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Griffiths Singularities in the Dynamics of Disordered Ising Models.

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Abstract. – We study the asymptotic behaviour of the correlation function $q(t) = \frac{1}{N}\sum_{i=1}^{N} \langle S_i(0)\, S_i(t)\rangle$ for dilute, short-range Ising ferromagnets and spin glasses with single spin-flip dynamics. Using an eigenfunction expansion for the time evolution operator and a variational estimate for the gap in the spectrum of this operator, we prove that, for a range of temperatures above the T_c of the random system $q(t) \geq A \exp[-C(\log t)^{\alpha}]$, with $\alpha = 2$ in two dimensions. The same inequality holds in d-dimensions, with $\alpha = d/(d-1)$, modulo a single conjecture in the equilibrium statistical mechanics of Ising ferromagnets. The slow relaxation of large «pure» clusters is responsible for this nonexponential bound.

1. Introduction.

Recently there has been much interest in the dynamics of disordered spin systems. However, there are very few exact results available for time-dependent correlation functions, in random systems. We have earlier given arguments to suggest that random magnets [1] and spin glasses [2] exhibit slow nonexponential relaxation even above their transition temperature T_c, a manifestation of the Griffiths singularities [3] in dynamics. In this paper we show that these arguments can be made rigorous in certain situations.

We study the asymptotic behaviour of the spin-spin autocorrelation function

$$q(t) = \frac{1}{N}\sum_{i=1}^{N} \langle S_i(0)\, S_i(t)\rangle \tag{1.1}$$

for random bond Ising models with dilution. We prove that in $d = 2$ dimensions

$$q(t) \geq A \exp[-C(\log t)^{\alpha}] \,, \tag{1.2}$$

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for a range of temperatures above T_c, with $\alpha = 2$. In d-dimensions we can prove the same inequality, with $\alpha = d/(d-1)$, provided a certain conjecture for the ferromagnetic Ising model holds (see eq. (2.7)).

The physical idea underlying (1.2) is as follows. It is well known that for random spin systems rare clusters of spins all of whose interactions are ferromagnetic, or more generally unfrustrated, lead to weak singularities [3] in the free energy as a function of the magnetic field in the temperature range between the T_c of the random system and that of the corresponding «pure» system. These same clusters also dominate the long-time dynamics in this temperature range by locking into one of two ground states and flipping from one to the other very infrequently. For a more detailed discussion of the physical significance of this result we refer the reader to ref. [2].

2. Outline of derivation.

We shall first outline a derivation of our main result and then present proofs for the various intermediate steps. Consider the model defined by the Hamiltonian $H = \sum_{(ij)} J_{ij} S_i S_j$ and single spin-flip relaxational dynamics (defined in sect. 3). $S_i = \pm 1$ and the summation extends over all pairs of nearest neighbors on a d-dimensional hypercubical lattice. The bond strengths J_{ij} are quenched, independent random variables with a nonzero probability for bonds of zero strength. The reasons for restricting attention to models with dilution will become clear below.

We consider the correlation function defined by (1.1). The angular brackets in this definition denote a double average: over all possible time evolutions starting from a given configuration *and* over an equilibrium distribution of initial conditions. We prove in sect. 3 that for a fixed site i, the autocorrelation function is necessarily nonnegative, namely $\langle S_i(0) S_i(t) \rangle \geq 0$. Thus each term in the summation in (1.1) is nonnegative and $q(t)$ is bounded below by a sum which runs over a subset of the lattice.

We will use the contribution of unfrustrated [4] clusters to compute a lower bound to $q(t)$. It will suffice for our purposes to restrict attention to hypercubical clusters surrounded by zero bonds (1). Let $P_0(L)$ be the probability that a given site belongs to such a cluster which is L sites to a side. As $L \to \infty$, $P_0(L) \simeq a \exp[-bL^d]$, where a and b can be explicitly calculated, though we shall never need them.

We show in sect. 4 that each cluster makes a contribution to $q(t)$ which is larger than $K \exp[-t/\tau(L)]$, where $\tau(L)$ is the relaxation time for that cluster and $K > 0$. Since these clusters are isolated from one another, they relax independently giving rise to the lower bound

$$q(t) \geq \sum_L P_0(L) K \exp[-t/\tau(L)] . \tag{2.1}$$

We further prove that $\tau(L)$ has an Arrhenius lower bound given by

$$\tau(L) \geq \tau_A(L) \equiv \exp[V(L)/k_B T] , \tag{2.2}$$

(1) In the absence of dilution, say for the $\pm J$ spin glass, we do not know how to rigorously control the effect of boundary conditions on the relaxation of clusters. See, however, ref. [2] for arguments suggesting the validity of the result in the presence of weak bonds as, for example, in a Gaussian distribution.

where the barrier height $V(L)$ is defined below. Combining (2.1) and (2.2), we obtain

$$q(t) \geqslant \sum_L P_0(L) K \exp[-t/\tau_A(L)]. \tag{2.3}$$

The barrier height $V(L)$ is defined by

$$V(L) \equiv F_L(M=0) - F_L, \tag{2.4}$$

where F_L is the free energy of an L^d Ising ferromagnet and $F_L(M=0)$ is the free energy of the same system *constrained* to have zero total magnetization (see sect. 4). To proceed further, we need to know how this barrier height scales with system size. Since, on physical grounds, $V(L)$ is closely related to the surface free energy of a domain wall, we would expect it to be proportional to the surface area below the ferromagnetic transition temperature T_F. This is rigorously known [5] only in $d=2$ dimensions, where $V(L) \sim L$ for all $T < T_F$. For $d > 2$, we make the very plausible, but unproven, conjecture (²) that, for $T < T_F$

$$V(L) \sim L^{d-1}, \qquad L \to \infty. \tag{2.5}$$

Using this, (2.3) may be estimated for $t \to \infty$ to give

$$q(t) \geqslant A \exp[-C(\log t)^{d/(d-1)}]. \tag{2.6}$$

If we consider a bounded distribution of bond strengths, (2.6) is expected to hold in the temperature range between the T_c of the random system and the ferromagnetic T_F for the largest bond strength. Since the barrier height $V(L) = 0$ for $T > T_F$, $q(t)$ is presumably exponential.

3. Nonnegativity of autocorrelations.

In this section we will prove that $\langle S_i(0) S_i(t) \rangle \geqslant 0$, under rather more general conditions (any relaxational dynamics; arbitrary multi-spin interactions) than are required for the rest of the paper.

Consider an N site Ising Hamiltonian $H[\{S_i\}]$. The states $\{S\}_\alpha \equiv \{S_1^\alpha, \dots, S_N^\alpha\}$ of the system are labelled by $\alpha = 1 \dots 2^N$. Let $P_\alpha(t)$ be the probability for the system to be in a state α at a time t. We define a continuous-time dynamics on the configuration space via the Master equation [6]

$$\frac{dP_\alpha}{dt} = \sum_\beta [\omega_{\alpha\beta} P_\beta(t) - \omega_{\beta\alpha} P_\alpha(t)]. \tag{3.1}$$

The (time-independent) transition rates $\omega_{\alpha\beta}$ satisfy the detailed balance condition

$$\omega_{\alpha\beta} P_\beta^E = \omega_{\beta\alpha} P_\alpha^E, \tag{3.2}$$

where P_α^E, the equilibrium probability at temperature T for the system to be in state α, is

(²) In fact, even the surface free energy, defined to be the difference in the free energies between periodic and antiperiodic boundary conditions, is rigorously known to scale as L^{d-1} only for sufficiently low temperatures and not for all $T < T_F$.

given, as usual, by $P^{E}_{\alpha} = \mathcal{Z}^{-1} \exp[-E_\alpha/k_B T]$, where $E_\alpha = H[\{S\}_\alpha]$ and the partition function $\mathcal{Z} = \sum_\beta \exp[-E_\beta/k_B T]$.

Following Abe [7], we find it convenient to define $\varphi_\alpha(t) = P_\alpha(t)/P^{E}_{\alpha}$. The equation of motion for φ is then given by

$$\frac{d\varphi_\alpha}{dt} = -\sum_\beta \mathcal{L}_{\alpha\beta}\varphi_\beta(t)\,, \tag{3.3}$$

where $\mathcal{L}_{\alpha\beta} \equiv \left(\sum_\gamma \omega_{\gamma\alpha}\right)\delta_{\alpha\beta} - \omega_{\beta\alpha}$ is the Liouville, or time evolution, operator. We next define an inner product [8]

$$\langle f|g\rangle \equiv \sum_\alpha P^{E}_{\alpha} f_\alpha g_\alpha = \langle fg\rangle \tag{3.4}$$

for arbitrary functions f and g defined on the configuration space. We further define the matrix element

$$\langle f|\mathcal{L}|g\rangle \equiv \sum_{\alpha\beta} P^{E}_{\alpha} f_\alpha \mathcal{L}_{\alpha\beta} g_\beta\,.$$

Using (3.2), it is then straightforward to show [7] that $\mathcal{L}$ is symmetric, *i.e.* for arbitrary functions f and g, $\langle f|\mathcal{L}|g\rangle = \langle g|\mathcal{L}|f\rangle$.

Now, since $\mathcal{L}$ is real and symmetric it has real eigenvalues λ^a, defined by

$$\sum_\beta \mathcal{L}_{\alpha\beta}\psi^a_\beta = \lambda^a\psi^a_\beta\,, \qquad a = 1\ldots 2^N\,, \tag{3.5}$$

or, in more compact notation $\mathcal{L}|\psi^a\rangle = \lambda^a|\psi^a\rangle$. For an arbitrary function f

$$\langle f|\mathcal{L}|f\rangle \equiv \sum_\alpha P^{E}_{\alpha} f_\alpha \mathcal{L}_{\alpha\beta} f_\beta = \frac{1}{2}\sum_{\alpha\beta} P^{E}_{\alpha}\omega_{\beta\alpha}(f_\alpha - f_\beta)^2\,, \tag{3.6}$$

where the second equality follows from the definition of $\mathcal{L}$ and (3.2). Thus $\langle f|\mathcal{L}|f\rangle \geqslant 0$ for any f, so that $\lambda^a \geqslant 0$ for $a = 1\ldots 2^N$. It is easy to verify that the smallest eigenvalue $\lambda^{(1)} = 0$ corresponds to the eigenfunction $\psi^{(1)}_\alpha \equiv 1$ (for all configurations α) which represents the equilibrium distribution.

We are now ready to prove the autocorrelation inequality. Abe's proof [7] for the ferromagnet goes through in the more general case with competing interactions. Let $S_A \equiv \prod_{i\in A} S_i$, for some finite subset A of points on the lattice. Define

$$\langle S_A(0)\,S_A(t)\rangle = \sum_{\alpha,\beta} P_\alpha(0) S^\alpha_A P_\beta(t|\alpha;\,0) S^\beta_A\,, \tag{3.7}$$

where $P_\beta(t|\alpha;0)$ is the conditional probability for the system to be in state β at time t, given that it was in a state α at time $t = 0$ and $P_\alpha(0) = P^{E}_{\alpha}$, since we are interested in fluctuations in the equilibrium state. Solving the time evolution equation (3.3), subject to the initial condition $\varphi_\alpha \equiv 1$, yields

$$P_\beta(t|\alpha;0) = P^{E}_{\beta}(\exp[-\mathcal{L}t])_{\beta\alpha}(P^{E}_{\alpha})^{-1}\,. \tag{3.8}$$

Substituting in (3.7), and using the eigenfunction expansion (3.5) immediately gives the required result

$$\langle S_A(0)S_A(t)\rangle = \langle S_A|\exp[-\mathcal{L}t]|S_A\rangle = \sum_a \exp[-\lambda^a t]\,|\langle S_A|\psi^a\rangle|^2 \geqslant 0\,. \tag{3.9}$$

Another useful way of rewriting this result is to use our knowledge of $\lambda^{(1)} = 0$ and $\psi_\alpha^{(1)} \equiv 1$, to obtain $\langle S_A(0) S_A(t)\rangle \geqslant \langle S_A\rangle^2$.

4. Bound on relaxation time.

We now turn to the contribution of the unfrustrated, or equivalently ferromagnetic, clusters to $q(t)$. Since these clusters are isolated, we shall study ferromagnets with free boundary conditions.

We restrict ourselves to single spin-flip dynamics with a nonconserved order parameter. A specific example of such a dynamics is that introduced by Glauber [6] in which $\omega_{\alpha\beta} = \frac{1}{2}\left(1 - S_j \operatorname{tgh}\left(\sum_k J_{ik} S_k / k_B T\right)\right)$ for states (α, β) which differ only by the sign of the j-th spin, and zero otherwise. While the arguments below are not tied to this particular form, it is important to assume that the transition rates are bounded above, *i.e.* $\omega_{\alpha\beta} \leqslant 1$ in appropriate units.

Using the results of the previous section, we obtain

$$\langle S_i(0) S_i(t)\rangle \geqslant \left|\langle S_i | \psi^{(2)}\rangle\right|^2 \exp[-\lambda^{(2)} t] \,. \tag{4.1}$$

Summing up the contribution of the independent clusters to $q(t)$, we then obtain (2.1), where the relaxation time $\tau(L) = 1/\lambda^{(2)}$.

We now use the variational principle to obtain an upper bound on the gap $\lambda^{(2)}$ in the spectrum of $\mathscr{L}$ for a cluster of $N = L^d$ spins. It can be checked easily that the stationary values of the function

$$\lambda(\{\psi_\alpha\}) = \frac{\langle \psi | \mathscr{L} | \psi\rangle}{\langle \psi | \psi\rangle} \tag{4.2}$$

with respect to variations in the «wave function» ψ_α are the eigenvalues λ^a and the stationary points ψ_α^a the corresponding eigenfunctions. Using (3.7), we can rewrite this in a more convenient form

$$\lambda(\{\psi_\alpha\}) = \frac{\sum_{\alpha\beta} P_\alpha^{\mathrm{E}} \omega_{\alpha\beta} (\psi_\alpha - \psi_\beta)^2}{2 \sum_\alpha P_\alpha^{\mathrm{E}} |\psi_\alpha|^2} \,. \tag{4.3}$$

The eigenfunction corresponding to the slowest decaying mode must be orthogonal to the «ground state» (or equilibrium) eigenfunction $\psi^{(1)}$. We thus make the simplest choice consistent with this requirement, namely $\psi = \operatorname{sgn} M_\alpha$, where $M_\alpha = \sum_{i=1}^N S_i^z$ is the *total* magnetization in state α. For simplicity, we assume N odd so that $M_\alpha \neq 0$. Using this trial wave function and the single spin-flip nature of transition rates, we obtain

$$\frac{1}{\tau(L)} = \lambda^{(2)} \leqslant \frac{2}{\mathscr{Z}} \sum_{\alpha,\beta}{}^{*} P_\alpha^{\mathrm{E}} \omega_{\beta\alpha} \,. \tag{4.4}$$

Here the sum is over pairs of states, with total magnetizations of opposite sign, which have a nonzero transition rate between them.

As noted above the transition rates are bounded, so that $\omega_{\alpha\beta} \leqslant 1$. Further there are exactly $(N+1)/2$ states with $M = -1$ connected to a given state with $M = +1$ by a single spin-flip. Thus, we have $\sum_{\beta}^{*} \omega_{\alpha\beta} \leqslant (N+1)/2$. Let $\mathcal{Z}(M=1)$ denote the restricted partition function (3) with fixed total magnetization $M=+1$. We thus obtain

$$\frac{1}{\tau(L)} \leqslant (N+1)\,\frac{\mathcal{Z}(M=1)}{\mathcal{Z}} = (L^d+1)\exp[-V(L)/k_{\rm B}T], \tag{4.5}$$

where we have defined the barrier height

$$V(L) \equiv F_L(M=1) - F_L, \tag{4.6}$$

with the free energy $F_L = -k_{\rm B}T \log \mathcal{Z}$. Note that even though the prefactor of (L^d+1) makes the Arrhenius bound (4.5) nonoptimal, this estimate will suffice for our purpose. For example, for a system of noninteracting spins, this bound gives $\lambda^{(2)} \leqslant \text{const}\sqrt{N}$ which is clearly not optimal, since we expect $\lambda^{(2)} \sim O(1)$, independent of system size. However, for the systems of our interest with unfrustrated interactions the prefactor is only a logarithmic correction to $V(L)$ which presumably grows like a power of L.

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(3) This corresponds to a canonical ensemble in contrast to the unrestricted partition function $\mathcal{Z}$, which corresponds to the grand canonical ensemble. See, *e.g.*, Gallavotti [9].

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