Internal Field Distribution in Spin-Glasses

Chaim Held and Michael W. Klein*
Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

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It is shown that the probability for the magnitude of the internal field $|\vec{H}|$ of a spin-glass is proportional to $H^2 d|\vec{H}|$ for very small internal fields. If one assumes that the spins are quantized in the magnitude of the field the low-temperature specific heat is proportional to T^3 in disagreement with the experimentally measured linear dependence.

Recent experiments by Fiory *et al.*[1] on polarized μ mesons slowed down in spin-glasses (dilute magnetic impurities distributed in a nonmagnetic metal host are referred to as spin-glasses) give a measure of the internal field distribution of the spin-glass system. It is also believed that the distribution of the internal fields for small fields may determine the origin of the excess low-temperature specific heat of spin-glasses. Experimentally it was found by Zimmerman and Hoare[2] that the low-temperature specific heat is linear in temperature T and independent of the fractional impurity concentration c for sufficiently low temperatures. Thus it is of considerable interest to determine the probability distribution of the internal fields for spin-glasses.

The purpose of this Letter is to obtain the self-consistent probability distribution of the magnitude of the molecular field $|\vec{H}|$ as well as the distribution of the vector field $\vec{H}$ experienced by the spins in the spin-glass system. We find that for both of these the probability distribution $P(\vec{H})$ is zero for zero field and has, for both cases, the form $P(|\vec{H}|)d|\vec{H}| = \text{const}H^2\,dH$, where H is the magnitude of the field. Thus if it is assumed that the spins are quantized in the magnitude of the field the molecular field model gives $P(|\vec{H}|) = 0$ for $|\vec{H}| = 0$ and hence *does not* explain the low-T behavior of spin-glasses. The specific heat C_v arising from the model still scales according to the relationship $C_v \propto c f(T/c)$. It is also shown that the previous treatment of one of the authors on this subject has an incorrect assumption in it.

Starting with the expression for the total molecular field vector $\vec{H}_T$ (internal plus external field) at an arbitrary spin located at the origin o, we have

$$\vec{H}_T = \vec{H}_o + \vec{H}_{\text{ext}}, \tag{1}$$

where $\vec{H}_{\text{ext}}$ is the externally applied field and

$$\vec{H}_o = \sum v_{oj} m_j (H_j) \vec{\mathfrak{u}}_j, \tag{2}$$

where v_{oj} is the Ruderman-Kittel-Kasuya-Yosida[3] (RKKY) potential assumed in this paper to have the form $v_{ij} = \pm a/r_{ij}^3$, each sign having a probability of $\frac{1}{2}$. Writing the RKKY potential in this form will allow us to evaluate our integrals exactly without changing the result obtained by using the full RKKY potential. m_j in Eq. (2) is the Brillouin function of the spin at site j in an effective field $\vec{H}_j$. $\vec{H}_j$ and $\vec{\mathfrak{u}}_j$ are random variables whose probability distribution has to be determined self-consistently. $\vec{\mathfrak{u}}_j$ is a unit vector in the direction of the vector field at site j since the direction of $\vec{H}_j$ is assumed to be the direction of quantization of the spin at site j. $\vec{H}_j$ is

$$\vec{H}_j = \sum v_{jk} m_k \vec{\mathfrak{u}}_k. \tag{3}$$

The magnitude of the field $|\vec{H}_o|$ at site o is obtained from Eqs. (1) and (2),

$$|\vec{H}_o| = [(\sum v_{oj} m_j \vec{\mathfrak{u}}_j + \vec{H}_{\text{ext}})^2]^{1/2}. \tag{4}$$

The calculation of the probability distribution is performed in the limit $\vec{H}_{\text{ext}} \to 0$. We use the statistical model of Margenau[4] in the form developed by Klein,[5] whose method we closely follow, to obtain $P(\vec{H}_o)$, where $\vec{H}_o$ is the vector internal field experienced by a spin placed at an arbitrary origin o. Thus

$$P(\vec{H}_o) = \int P_c(\vec{R}) \delta(\vec{H}_o - \sum v_{oj} m_j \vec{\mathfrak{u}}_j) d^3 r_N, \tag{5}$$

where $P_c(\vec{R}) = P(r_1, r_2, \ldots, r_N)$ is the N-particle distribution function of the spin coordinates (indicated by the subscript c), $d^3 r_N$ is a $3N$ dimensional integral over the $3N$ position coordinates of the impurities.

Similarly the formal expression for the probability distribution of the magnitude of the field H is given by[5]

$$P(|\vec{H}|) = \int P_c(\vec{R}) \delta(H - |\sum v_{oj} m_j \vec{\mathfrak{u}}_j|) d^3 r_N. \tag{6}$$

Rewriting Eq. (5) we obtain

$$P(\vec{H}_o) = (2\pi)^{-3}\int d^3\rho \exp(i\vec{\rho}\cdot\vec{H}_o)\int P_c(\vec{R})\, d^3r_N \prod_{j=1}^{N-1} \exp(-iv_{oj} m_j \vec{\rho}\cdot\vec{u}_j). \tag{7}$$

Note that m_j in the above equation is a function of H_j, where H_j is given by Eq. (3).

For convenience we rewrite Eq. (7) as follows,

$$P(\vec{H}_o) = (2\pi)^{-3}\int \exp(i\vec{\rho}\cdot\vec{H}_o) d^3\rho \int P_c(\vec{R})\, d^3r_N \prod\nolimits_j \int \exp(iv_{oj} m_j \vec{\rho}\cdot\vec{u}_j)\delta(\vec{H}_j - \textstyle\sum v_{jk} m_k \vec{u}_k)\, d^3H_j. \tag{8}$$

That Eq. (8) is identical with Eq. (7) can be seen by performing the integration over d^3H_j.

Equation (8) expresses the probability distribution of the vector field at site o in terms of the N random potentials v_{oj} at sites j ($j = 1$ to N) and the internal fields at all other (than the origin) sites in the system. In order to get a solution to Eq. (8) we will have to make an approximation. Let

$$D_j(\vec{H}_j) = \delta(\vec{H}_j - \textstyle\sum v_{jk} m_k \vec{u}_k). \tag{9}$$

We note that Eq. (8) contains the product of N such D_j's. However, once the N coordinates of the spins are fixed, so are all the r_{oj}'s and the D_j's. Now consider what happens when we change the position of a single spin, say spin 1 with position r_1^{o} to a new position r_1^{1}, where the subscript denotes the particle and the superscript denotes the position. As the position was changed from r_1^{o} to r_1^{1} all the D_j's take on new (fixed) values. Thus as the positions of all the particles are changed by allowing them to take various random values, all the D_j's change accordingly and for every set of new configurations the D_j's take on new *fixed* values. We now factor the D_j's, i.e., we assume that each D_j is independent of every other D_j [thereby giving the system $N(N-1)$ new degrees of freedom] and replace each D_j by its average over all coordinates [thereby reducing the number of degrees of freedom by $N(N-1)$]. We call this approximation the mean random field (MRF) approximation discussed previously in some detail.[5,6] In the MRF approximation we thus have

$$D_j \to \int P_c(\vec{R})\delta(\vec{H}_j - \textstyle\sum v_{jk} m_k \vec{u}_k)\, d^3r_N \equiv P(\vec{H}_j), \tag{10}$$

where the identity holds from the definition Eq. (5). Assuming next that the positions of all the particles are randomly and uniformly and independently distributed throughout the volume of the solid V, then $P_c(\vec{R}) = V^{-N}$. Substituting Eq. (10) into Eq. (8) and using the latter assumption gives

$$P(\vec{H}) = (2\pi)^{-3}\int \exp(i\vec{\rho}\cdot\vec{H}_o) d^3\rho [(1/V)\iint \exp(-iv_{oj} m_j \vec{\rho}\cdot\vec{u}_j) P(\vec{H}_j)\, d^3H_j\, d^3r_{oj}]^N. \tag{11}$$

We thus find that the introduction of the MRF approximation allows us to factor the j-fold product in Eq. (8) into a single integral raised to the Nth power. Equation (11) gives the probability distribution of the vector field $\vec{H}_o$ at site o in terms of the probability distribution of the field at site j. As a self-consistency condition we now require that $P(\vec{H})$ shall be site independent, and thus we drop the subscripts o and j. All that is left now is to solve the integral equation for $P(\vec{H})$ given in Eq. (11). This we do by using the following trick.[5] Let

$$P(\vec{H}) = (2\pi)^{-3}\int e^{i\vec{\rho}\cdot\vec{H}} d^3\rho [1 - V'(\vec{\rho})/V]^N, \qquad P(\vec{H}) = (2\pi)^{-3}\int \exp(i\vec{\rho}\cdot\vec{H}) \exp[-n_0 c V'(\rho)]\, d^3\rho, \tag{12}$$

where n_0 is the number of sites per unit cell, V' is

$$V'(\rho) = (8\pi/3)\rho a\langle m\rangle \int [(1 - \sin z/z)/z^2]\, dz = 2\rho\pi^2 a\langle m\rangle/3, \tag{13}$$

and

$$\langle m\rangle = \int m(H) P(\vec{H})\, d^3H. \tag{14}$$

Equation (12) can be readily integrated to give

$$P(\vec{H}) = \pi^{-2}\Delta/(\Delta^2 + H^2)^2, \tag{15}$$

where $\Delta = \pi^2 a n_0 c\langle m\rangle/3$. For later use it is convenient to exhibit the quantity $P(\vec{H})\, d^3H$. We have

$$P(\vec{H})\, d^3H = \pi^{-2}[\Delta/(\Delta^2 + H^2)^2] H^2\, dH \sin\theta\, d\theta\, d\varphi. \tag{16}$$

Equation (16) shows that the probability for small vector fields is proportional to $H^2 dH$.

We next obtain the probability distribution for the magnitude of the field H, where the formal expression for $P(H)$ is given in Eq. (6). We could go through the same steps as was done up till now to obtain $P(H)$, but instead we shall obtain $P(H)$ by a shorter method. We note that[7]

$$\delta(\vec{H}-v_{oj}m_j\hat{u}_j)=\delta(H-|\sum v_{oj}m_j\hat{u}_j|)\delta(\theta-\theta')\delta(\varphi-\varphi')(H^2\sin\theta)^{-1}. \tag{17}$$

Substituting the right-hand side of Eq. (17) into Eq. (5), multiplying the result by $H^2dH\sin\theta\, d\theta\, d\varphi$, and integrating over θ and φ gives

$$P(|\vec{H}|)\,dH=P(\vec{H})4\pi H^2\,dH=(4/\pi)\Delta\{\Delta^2+H^2\}^{-2}H^2\,dH. \tag{18}$$

Equations (16) and (18) are the central results of this paper. In both equations we find that the probability for small fields is proportional to H^2dH. The probability density for both the vector field and the magnitude of the field is zero for zero fields. An argument to this effect has been presented previously by Marshall[8] and Anderson,[9] however it has not been shown before.

Now we present a brief discussion of the present state of theoretical understanding of the molecular-field model in spin-glasses. The previous calculations[10, 11] were done using a molecular-field approximation and the Ising model neglecting all correlations. These Ising calculations gave the experimentally observed low-T specific heat. The calculations presented in this paper are also done in the molecular-field approximation and also neglect correlations. The present calculations are however believed to represent the correct physical picture. Thus we come to the conclusion that if (a) the spins are quantized in the magnitude of the field (the direction of quantization being the direction of the vector field) and (b) there is no preferred direction of spin orientation because of some internal constraint, the molecular-field model—with correlations neglected—does not explain the low-temperature specific heat of spin-glasses. Therefore, one must likely include correlations or do a more complete quantum mechanical calculation of the partition function to obtain the low-temperature specific heat. A recent quantum mechanical calculation[12] of the partition function following the lines developed by Edwards and Anderson[13] gives a specific heat linear in T, but the predicted concentration dependence of the specific heat is in disagreement with experiment.

Finally we comment on some previous work[14] of one of the authors on this subject. In the work of Ref. 14, the apparently incorrect assumption was made that the magnitude of the field at site o is given by the expression $|\vec{H}_o|=|\sum v_{oj}m_j\hat{u}_o\cdot\hat{u}_j|$ rather than the correct value given by Eq. (4) of the present paper. This assumption has forced the results of Ref. 14 to be Ising-like, and gave the incorrect Ising result, rather than the present Eq. (18).

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