Numerical Studies of Spin Glass Problems in Magnetism and Superconductivity

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Abstract

I will describe spin glass ideas as applied to magnetism and superconductivity, concentrating on numerical studies. The existence of a phase transition will be shown and some open problems discussed.

I. INTRODUCTION

Although phase transitions and critical phenomena have become quite well understood, particularly through the use of the renormalization group, there are several areas where our understanding is still quite primitive. In this lecture, I will discuss one of them, the spin glass [1]. Spin glasses are disordered systems in which the disorder is sufficiently strong that there is a competition, which is called "frustration", between different terms in the Hamiltonian. An example of a frustrated magnetic system *without* disorder is an antiferromagnet on a triangular lattice, where each spin would like to be anti-parallel to its neighbors, but this is impossible because some of its neighbors are also neighbors of each other. An example of a frustrated system *with* disorder (i.e. a spin glass) is a magnet in which the interactions are randomly ferromagnetic or antiferromagnet. This is, in fact, a popular spin glass model, due to Edwards and Anderson [2], which I will discuss below. Fig. 1 shows the concept of frustration for a single square.

Spin glasses have been widely studied because of the universal behavior seen in a wide variety of frustrated random systems, and because ideas from spin glass theory have been applied to phase transitions in related areas such as superconductors, as well as to areas of science which superficially seem quite far removed from magnetic systems, such as combinatorial optimization and neural networks. In this talk I will discuss spin glass ideas as applied to magnetism and superconductivity, the two principal themes of this meeting. I will emphasize the role of numerical simulations, since this is the aspect that I mainly work on.

Frustration means that it is non-trivial to find the ground state, and any low energy state will have to be a compromise between some terms in the energy which are "satisfied" and others which are "unsatisfied". In spin glasses, which also have disorder, it turns out that there are states close by in energy to the ground state which differ in the orientation of a large number of spins. In other words there are quite different ways of arranging the spins to get almost the best compromise. The resulting "energy landscape", is complicated, with different "valleys" (i.e. minima) separated by saddle points, which act as "barriers" which hinder the system from fluctuating from one minimum to another. There are barriers on all scales and so a spin glass at low temperatures will have very slow dynamics and never fully equilibrate. This is one of the difficulties in doing experiments and also in performing finite-temperature Monte Carlo simulations. Later I will discuss a recent technique, called parallel tempering, which speeds up Monte Carlo simulations at low temperature.

At a ferromagnetic transition, the susceptibility χ diverges, and this gives a strong indication that a phase transition takes place. For a spin glass, the susceptibility stays finite, because, in the low-T state, the spins point in random-looking directions [3]. However, a great impetus to spin glass studies came from the realization that the *non-linear* susceptibility $\chi_{\rm nl}$ will diverge. This is defined as the next term of the expansion of the magnetization, m in powers of an external field h:

$$m = \chi\, h - \chi_{\rm nl}\, h^3 + \cdots \, . \tag{1}$$

$\chi_{\rm nl}$ is expected diverge with a critical exponent γ as $T \to T_c$, i.e.

$$\chi_{\rm nl} \sim (T - T_c)^{-\gamma}. \tag{2}$$

The first spin glass systems to be studied consisted of a dilute concentration of a magnetic atom, such as Mn, in a non-magnetic host metal, such as Cu. The Mn spins interact through the RKKY interaction, mediated through the conduction electrons, which has the form $\cos(2k_F R)/R^3$, where R is the distance and k_F is the Fermi wave vector of the host metal. The rather long range, R^{-3}, nature of the interaction is possible the wave functions of the conduction electrons are extended. In insulators, by contrast, exchange interactions fall off exponentially at large distances. Thus, depending on the distance between the Mn ions (which is random) the interaction can either be positive or negative. Spin glass behavior is also observed in some insulating compounds which are magnetically diluted and have first and second neighbor interactions of opposite sign.

Spin glass behavior, which comprises slow dynamics, irreversibility, and a divergent non-linear susceptibility, are found in other problems as well as random magnetic alloys. In this lecture I will discuss one of them, a type-II superconductor in a magnetic field. If the field lies between the lower critical field H_{c_1} and the upper critical field H_{c_2}, magnetic flux partially penetrates in the form of flux lines which form a regular triangular lattice. At H_{c_2} the flux fully penetrates and the system goes normal. However, disorder destroys the long range positional order of the flux lattice [4,5] and individual flux lines can then move under the influence of a current which gives rise to dissipation. However, the suggestion was made [4] that there could be a transition to a phase called the "vortex glass", similar to a spin glass, in which there is a collective state (with zero dissipation in this case) without long-range translational order. The necessary conditions for a spin glass are present because the magnetic field twists the phase of the condensate (giving frustration) and we have assumed that there is disorder.

In fact, fluctuation effects are generally negligible in conventional low-T_c superconductors, and the traditional mean-field approaches, such as the Ginzburg-Landau theory, work very well there. It was only with the discovery of high-T_c materials, where fluctuation effects are much more important, that macroscopic fluctuation effects, such as a possible vortex glass phase, received attention.

II. MODEL AND TECHNIQUES

Because of universality, the microscopic details are unimportant so we can develop a theory with a simple model which has the right basic ingredients, which we argue are randomness and frustration. The simplest such model seems to be that proposed by Edwards and Anderson [2], whose Hamiltonian is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \,, \tag{3}$$

where we take Ising spins, $S_i = \pm 1$, which lie on the sites of a lattice with $N = L^d$ sites in d dimensions with periodic boundary conditions. The interactions J_{ij} are, for simplicity, taken between nearest neighbor sites only, and are assumed to be independent random variables. To avoid ferromagnetism or anti-ferromagnetism we set the mean equal to zero, and take the variance to be unity which sets the temperature scale, i.e.

$$[J_{ij}]_{\rm av} = 0, \qquad [J_{ij}^2]_{\rm av} = 1 \,, \tag{4}$$

where $[\cdots]_{\rm av}$ denotes an average over the disorder.

To describe the superconductor in a magnetic field, the elementary statistical variables must be an angle, describing the phase of the superconducting condensate. The magnetic field tends to twist the phase, giving rise to frustration. We can incorporate both this and the disorder in a compact way in the "gauge glass" model which is described by the following Hamiltonian:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j - A_{ij}) \,. \tag{5}$$

The ϕ_i lie in the range from 0 to 2π, and are allowed to fluctuate, while the A_{ij} are the quenched random variables, and also lie in the range from 0 to 2π.

For both models we assign the quenched random interactions (J_{ij} and A_{ij} respectively) and then fix them during the simulation while allowing the statistical variables (S_i and ϕ_i) to fluctuate. For the small sizes that can be simulated the results depend on the precise values of the random interactions chosen, and so many samples, with different choices of the random interactions, need to be averaged over.

III. RESULTS

There has been an enormous amount of numerical work on spin glasses and vortex glasses. For reasons of space I will not attempt to review the field, but just give a flavor of the sort of things that have been done by describing a piece of work I was involved in [6] which investigates whether there is a vortex glass phase in the gauge glass model, whose Hamiltonian is given by Eq. (5).

I have already mentioned that the dynamics becomes very slow at low temperatures, because the system takes a long time to fluctuate from one minimum to another in the complicated energy landscape. This is a problem for Monte Carlo simulations, and initially studies at very low temperature could not be done even for small sizes. However, this is not possible with the using the parallel tempering Monte Carlo method [7,8]. In this technique, one simulates several identical replicas of the system at different temperatures, and, in addition to the usual local moves, one performs global moves in which the temperatures of two replicas (with adjacent temperatures) are exchanged. It turns out to be straightforward to design an algorithm which satisfies the detailed balance condition, and it will also have a good acceptance ratio if the temperatures are fairly close together. In this way, the temperature of a given replica wanders up and down in a random manner, and each time the temperature goes low the system is likely to end up in a different valley of the energy landscape. Thus different valleys are sampled in much less time than it would take for the system to fluctuate between valleys if the temperature stayed fixed.

A sharp phase transition only occurs in an infinite system, and is rounded out in the finite size systems that can be studied numerically. In order to determine whether or not a transition occurs we use the technique of finite size scaling to extrapolate from data on *several* finite sizes to the thermodynamic limit.

The best quantity to analyze, to ascertain whether a transition occurs in the gauge glass model, seems to be the response of the system to a "twist" in the phase imposed by changing the boundary conditions. This works as follows.

We replace periodic boundary conditions with twisted boundary conditions along one of the axes $\hat{x}$, i.e.

$$\phi_{i+L\hat{x}} = \phi_i + \Theta, \tag{6}$$

where Θ is the twist angle. Note that $\Theta = 0$ corresponds to periodic boundary conditions, and $\Theta = \pi$ corresponds to anti-periodic boundary conditions. We then convert the model back to periodic boundary conditions by redefining ϕ through

$$\phi_{i+n\hat{x}} \to \phi_{i+n\hat{x}} - \frac{n}{L}\Theta. \tag{7}$$

The model then is precisely Eq. (5) with periodic boundary conditions but with the A_{ij} for bonds in the x-direction changed according to

$$A_{i,i+\hat{x}} \to A_{i,i+\hat{x}} - \frac{\Theta}{L}. \tag{8}$$

Using $F = -\ln(Z)/\beta$ we define a "current" as the response of the free energy to an infinitesimal Θ,

$$I(L) \equiv \lim_{\Theta \to 0} \frac{\partial F}{\partial \Theta} = \frac{1}{L} \sum_i \langle \sin(\phi_i - \phi_{i+\hat{x}} - A_{i,i+\hat{x}}) \rangle. \tag{9}$$

Because the A_{ij} are uniformly distributed over the entire period of the sine function, the the value of the current averaged over samples is zero, i.e.

$$[I(L)]_{\rm av} = 0. \tag{10}$$

Consequently we calculate the root-mean-square current, given by

$$I_{\rm rms} \equiv \sqrt{[\langle I_\alpha(L) \rangle \langle I_\beta(L) \rangle]_{\rm av}}, \tag{11}$$

where α and β denote two independent replicas with the same disorder.

$I_{\rm rms}$ is particularly useful because finite size scaling predicts [9] it is independent of the size at the critical point. Hence it is expected to vary near T_c as

$$I_{\rm rms} = \widetilde{I}(L^{1/\nu} t) \tag{12}$$

where ν is the exponent describing the divergence of the correlation length $\xi \sim t^{-\nu}$, and $t = (T - T_c)/T_c$ is the reduced temperature. The argument of the scaling function $\widetilde{I}$ can also be written as $(L/\xi)^{1/\nu}$, showing that the dependence on the system size only occurs through the ratio, L/ξ, which is the basic hypothesis of finite-size scaling.

In the spin glass-like phase below T_c the current should scale with the stiffness exponent [10] θ, i.e.

$$I_{\rm rms} \sim L^{\theta}, \qquad\qquad (T < T_c), \tag{13}$$

where $\theta > 0$ if $T_c > 0$, so $I_{\rm rms}$ *increases* with increasing size. Above T_c, where spin-spin correlations are small, we expect $I_{\rm rms}$ to *decrease* with increasing L and approach zero because larger systems are less sensitive to a twist at the boundaries. Hence the data for different sizes should *intersect* at T_c and splay out again below T_c. Hence, by using $I_{\rm rms}$ one can locate T_c "by eye", rather than by using a complicated fit with several correlated parameters.

Results for $I_{\rm rms}$ obtained in Ref. [6] for three dimensions are shown in Fig. (2) for a range of sizes up to $L = 12$. The data crossing is clearly seen, with splaying out on both sides of the intersection point, indicating a finite temperature transition with vortex glass (spin glass-like) order below T_c, which is estimated to be $T_c = 0.47 \pm 0.03$. Now that T_c has been determined the, correlation length exponent ν is then obtained by adjusting it until the data collapses on a scaling plot of $I_{\rm rms}$ against $L^{1/\nu}(T - T_c)$, see Eq. (12). This gives [6] $\nu = 1.39 \pm 0.20$.

Subsequent work [11], also using parallel tempering, investigated the region well below T_c to study the nature of the low temperature phase. The reader is referred to the original work [11,13,10] for details.

Considerable effort has also been expended to demonstrate the existence of a spin glass transition in the Ising spin glass in three dimensions. The most convincing work is that of Ballesteros et al. [12], which used a special purpose computer, applied the parallel tempering Monte Carlo technique, and used a very nice finite size scaling technique, analogous to the one I described above for the gauge glass, but with a different quantity which becomes independent of size at T_c. Again I refer the reader to the original paper for details.

IV. FOR THE FUTURE

I would like to conclude with a brief mention of two open topics:

- The nature of the low-temperature phase. The nature of the spin glass phase below T_c has been quite controversial. Two rival approaches have been discussed, "Replica Symmetry Breaking" [13] and the "droplet theory" [10]. Numerical work is difficult because, at least in three dimensions and higher, determination of the spin glass ground state is "NP-hard" [14], which means that all known algorithms take a time which increases exponentially with the system size, and so one is limited to quite small sizes. Similarly, Monte Carlo simulations are also restricted to small sizes at low temperature, even using the parallel tempering method that I have described above. Numerical work [15] suggests that the picture is closer to RSB than the droplet picture, but this may be due to the small sizes studied. In addition, an intermediate picture has been proposed [16].

  In two dimensions, highly efficient "polynomial" algorithms exist for finding ground states [17], so sizes with $N = L^2$ spins with L up to as large as 1800 can be studied. Unfortunately, though, the transition only occurs at $T = 0$ in two dimensions.

- Non-equilibrium effects. Because of very slow dynamics, a macroscopic system is never fully in equilibrium below T_c, so it is important to study *non-equilibrium* effects in a controlled manner. Particularly useful has been the "aging" experiments pioneered by Norblad et al [18], in which one studies, in a cooling experiment, how properties depend on the time that the system waited at a certain temperature. One of the remarkable aspects, still not understood, is the "memory" effect [19]. To explain what this is, suppose one measures the ac susceptibility, $\chi_{\rm ac}$, while slowly cooling the system, and waits for an additional time at some temperature T_w, below T_c. During the waiting period the value of $\chi_{\rm ac}$ decreases. On further cooling $\chi_{\rm ac}$ increases to the value it would have had without the wait at T_w, which is called "rejuvenation". On rewarming, $\chi_{\rm ac}$ tracks the values it had on cooling, *including the dip at* T_w. This indicates that that, while at lower temperature, the system maintained a memory that it waited at T_w. Surprisingly this behavior has *not* been reproduced by numerical simulations [20] on the Edwards-Anderson (EA) model. It is unclear whether this means that the EA model is inadequate, or that much longer simulations would be needed to see the effect. Note that the experiments are run over much longer time scales, relative to the microscopic time scale which is typically of order 10^{-12} sec., than the simulations.

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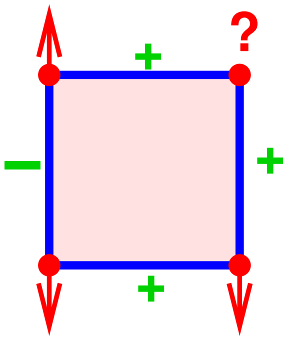

FIG. 1. The sketch illustrates the concept of frustration, one of the key ingredients of a spin glass system. The arrows represent (Ising) spins which can only point up or down. The "+" and "−" on the bonds connecting the spins represent interactions. A "+" denotes a ferromagnetic interaction, where parallel spins have the lowest energy, and a "−" indicates an antiferromagnetic interaction, where the lowest energy is for anti-parallel spins. Since there is an odd number of "−" interactions around the square, no spin configuration will will simultaneously minimize each contribution to the energy. The configuration shown minimizes the energy of the bottom and left hand interactions but then the top right spin, indicated by a "?", wants to be parallel to both of its neighbors, which is impossible. Hence there is competition or "frustration".

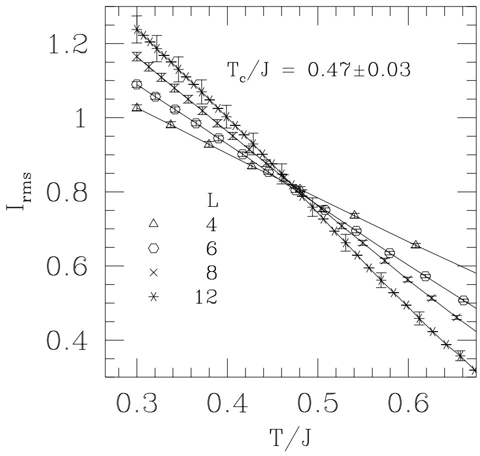

FIG. 2. A plot of $I_{\rm rms}$ from Eq. (11) for $L = 4, 6, 8,$ and 12 in three dimensions. For the point of intersection the critical temperature is estimated to be 0.47 ± 0.03. From Ref. [6].