, proposed by Swedsen and Wang (SW)[7]. In this algorithm instead of single spins, appropriately defined clusters of spins are flipped.

Static critical behaviour of random magnets

A second order thermal phase transition takes place

in the REIM at a non-zero temperature provided the concentration of the spins $p > p_c$, the so-called percolation threshold (see ref. 8 for a review). The transition temperature $T_c(p)$ is a monotonically decreasing function of the impurity concentration and T_c vanishes for all $p \leq p_c$. One of the fundamental questions is: are the critical exponents characterizing the thermal phase transition in the REIM at a given p ($p_c \leq p < 1$) identical to the corresponding ones for the pure Ising model ($p = 1$)? On the basis of a set of heuristic arguments Harris[9] derived the following criterion: if the specific heat exponent α_{pure} for the pure model is *positive* then the corresponding disordered model would belong to a different universality class. This criterion implies that the critical exponents for the three-dimensional REIM are different from the corresponding ones for the pure model for which $\alpha_{pure} = 0.11$. On the other hand, since α_{pure} is negative for the three-dimensional Heisenberg model the corresponding disordered model should belong to the same universality class as the pure model. So far as the two-dimensional Ising model is concerned the Harris criterion is inconclusive because the corresponding $\alpha_{pure} = 0$. Harris criterion has been supported by subsequent analytical calculations. However, the results of the computer simulation of the REIM remain controversial, primarily because the true critical regime for the latter model is too narrow to be probed by most of the traditional computational techniques. More precisely, critical slowing down prohibits the traditional simulations to be carried out sufficiently close to T_c (see ref. 5 and references therein). As stated earlier, the best algorithm to bypass the critical slowing down is the SW algorithm. Using this algorithm Wang and Chowdhury[10] have computed the effective exponents for various values of the reduced temperature $t' = (T - T_c)/T_c$ and extracted the asymptotic values of the exponents in the limit $t' \to 0$ by extrapolation. It turns out that $\gamma = 1.5 \pm 0.07$ and $\nu = 0.75 \pm 0.04$. These values are in good agreement with those obtained in a very recent simulation[11] carried out in the same range of temperature using a different algorithm.

Let us now compare the exponents obtained by the MC simulation with the corresponding values obtained from experimental investigations of the random Ising magnetic materials and with the corresponding theoretical predictions. To my knowledge, the best theoretical estimates of γ and ν are [12]$\gamma \approx 1.336$ and $\nu \approx 0.678$ whereas the most careful experiments (see ref. 13 for review) yield $\beta \approx 0.35$, $\gamma \approx 1.31$, $\nu \approx 0.69$. Surprisingly, the MC simulation seems to have overestimated the exponents although there are one or two experiments that yield exponents close to the MC estimates. A possible interpretation of this inconsistency between theory and MC simulation is that the effective exponents are nonmonotonic functions of the reduced temperature t' (ref. 14) and the higher values of γ and ν are consequences of a naive extrapolation to $t' \to 0$. However, a recent attempt[15] to detect such a maximum, if any, in $\gamma(t')$ using the so-called Wolff algorithm (which is little more efficient than the SW algorithm) on transputers (a type of parallel processing computer), has been inconclusive. Unfortunately, even the MC simulation using the SW algorithm at $t' \approx 10^{-3}$ cost about 500 h of CPU time on an IBM 3090 which is almost as fast as a Cray computer. Therefore, at present, the computer time required for simulation at $t' \approx 10^{-4}$ would be prohibitively large.

Critical dynamics of the REIM near the bicritical point

Theoretical activity in this field was triggered by the inelastic neutron scattering study of the site-diluted antiferromagnet $Rb_2Co_{1-x}Mg_xF_4$ with Co concentration near the percolation threshold[16]. The experimentally observed value $z \approx 2.4$ is much larger than the prediction $z \approx 1.67$ from the standard dynamical scaling. Aeppli *et al.* attributed this discrepancy to the fact that 'in a system as ramified as a percolating network, disturbances require a longer time to propagate between two points than they do on a regular lattice'. Using the known fractal properties of the percolating networks they proposed a scaling argument that apparently reconciled theory with experiment. More refined scaling arguments were proposed later[17]. However, all these attempts began with the *assumption* that the standard form of dynamical scaling applies to the system under investigation. On the other hand, most of the subsequent theoretical work[18-20] as well as computer simulation[21-26] indicate the breakdown of this standard form in the dilute Ising magnets near the percolation threshold. For example, Harris and Stinchcombe[20] suggested that the dynamic exponent 'z should really be infinite, and that the experiment sees a finite effective value limited by how close to the percolation bicitical point $T = 0$, $p = p_c$ the measurements are made.'

From these recent theories one concludes that at $p = p_c$ the standard dynamical scaling must be replaced by the so-called 'singular' dynamical scaling

$$\ln \tau = A (\ln \xi_T)2 + B (\ln \xi_T) + C \qquad (4)$$

where A, B and C are constants. Comparing this form (4) with the standard dynamical scaling form

$$\ln \tau = B (\ln \xi_T) + C, \qquad (5)$$

we conclude that both the forms (4) and (5) are special cases of a generalized dynamical scaling form

$$\ln \tau = f(\ln \xi_{\parallel}). \quad (6)$$

where f is a function of $\ln \xi_{\parallel}$. Thus, (4) corresponds to $f(x) = Ax^2 + Bx + C$ whereas in the case of the standard dynamical scaling (5) $f(x) = Bx + C$.

The singular dynamical scaling form (4) is a consequence of the fact that the most divergent energy barriers to overturning of spin-clusters of size L is $E_{max} \propto \ln L$, which, in turn, is a consequence of the (statistical-) self-similarity of the percolation clusters (see also ref. 27, 28 for related models and ref. 29 and 30 for reviews). MC simulation of the Ising model with quenched disorder in two dimension[24, 25] as well as in three dimension[26] demonstrate the breakdown of the standard dynamical scaling (5) and indicate the existence of a singular form (4). The existing experimental data, however, are not sufficiently accurate and can be fitted to both the forms (4) and (5); some more accurate experiments are in progress (G. Aeppli, private communication). Some aspects of this singular dynamical scaling, however, remain controversial; for example, whether the constant A is an universal quantity in the same sense as the critical exponents.

Kinetics of domain growth in random magnets far from equilibrium

When an Ising magnet is quenched, i.e. cooled rapidly, domains of up (down) spins grow at the cost of the domains of down (up) spins. It is now well known that the linear size R of a domain grows with time t following the so-called Allen–Cahn law $R^2 \propto t$. This law is a consequence of the fact that the local velocity of the interface separating the up and down spins is proportional to the local curvature.

Recently, the effects of random field[31, 32] as well as that of random impurities (ref. 33 and references therein) have been investigated by MC simulation. A 'crossover' from the power-law growth (during the very early stages) to a logarithmically slow growth (in the late stages) has been observed in both the cases. Such observations are consistent with the theoretical conjectures that domain growth would be slowed down by the pinning effects of the random fields and the random impurities which roughen the interfaces. However, a detailed discussion on the various aspects of roughening of the interfaces is beyond the scope of this paper.

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