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Theoretical Aspects of Realistic Spin Glass Models

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ABSTRACT

This note investigates the universality of spin glass models by calculating the distribution of instantaneous local magnetic fields, $p(h)$. It is found that short range Ising models with Gaussian bond disorder fall into a different universality class than realistic models with RKKY-interactions and randomly positioned spins. The result is obtained from an analysis of $p(h)$ at high temperatures where the local fields are sums of independent random variables. It is found that for realistic models these sums are in general not governed by the central limit theorem. In three dimensions a cutoff Cauchy distribution is obtained for $p(h)$ instead of a Gaussian distribution. In general $p(h)$ is a cutoff stable law whose characteristic exponent depends strongly on the dimension and the decay of the interactions. As a consequence a new short range model is proposed for dilute metallic spin glasses in three dimensions in which the bond disorder is taken to be a cutoff Cauchy distribution instead of a Gaussian. Preliminary considerations indicate a much smoother specific heat for models in this universality class and suggest the existence of strong precursor effects in qualitative agreement with experiment.

1. INTRODUCTION

According to the central limit theorem of probability theory the Gaussian distribution arises as the limit distribution for (properly normalized) sums of mutually independent random variables having a common distribution with finite moments[1)]. This theorem lies at the heart of much of statistical physics, and it is therefore important to note exceptions from it. Such an exception arises in the context of the spin glass problem. In the classical spin glass models the central limit theorem is invoked to argue that the distribution of instantaneous local magnetic fields experienced for example by the Mn spins in CuMn is a Gaussian[2)]. Combining this argument with an appeal to the universality of the Ising model for phase transitions in ordered systems it was proposed to study the short range Ising model with a gaussian distribution for random exchange couplings as a generic model for metallic (and insulating) spin glasses[2)]. This model and in particular its mean field theory have been the subject of intense interest[3)]. Relatively little attention has been paid on the other hand to more realistic models in which the spins are placed at random positions in a lattice.[3)] In particular it seems that the question whether short range models with bond disorder fall into the same universality class as realistic models with positional disorder and RKKY-interactions has not been theoretically investigated.

My purpose in these notes is to approach this question. It will be found that within a straightforward idealization the limiting distribution of local fields in a realistic model of a diluted metallic spin glass is in general not governed by the central limit theorem. Instead other limit theorems from probability theory apply. This finding is potentially very important because it seems to imply that realistic models with positional disorder and RKKY-interactions belong to a different universality class than short range models with Gaussian bond disorder. The results also suggest how the conventional short range models must be modified to remedy this defect.

Dilute metallic spin glasses may be straightforwardly idealized as a system of point particles which are scattered randomly in space with fixed positions. Each particle carries a spin $S_i = \pm 1$ which for simplicity is taken to be Ising like, but the arguments are easily generalized to the case of more realistic Heisenberg spins. The underlying space will be assumed to be a continuum and the spatial density of spins is taken to be uniform. The Hamiltonian of the system in zero external field may be written as

$$H = -\sum_{i,j} J_{i,j} S_i S_j \tag{1.1}$$

where the spin S_i is located at position $\vec{r}_i$, and $J_{ij} = J(|\vec{r}_i - \vec{r}_j|)$ is an exchange interaction which depends on the distance between spin i and j. The summation in Eq. (1.1) runs over all spins in the sample. The exchange interaction for CuMn is usually taken to be approximated by the RKKY-form

$$J_{ij} = J_0 \frac{\cos(2k_F|\vec{r}_i - \vec{r}_j|)}{|\vec{r}_i - \vec{r}_j|^3}$$

where k_F is the value of the Fermi wave vector of the host metal and $J_0 > 0$ denotes a constant.

Given some fixed site 0 (chosen to be the origin) one defines the instantaneous local magnetic field at this site as

$$h = \sum_j J_{0j} S_j = \sum_j h_j \,. \tag{1.2}$$

The magnetic field h at the origin is generated as the sum of all other spins in the system. As such it is the sum of the random variables h_j which represent the field generated at the origin by the spin located at position $\vec{r}_j$. Its probability density will be denoted by $p(h)$. There are two sources of randomness in the random variables h_i. One is the random position of the corresponding spin, the other its random value. In this note general power law interactions will be considered so that h_i may be written as

$$h_i = \frac{J_i \tilde{S}_i}{|\vec{r}_i|^\sigma} \tag{1.3}$$

where J_i is a positive random variable and $\tilde{S}_i$ is a random sign. The case of a

dilute RKKY-system is recovered by setting $\sigma = 3$, $J_i = J_0|\cos(2k_F|\vec{r}_i|)|$ and $\tilde{S}_i = S_i \mathrm{sgn}[J_0 \cos(2k_F|\vec{r}_i|)]$.

Let me conclude this introduction with an important remark about the general strategy followed in this note. It is the objective to investigate the question which general class of distributions of coupling strengths are appropriate for short range Ising models of realistic RKKY spin glasses. The idea is to use limit theorems for sums of independent random variables to calculate the distribution of local fields $p(h)$, and then to infer the distribution of couplings in a short range model from the requirement that it must be able to reproduce the fundamental scaling properties of the correct $p(h)$. It is important to note that one assumes independence of the h_j in Eq. (1.2) which is equivalent to assuming that the system is at very high temperatures. At low temperatures correlations develop between the spins S_j, which implies that the random variables h_j are no longer independent.

2. THE DISTRIBUTION OF LOCAL FIELDS AT HIGH T

To calculate the probability density function $p(h)$ of the instantaneous local magnetic field one employs the method of charcteristic functions[1)]. Consider a finite subset of the infinite spin system. Suppose that the subset has volume V, includes the origin, and contains exactly N spins. Let $p_N(h)$ denote the probability density function of the finite sum $h = \sum_{j=1}^{N} h_j$ and $C_N(k)$ its charcteristic function. Then

$$p_N(h) = (2\pi)^{-3} \int_{-\infty}^{\infty} \exp[-ikh]\, C_N(k)\, dk \tag{2.1}$$

and

$$C_N(k) = \prod_{j=1}^{N} c_j(k) \tag{2.2}$$

where $c_j(k)$ is the charcteristic function of the random variable corresponding to the random variable h_j. Equation (2.2) assumes that the h_j are independent, and is therefore srictly valid only in the high temperature limit. The $c_j(k)$ are given by

$$c_j(k) = \int_{-\infty}^{\infty}\int_{0}^{\infty}\int_{V} \exp[ikh_j]\; p_j(\vec{r}_j,J_j,\tilde{S}_j)\; d^3\vec{r}_j\,dJ_j\,d\tilde{S}_j \qquad (2.3)$$

where $p_j(\vec{r}_j,J_j,\tilde{S}_j)$ is the probability density to find a spin at $\vec{r}_j$ with value J_j for its coupling and $\tilde{S}_j$ for its random sign such that it contributes the field h_j at the origin.

In order to proceed it is now assumed that the spins are distributed with uniform spatial density ρ. It is further assumed that the signs are completely random with mean zero, and that the values of J_j are governed by the same density $p(J)$ for all j. Also, any correlations between the variables $\vec{r}$, J and $\tilde{S}$ are ignored. With these assumptions p_j can be written

$$p_j(\vec{r}_j,J_j,\tilde{S}_j) = \frac{1}{V}\; p(J)\; \frac{1}{2}[\delta(\tilde{S}-1)+\delta(\tilde{S}+1)] \qquad (2.4)$$

where $\delta(x)$ denotes the δ-distribution.

Inserting Eq. (2.3) into (2.2) and (2.3) one finds that

$$C_N(k) = \Big\{\frac{1}{V}\frac{1}{2}\sum_{\tilde{S}=1,-1}\int_0^{\infty}\int_V \exp[ikf]\; p(J)\; d^3\vec{r}\,dJ\Big\}^N$$

where the field has been written as $f=J\tilde{S}r^{-\sigma}$ and $r=|\vec{r}|$. One realizes that $\mathrm{sgn} f=\tilde{S}$, and together with the symmetry of the cosine this gives

$$C_N(k) = \Big\{\frac{1}{V}\int_0^{\infty}\int_V \cos[|k|\;|f|]\; p(J)\; d^3\vec{r}\,dJ\Big\}^N$$

where $|f|=Jr^{-\sigma}$. To calculate the volume integral it is assumed that V has the shape of a sphere of radius R centered at the origin so that $V=\frac{4\pi}{3}R^3$. Introducing spherical coordinates one arrives at

$$C_N(k) = \Big\{\frac{4\pi}{V}\int_0^{\infty}\int_0^{R} \cos[|k|\;|f|]\; p(J)\; r^2\,dr\,dJ\Big\}^N. \qquad (2.5)$$

The next step is to take the limit of infinite volume, $V\to\infty$, in such a way that the density $\rho=\frac{N}{V}$ remains constant. To do this it is convenient to insert a zero in the bracket of Eq. (2.5) in the form of

$$0 = 1 - \frac{4\pi}{V}\int_0^{\infty}\int_0^{R} p(J)\; r^2\,dr\,dJ\,.$$

Writing $C(k) = \lim_{\substack{V,N\to\infty\\ \rho=const}} C_N(k)$ this gives

$$C(k) = \lim_{\substack{V,N\to\infty\\ \rho=const}}\Big\{1 - \frac{4\pi}{V}\int_0^{\infty}\int_0^{(\frac{3V}{4\pi})^{\frac{1}{3}}} \Big(1-\cos[|k|\;|f|]\Big)\; p(J)\; r^2\,dr\,dJ\Big\}^{\rho V},$$

and leads to the following expression for the characteristic function

$$C(k) = \exp[-\rho B(k)] \qquad (2.6)$$

where

$$B(k) = 4\pi\int_0^{\infty}\int_0^{\infty} \Big(1-\cos[|k|\;|f|]\Big)\; p(J)\; r^2\,dr\,dJ\,. \qquad (2.7)$$

To calculate $B(k)$ from Eq. (2.7) it is convenient to change variables from r to $|f|$. In this way one finds

$$B(k) = \frac{4\pi}{\sigma}\int_0^{\infty}\int_0^{\infty} \Big(1-\cos[|k|\;|f|]\Big)\; J^{\frac{3}{\sigma}}|f|^{-1-\frac{3}{\sigma}}p(J)\; d|f|\,dJ\,.$$

Changing variables again to $z=|k|\;|f|$ gives

$$B(k) = \frac{4\pi}{\sigma}\;\overline{J^{3/\sigma}}\;|k|^{\frac{3}{\sigma}}\int_0^{\infty}\Big(1-\cos z\Big)\; z^{-1-\frac{3}{\sigma}}dz \qquad (2.8)$$

where the notation $\overline{J^{3/\sigma}}=\int_0^{\infty} J^{\frac{3}{\sigma}}p(J)dJ$ was introduced. The remaining integral

$$I_\sigma = \int_0^{\infty} (1-\cos z)z^{-1-\frac{3}{\sigma}}dz \qquad (2.9)$$

is found to be convergent for all $\sigma>\frac{3}{2}$. Integrating by parts one finds explicitly

$$I_\sigma = \frac{\sigma}{3}\Gamma(1-\tfrac{3}{\sigma})\sin[\tfrac{\pi}{2}(1-\tfrac{3}{\sigma})] \tag{2.10a}$$

for $\sigma>3$, and

$$I_\sigma = \frac{\sigma^2}{3(3-\sigma)}\Gamma(2-\tfrac{3}{\sigma})\cos[\tfrac{\pi}{2}(2-\tfrac{3}{\sigma})] \tag{2.10b}$$

for $\frac{3}{2}<\sigma<3$. Combining equations (2.1),(2.6) and (2.8)-(2.10) one finally obtains the result

$$p(h) = (2\pi)^{-3}\int_{-\infty}^{\infty} \exp[-ikh-\lambda|k|^{\frac{3}{\sigma}}]\, dk \tag{2.11}$$

where $\lambda=\frac{4\pi}{\sigma}\ \overline{J^{3/\sigma}}\, I_\sigma\rho$.

Thus the distribution $p(h)$ of instantaneous local magnetic fields is given by a symmetric stable distribution with characteristic exponent $\alpha=\frac{3}{\sigma}$ and scale parameter λ proportional to the density ρ. For the case of RKKY interactions, $\sigma=3$, one obtains a stable law with exponent 1, the symmetric Cauchy distribution. The fact that the integral I_σ in Eq. (2.9) converges only for $\sigma>\frac{3}{2}$ expresses the well known restriction of the characteristic exponent to the range $0\leq\alpha\leq2$. For exponents $\sigma\leq\frac{3}{2}$ the above calculation no longer applies and one obtains the Gaussian distribution for $p(h)$.

3. PROBABILISTIC SCALING ARGUMENT

Before proceeding with a discussion of this result, and its immediate problems, it is instructive to derive it in a different way and at the same time to generalize it. The fundamental nature of the result is apparent from the fact that the characteristic exponent can also be derived from a simple probabilistic scaling argument combined with the use of general theorems from the theory of stable laws.

Consider two very dilute samples with spin densities ρ_1 and ρ_2. A third sample of density $\rho_1+\rho_2$ is obtained as their superposition. The random variable

$h(\rho)$ is defined as the field at the origin generated by the spins in a given sample of density ρ. This random variable obeys the relation

$$h(\rho_1)+h(\rho_2)=h(\rho_1+\rho_2) \tag{3.1}$$

where the equality sign means equality in distribution, i.e. the random variables on the right and the left hand side have the same probability densities.

To each density ρ there corresponds a characteristic length scale which is the average distance between two particles. Let l_0 be this length scale for the density ρ_0. Now imagine changing the density by some factor λ from ρ_0 to $\lambda\rho_0$. Then the corresponding length scale will change from l_0 to $\lambda^{-1/d}l_0$. Assuming for the fields the same spatial dependence as that of Eq. (1.3) one finds that the fields must scale as

$$h(\lambda\rho_0) = \lambda^{\frac{\sigma}{d}}h(\rho_0) \tag{3.2}$$

where the equality means again equality in distribution.

Therefore the family of distributions $p_\rho(h)$ of the random variables $h(\rho)$ constitutes a one parameter family of distributions which form a convolution semigroup by virtue of Eq. (3.1) and which differ only by a scale parameter. One can thus use general theorems from the theory of stable distributions[1)] to conclude that the distribution of h must be a stable law with characteristic exponent $\alpha=\frac{d}{\sigma}$. It also follows from the general theory that the exponent is restricted to the range $0\leq\alpha\leq2$.

4. DISCUSSION

4.1 Short Range Behaviour

The central result of the previous sections is the fact that combining RKKY-interactions and disorder gives rise to new and fundamental scaling properties. They are reflected in the occurrence of a non-gaussian stable law for $p(h)$, at least at sufficiently high temperatures, and imply much stronger fluctuations than in a gaussian system. A realistic short range Ising model with nearest neighbour random exchange which wants to reproduce the correct $p(h)$ in the high temperature limit must incorporate the correct scaling in its distribution of couplings. The distribution of couplings must belong to the domain of attraction of the appropriate stable law. It follows that the Edwards-Anderson model is only realistic for dimensions $d \geq 6$. For a realistic model of a dilute RKKY spin glass in $d=3$ the distribution of random nearest neighbour couplings must be chosen from the domain of attraction of the Cauchy distribution.

There is however a serious problem: The Cauchy distribution for example has no moments and that is unphysical. As a consequence the internal energy per particle in a model with a Cauchy distribution of local fields would be divergent. The problem can be traced back to the idealization that the particles are pointlike and their positions can assume a continuum of possible values. One can show[4] that the power law decay of $p(h)$ results entirely from configurations in which two spins are only a short distance apart (cf. Eq. (1.3)). In reality the particles are restricted to lie on a lattice. This implies that there exists a minimum distance between two particles, and consequently a maximum possible field. Similarly, the fact that the RKKY interaction does not diverge at the origin also implies a high field cutoff for $p(h)$. One concludes that the true distribution of local fields at high temperatures is given by a stable law with a cutoff at high fields corresponding to the minimum distance between particles.

One might now argue that if the wings of $p(h)$ are cut off then all its moments exist, and $p(h)$ must belong to the domain of attraction of the Gaussian distribution. One could then conclude that a Gaussian distribution of local fields is universal, and its actual form obtained above is irrelevant. Such a conclusion, however, would be premature. The existence of a cutoff means only that the basic scaling properties implied by $p(h)$ are restricted to a limited range. Such a phenomenon is ubiquitous in scaling theories and therefore the question becomes: How important is the cutoff for the physics of the spin glass transition ?

To answer this question consider a dilute system of density $\rho(\ll 1)$ in continuum space. For any given particle the probability of finding a second particle within a distance of order unity will be of order ρ and hence very small. Consider now a second system with a cutoff of order unity which is obtained from an exact copy of the first system by removing one particle whenever two particles have distance less than unity. The main difference between the two systems is the existence of a finite temperature T_{co} for the system with cutoff above which all spins fluctuate independently. By contrast such a temperature does not exist for the system without cutoff because there will always be a very small number of strongly coupled spins whose interaction energy is higher than the thermal energy. For low densities ρ the temperature T_{co} will lie well above the glass transition temperature. For temperatures below T_{co} the two systems will behave almost identically because they differ only by a small number (order ρ^2) of strongly coupled spins. Therefore the introduction of a cutoff is expected to be only a small perturbation as far as the freezing behaviour of the system is concerned. On the other hand if one were to change $p(h)$ into a Gaussian then the fluctuation and scaling properties of the system are changed and the freezing process must be expected to be very different.

4.2 The Specific Heat

The occurrence of a non-gaussian stable law implies much stronger fluctuations than in a gaussian system. This is reflected in a simple consideration of the specific heat. As mentioned above the tails of $p(h)$ are governed by the field arising from nearest neighbours. This is true at all temperatures and therefore the tails are temperature independent. Assuming for the moment that not only the tail but the full distribution $p(h)$ is independent of temperature one finds for the specific heat

$$C_V \sim \int_{-\infty}^{\infty} p(h)\beta^2 h^2 \cosh^{-2}(\beta h)\, dh ,$$

where $\beta = 1/T$ is the inverse temperature. It is very instructive to compare the results obtained from an evaluation of the integral using a Gaussian for $p(h)$ with those using a cutoff Cauchy distribution. In both distributions the same width w is used, and for the Cauchy case the cutoff is called h^{max}. For temperatures $T \gg w$ one obtains for the Gaussian $C_V \sim T^{-2}$ as in the Edwards-Anderson model. For the cutoff Cauchy distribution the situation is different. The T^{-2}-law is now only obtained for $T \gg h^{max}$, while for $w \ll T \ll h^{max}$ one has $C_V \sim T^{-1}$. At low temperatures both cases give a linear specific heat, but that results from the behaviour of $p(h)$ near the origin for which the assumption of temperature independence is no longer valid. Nevertheless it is interesting to note that the maximum obtained with a Gaussian is relatively pronounced while the maximum in the Cauchy case is very broad. This is also in line with the existence of much stronger precursor effects for the Cauchy case which result from the existence of many strongly coupled spins well above the freezing temeperature. In summary it appears that new models with a cutoff Cauchy distribution for $p(h)$ have a better chance to be in qualitative agreement with experiment.

4.2 "Universality" and "critical" dimensions

Finally I would like to remark two interesting consequences of the results. Each stable distribution characterized by its exponent defines a "universality class" by virtue of its domain of attraction. Thus one has the curious consequence that for the positionally disordered spin systems discussed in these notes the universality class depends sensitively on the details of the interaction (except when $\sigma \leq d/2$).

A second interesting point might be to note that the relation $\alpha = \frac{d}{3}$ for the dilute RKKY systems implies that the dimensions $d=3$ and $d=6$ are "special" or perhaps "critical" dimensions. This follows from the very "special" role played by the Gaussian and the Cauchy distribution in the family of stable laws.

5. CONCLUSIONS

The purpose of this paper was to motivate and introduce a new generic model for dilute RKKY spin glasses in low dimensions. In three dimensions the model is defined by the usual Ising Hamiltonian

$$H = -\sum_{<j,i>} J_{ij} S_i S_j$$

on a regular lattice. The sum runs over all nearest neighbour pairs of Ising spins $S_i = \pm 1$, and the random variables J_{ij} for the couplings are chosen from the cutoff Cauchy density

$$p(J_{ij}) = \frac{J}{\arctan J^{max}} \frac{1}{J^2 + J_{ij}^2} \quad .$$

for $|J_{ij}| < J^{max}$ and 0 otherwise. It is argued that the new distribution is necessary to capture the essential fluctuation properties of real materials, and preliminary results indicate[4)] that the new model is indeed able to achieve a broader correspondence between theory and experiment.

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