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Restrictions concerning the internal field in spin glasses

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Abstract. In addition to the fact that the spin-glass system is situated within a stationary point of the energy surface, energetic correlations have been taken into account between groups of p spins, which lead to restrictions concerning the simultaneous internal field values on different sites. The physical implications of this fact are also analysed.

1. Introduction

The internal field distribution in random systems in general and in spin glasses in particular represents an essential problem [1]. Knowledge of this property helps us in the elaboration of the theoretical description of the quenched state [1, 2] and also in the interpretation of much experimental data [1, 3] concerning this domain.

If we suppose that the spin directions at different sites are totally random variables, we obtain two types of classical distribution functions: if the interspin distances are non-restricted, the distribution is Lorentzian (or double Lorentzian) [4], and if the interspin distances are restricted, in conformity with the central limit theorem, the distribution is Gaussian [5].

Recent results on this subject show that this image is unacceptable. Correlations between the spins in the quenched systems can be directly explicit [5, 6]; theoretical and Monte Carlo studies of the internal field distributions show that near the low field limit a cavity [5] or a hole [7] appears, results which cannot be explained using totally random and independent spin directions and values.

For theoretical descriptions and for interpretation of the experimental data, in the majority of the cases, one uses distribution functions for the modulus of the internal field $|\boldsymbol{H}_i|$. When we take classical distributions, we consider that the $|\boldsymbol{H}_i|$ values are not correlated from site to site and can independently take any positive values. In contrast, if the spins correlate with each other and the classical field distributions fall, then there must exist restrictions over the different $|\boldsymbol{H}_i|$ values. The knowledge of these restrictions will contribute to a better understanding of the different phenomena which characterise the systems under study.

In this paper we try to obtain, in the vector spin case, a mathematical description for the energetic correlation of spins and to deduce from it the restrictions concerning the $|\boldsymbol{H}_i|$ values. We do not express the interaction between the spins; we impose only that the i spin contribution in the Hamiltonian be given by the expression $\boldsymbol{\mu}_i\boldsymbol{H}_i$, where $\boldsymbol{\mu}_i$ is the dipole moment on the site i. In this way, our results can be applied to any kind of interspin interaction which satisfies this condition, and it can also be generalised to electric dipole moments.

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The paper is organised as follows: in § 2 we analyse the energetic correlation conditions between the spins, which are used in § 3 for the deduction of the restriction conditions concerning the $|\boldsymbol{H}_i|$ values. Section 4 presents a discussion and conclusions.

2. The energetic correlation conditions

If we take p spins and write their energy, we obtain

$$E_p = -\tfrac{1}{2} \sum_{i=1}^{p} \boldsymbol{\mu}_i \cdot \boldsymbol{H}_i \tag{1}$$

where $\boldsymbol{H}_i$ is the total internal field and $\boldsymbol{\mu}_i = \boldsymbol{\mu} \cdot \boldsymbol{n}_i$ is the dipole moment on site i. $\boldsymbol{H}_i$ can be explained as

$$\boldsymbol{H}_i = \boldsymbol{H}_i^{\mathrm{E}} + \boldsymbol{H}_i^{\mathrm{I}} \tag{2}$$

where $\boldsymbol{H}_i^{\mathrm{E}}$ is the field created at site i by the external magnetic moments (all spins from the system, except the chosen p spins) and

$$\boldsymbol{H}_i^{\mathrm{I}} = \sum_{\substack{j=1 \\ j \neq i}}^{p} \boldsymbol{H}_{ij} \tag{3}$$

is the internal field created at site i (by the chosen p spins). We denote by $\boldsymbol{H}_{ij}$ the field created at site i by the magnetic moment from the site j.

We suppose that the whole system is situated at a stationary point of the energy surface, so $\boldsymbol{n}_i$ is directed along $\boldsymbol{H}_i$ [5, 8]. On the other hand we consider that the chosen p spins correlate with each other so that their energy contribution E_p will be a minimum value. If this supposition is true, then a simultaneous flip of all p spins in (1) will increase E_p, so one obtains

$$\sum_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{E}} > 0. \tag{4}$$

By analogy, if we flip only one spin from the p spins, we obtain

$$\sum_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i + \sum_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{I}} > 0. \tag{5}$$

Equations (4) and (5) and the $\Sigma_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i > 0$ condition gives the following relations:

$$\sum_{i=1}^{p} |\boldsymbol{H}_i| > \left| \sum_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{I}} \right| > 0 \tag{6}$$

$$\sum_{i=1}^{p} |\boldsymbol{H}_i| > \tfrac{1}{2} \sum_{i=1}^{p} \boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{E}} > 0. \tag{7}$$

These two relations can be considered as simple expressions of the energetic correlations between the spins within the system. Based on these inequalities one can deduce conditions which restrict the simultaneous $|\boldsymbol{H}_i|$ values on different sites depending on the $\boldsymbol{H}_{ij}$ values.

This problem will be treated in § 3.

3. The restriction conditions concerning the $|H_i|$ values

It can easily be demonstrated that for $p \geqslant 3$ and $x_i \geqslant 0$ the following relation exists:

$$Z(p)\left(\sum_{\substack{i,j=1\\ i<j}}^{p}(x_i x_j)\right)^{(p+1)/2} \geqslant \left(\prod_{i=1}^{p} x_i\right)\left(\sum_{i=1}^{p} x_i\right) \tag{8}$$

where

$$Z(p)=\sum_{i=2}^{\infty} a_i \delta i, p \qquad a_3=\tfrac{1}{3} \qquad a_{2k+1}|_{k>1}=(k+1)^{-1} \qquad a_{2k}|_{k>1}=(2k+1)^{-1/2}. \tag{9}$$

The introduction of a_2 in (9) will be clarified below. It can be observed that from (6) we obtain

$$\left(\sum_{i=1}^{p}|\boldsymbol{H}_i|\right)^2 > \sum_{\substack{i,j=1\\ i<j}}^{p}(\boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{I}})(\boldsymbol{n}_j \cdot \boldsymbol{H}_j^{\mathrm{I}}). \tag{10}$$

Now using $x_i=|\boldsymbol{H}_i|$, (3), (8) and (10) and the well known inequality

$$\frac{1}{n}\sum_{i=1}^{n} x_i^m \geqslant \left(\sum_{i=1}^{n}\frac{x_i}{n}\right)^m \tag{11}$$

we obtain the restriction conditions for the $|\boldsymbol{H}_i|$ values:

$$Q(p)\left(\prod_{i=1}^{p}|\boldsymbol{H}_i|^{-2}\right)\left(\sum_{\substack{i,j=1\\ i<j}}^{p}(|\boldsymbol{H}_i|\cdot|\boldsymbol{H}_j|)^{p+1}\right) > \sum_{\substack{i,j=1\\ i<j}}^{p}\left(\sum_{\substack{l=1\\ l\neq i}}^{p}\boldsymbol{n}_i \cdot \boldsymbol{H}_{il}\right)\left(\sum_{\substack{k=1\\ k\neq j}}^{p}\boldsymbol{n}_j \cdot \boldsymbol{H}_{jk}\right) \tag{12}$$

where

$$Q(p)=[p(p-1)/2]^p Z^2(p). \tag{13}$$

We recall that $\boldsymbol{n}_i$ is the unit vector of $\boldsymbol{\mu}_i$ and $\boldsymbol{H}_i$, $\boldsymbol{H}_i$ is the total internal field on site i and $\boldsymbol{H}_{ij}$ is the field acting on site i created by the spin situated at site j. The relation arising from (12) is true in any case where (1) and (2) take place.

Now we must analyse the $p=2$ case. Because the inequality (8) is true only for $p \geqslant 3$, the $p=2$ case of (12)

$$Q(2)|\boldsymbol{H}_i|\cdot|\boldsymbol{H}_j| > (\boldsymbol{n}_i \cdot \boldsymbol{H}_{ij})(\boldsymbol{n}_j \cdot \boldsymbol{H}_{ji}) \qquad Q(2)=a_2^2 \tag{14}$$

is insufficiently argued. In the following we demonstrate that (14) is also a correct result, and we estimate the a_2 value.

If we denote, in accordance with (7), $\xi_{ij}=\frac{1}{2}(\boldsymbol{n}_i \cdot \boldsymbol{H}_i^{\mathrm{E}}+\boldsymbol{n}_j \cdot \boldsymbol{H}_j^{\mathrm{E}})>0$, then we obtain for the all-site pair

$$|\boldsymbol{H}_i|+|\boldsymbol{H}_j| > \xi_{ij}. \tag{15}$$

Suppose that we have in a crystal a site i, where $|\boldsymbol{H}_i|=0$. Then, in accordance with (15), for all the other sites the internal field must be greater than ξ_{ij}. On the other hand, the existence of an $|\boldsymbol{H}_i|=0$ site leads to an energy variation proportional to $\delta \boldsymbol{n}_j$, which decreases the energy [5]. So on every site $|\boldsymbol{H}_i|=\eta_i$ must be a strictly positive value. This conclusion also agrees well with Monte Carlo simulations [7].

The minimum of η_i is comparable with $\xi = \min \xi_{ij}$. Under these conditions relation (14) is correct, with

$$a_2 \rightleftharpoons (\xi/\varepsilon) \tag{16}$$

where $\varepsilon = \max(\boldsymbol{n}_i \cdot \boldsymbol{H}_{ij})$ and a_2 is a positive finite value.

An inequality resembling that given in (14) has been obtained by mathematical tricks in reference [5] in the RKKY case where, because the $\boldsymbol{H}^{\mathrm{E}}$ and $\boldsymbol{H}^{\mathrm{I}}$ components of the total local fields for the pair lie in the same plane, $a_2 = 1$.

4. Discussion and conclusions

It can be observed that if we consider classical distributions for the internal field in a random system, the $|\boldsymbol{H}_i|$ values from site to site are not correlated with each other and could independently take any positive values. Recent results [7, 8] concerning spin-glass systems show that the classical field distributions fall, which indicates that the $|\boldsymbol{H}_i|$ values must correlate with each other and so the internal fields at different sites cannot independently take any value. In other words, there must exist restriction conditions concerning the simultaneous internal field at different sites.

In this paper we have attempted to deduce, in the vector spin case, these restriction conditions, taking into account that, apart from the fact that the whole system is situated within a stationary point of the energy surface, groups of p spins will correlate (accommodate) with each other in such a way that they give a minimum energy contribution to the total energy of the system.

The restriction conditions can be used in different ways in the description of spin-glass systems. For example, they can indicate in the Monte Carlo experiments how the chosen state in the simulation process is situated in comparison with the real state of the system. On the other hand, some of the restriction conditions can be used to calculate analytically the internal field distribution $P(H)$. The standard procedures which can be used for this [5] give a correction factor $f_c(H)$ to the classical field distributions, which describe analytically the appearance of a cavity or hole in $P(H)$ and the cavity depth modification as a function of the anisotropy factor which enters into the Hamiltonian of the system. $f_c(H)$ is of the form

$$f_c(H) \sim \exp[-\alpha/(\beta + H)^{1/2}]. \tag{17}$$

Furthermore, because of the generality of (12) and (13), we also have the possibility of treating the RKKY and dipolar interactions together in a description of the realistic internal field distribution in spin-glass systems [9].

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