Internal-field distribution in spin-glasses with dipolar interactions

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We analyze the internal-field distribution functions for dipolar coupling and for dipolar and Ruderman-Kittel-Kasuya-Yosida interactions together. First a totally random spin system is considered. After this a local correlation between the spins is taken into account, which causes a cavity to appear within the internal-field distribution functions. We also analyze the cavity-depth-modification problem and present an application in the μ^+ relaxation domain.

I. INTRODUCTION

In recent years many theoretical and experimental papers have analyzed the spin glass (SG) phase in different materials. The interactions which exist in these materials are diverse. The most frequently analyzed interaction of these is the Ruderman-Kittel-Kasuya-Yosida (RKKY) coupling[1] which causes the appearance of the SG phase in the greatest part of the materials within which the frozen phase takes place. Other interactions are overshadowed despite the fact that many of them play an important role in diverse situations. One of these is the dipolar interaction. This interaction contributes in an essential fashion to the occurrence of the SG phase in general,[2] and in insulators in particular,[3] determines the muon-spin relaxation in most of the frozen and random systems,[4] influences the NMR line broadening,[5] and cannot be neglected in many situations in which the stronger RKKY long-range coupling cannot be realized or is damped in the analyzed materials.[6] All of these applications necessitate a reanalyzation of the dipolar interaction, especially its internal-field probability-density function, taking into account the new results concerning the internal-field distribution problem for SG.[7–9]

The possibility of existence of the SG phase caused by dipolar interactions was demonstrated theoretically,[10] and it seems to have been proved experimentally too.[3,11] The internal-field distribution was first analyzed in connection with the NMR line broadening. A Lorentzian shape for dilute dipole-dipole broadening was derived for $S=\frac{1}{2}$ from statistical arguments,[12] and by the method of moments.[13] Walstedt and Walker[5] have generalized this result to higher spin values and have analyzed the dipolar interaction in the high-field approximation.[14] They conjectured that in the dilute limit the NMR line shape is Lorentzian for any coupling which varies as R^{-3}. Describing a mathematically analogous situation, Klein *et al.*[15] considered a set of electric-dipole impurities, randomly distributed in a medium. The dipoles were assumed to be orientated only in the six equivalent cubic directions. Using a complicated approximation (mean-random-molecular field, denoted by MRF in Ref. 15), they obtained a double Lorentzian distribution for the internal electric field. The internal-field distribution for dipole-dipole coupling is reanalyzed in other papers,[16] but without giving qualitative new results.

As can be seen, the description of the dipolar internal-field distribution is relatively poor considering the importance of this interaction in the interpretation of many physical situations concerning random systems.[2–11] Furthermore, physical applications[3–6] have been claimed to take into account the new results obtained in these directions. Dasgupta, Ma, and Hu,[7] Ma,[8] and at approximately the same time Walker and Walstedt,[9] directed attention to the fact that one obtains the classical internal-field distributions when one considers a totally random spin system. But this model is static and neglects the dynamic processes which allow each spin to accommodate to others. In this way, the supposition of totally random spin-direction distribution is incorrect. One consequence of local correlations is the appearance of a cavity within the field-distribution function, the shape of which is greatly modified, especially in the low-field domain. This is confirmed also by Monte Carlo simulations.[17]

For the RKKY interaction the above-mentioned effect is already taken into account.[7,8] The purpose of this paper is to reanalyze the internal-field distributions for the dipolar coupling from this point of view. To extend the applicability of the paper, in all the described cases we analyze the RKKY-dipolar combined coupling too. We consider vector spins.

The paper is organized as follows. In Sec. II we analyze in the most general case the internal-field distribution for the totally random distributed spins, taking into account dipolar coupling alone and the dipolar and RKKY interactions together. In Sec. III we analyze the minimization conditions. These will be taken into account in Sec. IV, to correct the field-density distributions deduced in Sec. II. In Sec. V we analyze the cavity-depth problem, and in Sec. VI we present a discussion and an application in the μ^+ relaxation domain.

II. CLASSICAL FIELD DISTRIBUTIONS

First of all, we determine the distribution function of the local dipolar field in the most general case. We consider N dipoles randomly distributed in position and direction throughout the volume V. An arbitrary directed dipole situated at a distance $\mathbf{r}_i$ from the origin produces a vector potential at the origin given by

$$\mathbf{A}_i=\frac{\boldsymbol{\mu}\times\mathbf{r}_i}{|\mathbf{r}_i|^3}\ , \tag{1}$$

where $\boldsymbol{\mu}$ is the dipolar moment.

From Eq. (1), using the relation $\mathbf{H}=\nabla\times\mathbf{A}$, we obtain the magnetic field produced at the origin by the analyzed dipole:

$$\mathbf{H}_i=\frac{|\boldsymbol{\mu}|}{|\mathbf{r}_i|^3}\boldsymbol{\phi}\ , \tag{2}$$

where $\boldsymbol{\phi}=\mathbf{i}\phi_x+\mathbf{j}\phi_y+\mathbf{k}\phi_z$ is the angular anisotropy factor given by

$$\begin{aligned}
\phi_x&=\sin\theta_r\cos\varphi_r[\cos\theta_\mu\cos\theta_r+\cos(\varphi_\mu-\varphi_r)\sin\theta_\mu\sin\theta_r]-\sin\theta_\mu\cos\varphi_\mu\ ,\\
\phi_y&=\sin\theta_r\sin\varphi_r[\cos\theta_\mu\cos\theta_r+\cos(\varphi_\mu-\varphi_r)\sin\theta_\mu\sin\theta_r]-\sin\theta_\mu\sin\varphi_\mu\ ,\\
\phi_z&=\cos\theta_r[\cos\theta_\mu\cos\theta_r+\cos(\varphi_\mu-\varphi_r)\sin\theta_\mu\sin\theta_r]-\cos\theta_\mu\ .
\end{aligned} \tag{3}$$

In Eq. (3) the θ and φ represent the polar and azimuthal angles, for the vectors $\boldsymbol{\mu}$ and $\mathbf{r}_i$, respectively.

We define $P_0(\mathbf{H})$ as the distribution, normalized to unity for the local field:[8]

$$P_0(\mathbf{H})=\left\langle\delta\left[\mathbf{H}-\sum_i\mathbf{H}_i\right]\right\rangle\ , \tag{4}$$

where $\mathbf{H}_i$ is given in Eq. (2), and the average is taken over all positions $\mathbf{r}_i$ and all possible directions of the dipoles. Using the Fourier integral representation for the δ function, we get from Eq. (4)

$$P_0(\mathbf{H})=(2\pi)^{-3}\int d^3\xi\, e^{-i\boldsymbol{\xi}\cdot\mathbf{H}}\prod_i\langle e^{-i\boldsymbol{\xi}\cdot\mathbf{H}_i}\rangle\ . \tag{5}$$

For $C(\xi)=\langle e^{-i\boldsymbol{\xi}\cdot\mathbf{H}_i}\rangle$ we have

$$C(\xi)=\frac{1}{V-V_0}\int_{r_0}^{r}r^2dr\int_0^\pi d\theta_r\sin\theta_r\int_0^{2\pi}d\varphi_r\frac{1}{\pi}\int_0^\pi d\theta_\mu\frac{1}{2\pi}\int_0^{2\pi}d\varphi_\mu\exp\left[-i\frac{\mu}{r^3}\boldsymbol{\xi}\cdot\boldsymbol{\phi}\right]\ , \tag{6}$$

where $\mu=|\boldsymbol{\mu}|$, and the lower cutoff r_0 is the minimum distance between two particles. After some algebra, the expression of $C(\xi)$ becomes

$$C(\xi)=1-\frac{1}{V-V_0}\frac{\mu}{3}\int_z^{z_0}\frac{dz}{z^2}\int_0^\pi d\theta_r\sin\theta_r\int_0^{2\pi}d\varphi_r\frac{1}{\pi}\int_0^\pi d\theta_\mu\frac{1}{2\pi}\int_0^{2\pi}d\varphi_\mu|\boldsymbol{\xi}\cdot\boldsymbol{\phi}|[1-\cos z+i\,\mathrm{sgn}(\boldsymbol{\xi}\cdot\boldsymbol{\phi})\sin z] \tag{7}$$

where $z=|\boldsymbol{\xi}\cdot\boldsymbol{\phi}|\mu/r^3$ and $z_0=|\boldsymbol{\xi}\cdot\boldsymbol{\phi}|\mu/r_0^3$. The integral over the angles from the last term in Eq. (7) vanish, so we obtain

$$C(\xi)=1-\frac{1}{3}\frac{\mu}{V-V_0}\int_z^{z_0}dz\frac{1-\cos z}{z^2}\int_0^\pi d\theta_r\sin\theta_r\int_0^{2\pi}\frac{d\varphi_r}{\pi}\int_0^\pi\frac{d\theta_\mu}{2\pi}\int_0^{2\pi}d\varphi_\mu|\boldsymbol{\xi}\cdot\boldsymbol{\phi}|\ . \tag{8}$$

For $C(\xi)$, the ξ vector is fixed in space. Then, we can rotate the local coordinate system from the origin, so that its z axis will coincide with the direction of the ξ vector. In this way the integral in Eq. (8) can be performed.

Let us assume in the first case that $r_0\to 0$. In the large-V limit we get

$$C(\xi)=1-\frac{\xi\mu}{V}\frac{\pi}{6}\langle\phi\rangle\ , \tag{9}$$

where

$$\langle\phi\rangle=\int_0^\pi d\theta_r\sin\theta_r\int_0^{2\pi}d\varphi_r\frac{1}{\pi}\int_0^\pi d\theta_\mu\frac{1}{2\pi}\int_0^{2\pi}d\varphi_\mu\phi_z\ . \tag{10}$$

Returning to Eq. (5), the ξ integral is then easily evaluated to give

$$P_{0L}(\mathbf{H})=\frac{1}{\pi^2}\frac{A_{DL}}{(A_{DL}^2+H^2)^2}\ , \tag{11}$$

where $A_{DL}=\mu(\pi/6)n\langle\phi\rangle$ is the width of the local-field distribution and

$$n=(N/V)|_{N\to\infty,V\to\infty}$$

is the volume concentration of the dipoles in the system.

In the second case, we take a small but finite r_0. Then, from Eq. (8) we obtain

$$C(\xi)=1-\frac{1}{3}\frac{\mu}{V-V_0}\int_0^\pi d\theta_r\sin\theta_r\int_0^{2\pi}d\varphi_r\frac{1}{\pi}\int_0^\pi d\theta_\mu\frac{1}{2\pi}\int_0^{2\pi}d\varphi_\mu|\boldsymbol{\xi}\cdot\boldsymbol{\phi}|\left[\mathrm{Si}(z_0)+\frac{\pi}{2}-\frac{1-\cos z_0}{z_0}\right]\ , \tag{12}$$

where $\mathrm{Si}(x)=-\int_x^\infty t^{-1}\sin t\,dt$, is the sin-integral function.[18] Following the method presented in the previous case, we get

$$C(\xi)=1-\frac{1}{6}\frac{\xi^2\mu^2}{r_0^3}\frac{\langle\phi^2\rangle}{V-V_0}\;, \tag{13}$$

where $\langle\phi^2\rangle$ is defined with the use of Eq. (10), in which ϕ_z must be replaced by ϕ_z^2.

The evaluation of the ξ integral in this case leads to an expression that the central limit theorem would imply:

$$P_{0G}(\mathbf{H})=(4\pi A_{DG}^2)^{-3/2}\exp\left[-\frac{H^2}{4A_{DG}^2}\right]\;, \tag{14}$$

where $A_{DG}^2=(\mu^2 n/6r_0^3)\langle\phi^2\rangle$.

We mention now some aspects concerning the applications of the deduced local-field distribution functions. As can be seen from Eqs. (11) and (14), the assumption of a totally random spin distribution leads to classical probability functions. From these, the double Lorentzian is usually taken into account,[15,16] but this is acceptable only for not very high field limit, because $P_{0L}(\mathbf{H})$ defined in Eq. (11) give rise to logarithmically divergent $\langle H\rangle$ and linearly divergent $\langle H^2\rangle$ for large H. This means that in the large internal-field limit one had to use the Gaussian distribution function given in Eq. (14).

In many analyzed systems the dipolar interaction together with the RKKY indirect exchange couples the spins. For these cases we must also calculate the density distribution function of the local field. In the mentioned situation the internal field is

$$\mathbf{H}_i=\mathbf{H}_D+\mathbf{H}_R \tag{15}$$

where $\mathbf{H}_D$ is given in Eq. (2), and

$$\mathbf{H}_R=g_R\frac{q}{r^3}\boldsymbol{\mu},\;\; q=\cos(2k_F r)\;. \tag{16}$$

We denote the $\boldsymbol{\mu}$ vector components in the local coordinate axis by φ_i, $i=x,y,z$ obtaining the following expression for the local field at the origin:

$$\mathbf{H}=\frac{\mu}{r^3}[(\phi_x+qg_R\varphi_x)\mathbf{i}+(\phi_y+qg_R\varphi_y)\mathbf{j}+(\phi_z+qg_R\varphi_z)\mathbf{k}]\;. \tag{17}$$

In this way, the density distribution functions can be determined replacing $\boldsymbol{\phi}$ in Eq. (6) with $\boldsymbol{\psi}=\boldsymbol{\phi}+qg_R\boldsymbol{\varphi}$, and taking into account in the average a supplementary integral over the density distribution of q:[19]

$$P(q)=\frac{1}{\pi}\frac{1}{(1-q^2)^{1/2}}\;. \tag{18}$$

Using this method one reobtains Eqs. (11) and (14) with the remark that in the expression of A_{DL} and A_{DG} in place of $\langle\phi\rangle$ and $\langle\phi^2\rangle$ will enter $\langle\psi\rangle$ and $\langle\psi^2\rangle$, respectively.

III. THE ENERGY EXTREMA CONDITIONS

The question which now arises is whether the results given in Eq. (11) or Eq. (14) represent the real distribution functions. The main assumption that we made in the preceding section was that all the spins are randomly distributed in their position and direction. But this assumption seems to be incorrect. The spin directions within the system are not totally independent, because each spin will accommodate to others so that the local spin configuration will try to decrease the energy of the system. In other words, the spin directions are not totally random, being influenced by the local correlation tendency of the spins.

A simple model of this process can be obtained in the following way: Let us consider a system of randomly oriented $N\gg 1$ magnetic moments $\boldsymbol{\mu}_i$, with unit vector $\mathbf{n}_i$. For simplicity we take (during this section) $|\boldsymbol{\mu}_i|=1$ and so the total energy of the system can be written as

$$E=-\frac{1}{2}\sum_{i,j=1}^{N}\mathbf{n}_i\cdot\mathbf{H}_{ij}\;, \tag{19}$$

where $\mathbf{H}_{ij}$ is the internal field acting on site i and which was created by the magnetic moment situated at the site j. In the following we will always explicate the $\mathbf{n}_j$ dependence of $\mathbf{H}_{ij}$: $\mathbf{H}_{ij}=\mathbf{H}_{ij}(\mathbf{n}_j)$. About $\mathbf{H}_{ij}(\mathbf{n}_j)$ we consider only that it is linear concerning its variable $\mathbf{n}_j$:

$$\mathbf{H}_{ij}\left[\mathbf{A}_j=\sum_k x_k\mathbf{A}_k\right]=\sum_k x_k\mathbf{H}_{ij}(\mathbf{A}_k)\;, \tag{20}$$

where $\mathbf{A}_k$ is an arbitrary vector set.

We consider that our system has a configuration $\{\mathbf{n}_i^0\}$ which represents a stationary point of the energy surface, so we can write

$$\sum_{\substack{j=1\\ j\neq i}}^{N}\mathbf{H}_{ij}(\mathbf{n}_j)=\lambda_i\mathbf{n}_i,\;\;\lambda_i=|\mathbf{H}_i|\;, \tag{21}$$

where $\mathbf{H}_i$ is the total internal field acting on site i:

$$\mathbf{H}_i=\sum_{\substack{j=1\\ j\neq i}}^{N}\mathbf{H}_{ij}(\mathbf{n}_j)\;. \tag{22}$$

The image presented up to now gives the classical distribution functions for the internal fields.

As we mentioned above, the spins are not totally independent, but correlate locally each other, so that the local spin configuration will try to decrease the energy of the system. To describe this process mathematically we choose p spins and impose that its configuration give a minimum energy contribution in the total energy of the system. To do this first we renote the spin indices to ensure the first indices for the chosen p spins and rewrite the total energy from Eq. (19) as

$$E=-\sum_{i=1}^{p}\mathbf{n}_i\mathbf{H}_i-\frac{1}{2}\sum_{l=p+1}^{N}\mathbf{n}_l\widetilde{\mathbf{H}}_l\;, \tag{23}$$

where

$$\mathbf{H}_i\,|_{i\le p}=\mathbf{H}_i^E+\mathbf{H}_i^I,\quad \mathbf{H}_i^I\,|_{i\le p}=\sum_{\substack{j=1\\ j\neq i}}^{p}\mathbf{H}_{ij}(\mathbf{n}_j),$$
$$\mathbf{H}_i^E\,|_{i\le p}=\sum_{l=p+1}^{N}\mathbf{H}_{il}(\mathbf{n}_l),\quad \widetilde{\mathbf{H}}_l=\mathbf{H}_l-\sum_{k=1}^{p}\mathbf{H}_{lk}(\mathbf{n}_k)\ . \tag{24}$$

$\mathbf{H}_i^E$ and $\mathbf{H}_i^I$ are the two components of the internal field acting on the chosen p sites: The first ($\mathbf{H}_i^E$) is created by the spins other then the p spins (it is an "external" field from the point of view of the chosen spins), and the second ($\mathbf{H}_i^I$) is the field created by the p particles themselves (it is an "internal" field from the point of view of the chosen group). $\widetilde{\mathbf{H}}_l$ is a truncated field which acts on the magnetic moments situated outside of the chosen magnetic moments and which can be obtained by subtraction of the first p contribution from the total internal field H_l.

The first term from Eq. (23) gives the contribution in the total energy of the p spins:

$$E_p=-\sum_{i=1}^{p}\mathbf{n}_i\cdot\left[\mathbf{H}_i^E+\sum_{\substack{j=1\\ j\neq i}}^{p}\mathbf{H}_{ij}\right] \tag{25}$$

Let us now perturb the analyzed p group of spins by a small displacement $\mathbf{m}_i$ ($|\mathbf{m}_i\cdot\mathbf{m}_i|\ll 1$, $\mathbf{n}_i^0\cdot\mathbf{m}_i=0$); then for $i\le p$ we may write

$$\mathbf{n}_i=\mathbf{n}_i^0+\mathbf{m}_i-\tfrac{1}{2}(\mathbf{m}_i\cdot\mathbf{m}_i)\mathbf{n}_i^0+\cdots\ . \tag{26}$$

Introducing $\mathbf{n}_i$ from (26) in Eq. (23) and using the property (20) we get the second-order change in the energy as

$$E_2=\sum_{i=1}^{p}\frac{\lambda_i}{2}(\mathbf{m}_i\cdot\mathbf{m}_i)-\sum_{i=1}^{p}\sum_{\substack{j=1\\ j\neq i}}^{p}\mathbf{m}_i\mathbf{H}_{ij}(\mathbf{m}_j)+\sum_{i=1}^{p}\sum_{\substack{j=1\\ j\neq i}}^{p}\tfrac{1}{2}(\mathbf{m}_i\cdot\mathbf{m}_j)\mathbf{n}_i^0\mathbf{H}_{ij}(\mathbf{n}_j^0) \tag{27}$$

Furthermore, the p spins will give a minimum energy contribution in E (in other words will minimize E_p) if E_2 is positive definite.

Introducing unit vectors $\mathbf{a}_i$ and $\mathbf{b}_i$, with $\mathbf{a}_i\mathbf{n}_i^0=\mathbf{b}_i\mathbf{n}_i^0=\mathbf{a}_i\mathbf{b}_i=0$ at each p sites, we can put

$$\mathbf{m}_i=\alpha_i\mathbf{a}_i+\beta_i\mathbf{b}_i\ , \tag{28}$$

and E_2 becomes

$$E_2=\sum_{i=1}^{p}\left[(\alpha_i^2+\beta_i^2)\frac{\lambda_i}{2}+\frac{1}{2}\sum_{\substack{j=1\\ j\neq i}}^{p}(\alpha_j^2+\beta_j^2)h_{ij}-\sum_{\substack{j=1\\ j\neq i}}^{p}(\alpha_i\alpha_jx_{ij}+\beta_i\beta_jy_{ij}+\alpha_i\beta_ju_{ij}+\beta_i\alpha_jv_{ij})\right], \tag{29}$$

where

$$h_{ij}=\mathbf{n}_i^0\cdot\mathbf{H}_{ij}(\mathbf{n}_j^0),\quad x_{ij}=\mathbf{a}_i\cdot\mathbf{H}_{ij}(\mathbf{a}_j)\ ,$$
$$y_{ij}=\mathbf{b}_i\cdot\mathbf{H}_{ij}(\mathbf{b}_j),\quad u_{ij}=\mathbf{a}_i\cdot\mathbf{H}_{ij}(\mathbf{b}_j)\ ,$$
$$v_{ij}=\mathbf{b}_i\cdot\mathbf{H}_{ij}(\mathbf{a}_j)\ . \tag{30}$$

Now E_2 is a quadratic form in $2p$ variables α_i,β_i which must be positive definite.

If we take $p=2$, the eigenvalues of the Hessian matrix associated with E_2 from Eq. (29) can be obtained from the equation (Λ_k stands for the eigenvalues of the Hessian matrix)

$$\left[\frac{\lambda_1+h}{2}-\Lambda_k\right]^2\left[\frac{\lambda_2+h}{2}-\Lambda_k\right]^2-\left[\frac{\lambda_1+h}{2}-\Lambda_k\right]\left[\frac{\lambda_2+h}{2}-\Lambda_k\right](x^2+y^2+u^2+v^2)+(xy-uv)^2=0\ , \tag{31}$$

and must be positive definite. We used the notations $x=x_{12}=x_{21}$, $y=y_{12}=y_{21}$, $u=u_{12}=v_{21}$, $v=v_{12}=u_{21}$, and $k=1,2$. After some algebra this condition leads to

$$\sum_{i=1}^{2}|\mathbf{H}_i|>\tfrac{1}{2}\sum_{i=1}^{2}\mathbf{n}_i^0\cdot\mathbf{H}_i^E\ . \tag{32}$$

With the $|\mathbf{m}_i\cdot\mathbf{m}_i|\ll 1$ small displacements we can perturb only infinitesimally the $\{\mathbf{n}_i^0\}$ stationary configuration. If we want to be sure that E_p has an absolute minimum value, we must check also for great perturbations, for example with momentum inversion $\mathbf{n}_i\to-\mathbf{n}_i, i=1,2,\ldots,p$ (which cannot be obtained with small displacements). This inversion leaves the second term from Eq. (25) unchanged, and so the energy minimization is governed by the first term. So we must have

$$\sum_{i=1}^{p}\mathbf{n}_i\cdot\mathbf{H}_i^E>0\ . \tag{33}$$

From Eq. (33) for $p=2$ we get

$$\xi_{ij}=\tfrac{1}{2}(\mathbf{n}_i\cdot\mathbf{H}_i^E+\mathbf{n}_j\cdot\mathbf{H}_j^E)>0\ . \tag{34}$$

If there exists one site in the system where $|\mathbf{H}_i|=0$, then for all $j\neq i$ one obtains $|\mathbf{H}_j|>\xi_{ij}$. But the existence of the $|\mathbf{H}_i|=0$ case, in a stationary point of E, leads to an energy variation which is proportional with $\delta\mathbf{n}_j$ and decreases the energy of the system.[8] So $|\mathbf{H}_i|$ must be a strict positive number for every site. This gives the necessary condition for the local energy extremum requirement obtained for the RKKY case by Walker and Walstedt[9] in agreement with other authors' results,[17] and shows that the probability of finding zero local field must be zero and not a maximum value as the classical distribution functions in Eqs. (11) and (14) predict. This is the reason why the local energy extremum condition modifies the internal-field distribution functions.

If we denote $\xi=\min\{\xi_{ij}\}$ and $\eta=\max\{\mathbf{n}_i\cdot\mathbf{H}_{ij}\}$ for all $i,j=1,2,\ldots,N$, then

$$|\mathbf{H}_i|\cdot|\mathbf{H}_j|Q>(\mathbf{n}_i\cdot\mathbf{H}_{ij})(\mathbf{n}_j\cdot\mathbf{H}_{ji}), \tag{35}$$

where $Q=\eta/\xi$ is a positive, finite number. This inequality exists for any kind of interaction between magnetic moments which satisfy the relations from Eqs. (19) and (20). In the case of RKKY interaction for any pair of spins $\mathbf{H}_i$, $\mathbf{H}_i^E$, $\mathbf{H}_{12}$, and $\mathbf{H}_{21}$ lie in the same plane. In this situation one reobtains the relation (3.12) from Ref. 8, deduced by mathematical artifacts, obtaining for this case $Q=1$.

For $p\geq 3$ a general formula is obtained[20] to describe the local energy minimization condition:

$$\left[\frac{p(p-1)}{2}\right]^p\left[\prod_{i=1}^{p}|\mathbf{H}_i|^{-2}\right]\left[\sum_{i=1}^{p}\sum_{\substack{j=1\\i<j}}^{p}(|\mathbf{H}_i|\;|\mathbf{H}_j|)^{p+1}\right]>\sum_{i=1}^{p}\sum_{\substack{j=1\\i<j}}^{p}\left[\left[\sum_{\substack{l=1\\l\neq i}}^{p}\mathbf{n}_i\cdot\mathbf{H}_{il}\right]\left[\sum_{\substack{k=1\\k\neq j}}^{p}\mathbf{n}_j\cdot\mathbf{H}_{jk}\right]\right]. \tag{36}$$

Returning to Eq. (35), for dipolar interaction we find

$$|\mathbf{H}_i|\;|\mathbf{H}_j|>\frac{(g\mu_B S)^2}{Q}\left[3\frac{(\mathbf{n}_i\cdot\mathbf{r}_{ij})(\mathbf{n}_j\cdot\mathbf{r}_{ji})}{|\mathbf{r}_{ij}|^5}-\frac{\mathbf{n}_i\cdot\mathbf{n}_j}{|\mathbf{r}_{ij}|^3}\right]^2. \tag{37}$$

Furthermore, taking into account the RKKY and dipolar couplings together, one gets

$$|\mathbf{H}_i|\;|\mathbf{H}_j|>\frac{(g\mu_B S)^2}{Q}\left[3\frac{(\mathbf{n}_i\cdot\mathbf{r}_{ij})(\mathbf{n}_j\cdot\mathbf{r}_{ji})}{|\mathbf{r}_{ij}|^5}+(qg_R-1)\frac{\mathbf{n}_i\cdot\mathbf{n}_j}{|\mathbf{r}_{ij}|^3}\right]^2. \tag{38}$$

In the next section we will use these results to deduce the corrections to the classical distribution functions.

IV. THE CORRECTED DISTRIBUTION FUNCTIONS

As we mention in the preceding section, the energy extremum condition modifies substantially the classical distribution functions. From the physical point of view this modification means that at the impurity sites, it is not the $H=0$ internal-field value that is the most probable, but on the contrary the probability of finding a vanishing local field is greatly diminished. In this condition a cavity appears in the distribution function around the value $H=0$. The effect of the cavity was analyzed by many authors[8,9,17] in the case of RKKY interaction. The purpose of this section is to generalize the cavity calculations for other then RKKY couplings.

From a mathematical point of view the presence of the cavity means that the classical distribution function is multiplied by a correction term which modifies its shape for not very high H values.

First we will exemplify the calculation of the mentioned correction term for dipolar coupling. If we use in Eq. (37) the notation $\mathbf{r}_{ij}=r\mathbf{u}_{ij}$, $\mu_0=g\mu_B S/\sqrt{Q}$, and $|\mathbf{H}_i|=H_i$, one obtains

$$H_iH_j>\frac{\mu_0^2}{r^6}[3(\mathbf{n}_i\cdot\mathbf{u}_{ij})(\mathbf{n}_j\cdot\mathbf{u}_{ij})-\mathbf{n}_i\cdot\mathbf{n}_j]^2. \tag{39}$$

For a given $H_j=H$ the restriction introduced by Eq. (39) in the space of all H_i is

$$\prod_i\Theta\left[H_i-\frac{\xi_D}{Hr^6}\right], \tag{40}$$

where

$$\Theta(x)=\begin{cases}1 & \text{for } x\geq 0\\ 0 & \text{for } x<0,\end{cases}$$

and

$$\xi_D=\mu_0^2[3(\mathbf{n}_i\cdot\mathbf{u}_{ij})(\mathbf{n}_j\cdot\mathbf{u}_{ij})-(\mathbf{n}_i\cdot\mathbf{n}_j)]^2. \tag{41}$$

Taking the average of this product over the random distribution of $\mathbf{H}_i$, we obtain

$$P_L(\mathbf{H})=K_LP_{0L}(\mathbf{H})C_{0L}(H), \tag{42}$$

where

$$C_{0L}(H)=\prod_i\langle\Theta(H_i-\xi_D/Hr^6)\rangle \tag{43}$$

is the correction factor and K_L is the constant which accomplish the normalization to unity. In order to calculate the correction factor one can write

$$\ln C_{0L}(H)=\sum_i \ln g_L\left[\frac{\xi_D}{Hr^6}\right], \tag{44}$$

where

$$g_L\left[\frac{\xi_D}{Hr^6}\right]=\langle\Theta(H_i-\xi_D/Hr^6)\rangle$$

$$=\int_{H_i=\xi_D/Hr^6}^{\infty}P_{0L}(\mathbf{H})\,d\mathbf{H}. \tag{45}$$

Integrating in Eq. (45) we find

$$g_L\left[\frac{\xi_D}{Hr^6}\right]=1+\frac{2}{\pi}\frac{z_L\xi_D}{z_L^2+\xi_D^2}-\frac{2}{\pi}\arctan\frac{\xi_D}{z_L}\,, \quad (46)$$

where $z_L=A_{DL}Hr^6$. Now we transform the sum over i in Eq. (44) in an integral over r, for which (because of the fixed $H_j=H$) one takes the polar angle θ_j defined as $\mathbf{n}_j\cdot\mathbf{u}_{ij}=\cos\theta_j$. The obtained result must be than averaged over all possible directions of n_i, after which, changing the integration variable r in z_L, one gets

$$\ln C_{0L}(H)=-H^{-1/2}\frac{B_{DL}}{(A_{DL})^{1/2}}\,, \quad (47)$$

where

$$B_{DL}=\frac{n}{3}\int_0^{\pi}d\theta_i\int_0^{\pi}d\theta_j\sin\theta_j\int_0^{\infty}\frac{dz_L}{(z_L)^{1/2}}\ln\left[1+\frac{2}{\pi}\frac{z_L\xi_D}{z_L^2+\xi_D^2}-\frac{2}{\pi}\arctan\frac{\xi_D}{z_L}\right]^{-1}. \quad (48)$$

It can be checked that the constant B_{DL} always has a positive value. Now from Eqs. (42) and (47) we obtain

$$P_L(\mathbf{H})=\frac{K_L}{\pi^2}\frac{A_{DL}}{(A_{DL}^2+H^2)^2}\exp\left[-H^{-1/2}\frac{B_{DL}}{(A_{DL})^{1/2}}\right]. \quad (49)$$

Analytically it can be shown that K_L is always a positive, finite number.[21]

In the case of Gaussian distribution the correction term can be determined using the same method. Integrating over H within the g_G function

$$g_G\left[\frac{\xi_D}{Hr^6}\right]=\int_{H_i=\xi_D/Hr^6}^{\infty}P_{0G}(\mathbf{H})d\mathbf{H}\,, \quad (50)$$

we obtain

$$g_G\left[\frac{\xi_D}{Hr^6}\right]=1-\phi\left[\frac{\xi_D}{z_G}\right]-\frac{2}{\sqrt{\pi}}\frac{\xi_D}{z_G}\exp\left[-\frac{\xi_D^2}{z_G^2}\right], \quad (51)$$

where $z_G=2A_{DG}Hr^6$ and

$$\phi(x)=2/\sqrt{\pi}\int_0^x\exp(-t^2)dt$$

is the error function.[18] Using the same procedure as above, one gets

$$C_{0G}(H)=\exp\left[-H^{-1/2}\frac{B_{DG}}{(A_{DG})^{1/2}}\right], \quad (52)$$

where

$$B_{DG}=\frac{n}{3\sqrt{2}}\int_0^{\pi}d\theta_i\int_0^{\pi}d\theta_j\sin\theta_j\int_0^{\infty}\frac{dz_G}{(z_G)^{1/2}}\ln\left[1-\phi\left[\frac{\xi_D}{z_G}\right]-\frac{2}{\sqrt{\pi}}\frac{\xi_D}{z_G}\exp\left[-\frac{\xi_D^2}{z_G^2}\right]\right]^{-1}. \quad (53)$$

So, the corrected Gaussian distribution function becomes

$$P_G(\mathbf{H})=K_G(4\pi A_{DG}^2)^{-3/2}\exp\left[-\frac{H^2}{4A_{DG}^2}-H^{-1/2}\frac{B_{DG}}{(A_{DG})^{1/2}}\right]. \quad (54)$$

The normalization constant K_G can be easily determined.[21]

If we take into consideration the dipolar and RKKY interactions together, one must start with Eq. (38) and must take into account a supplementary average over $P(q)$ given in Eq. (18). The corrected internal-field distributions do not have a qualitative new shape, so we exemplify the correction term only in the double Lorentzian case:

$$C_0(H)=\exp\left[-H^{-1/2}\frac{B_{DRL}}{(A_{DRL})^{1/2}}\right], \quad (55)$$

where

$$B_{DRL}=\frac{n}{3\pi}\int_{-1}^{+1}\frac{dq}{(1-q^2)^{1/2}}\int_0^{\pi}d\theta_i\int_0^{\pi}d\theta_j\sin\theta_j\int_0^{\infty}\frac{dz}{\sqrt{z}}\ln\left[1+\frac{2}{\pi}\frac{z\xi_{DR}}{z^2+\xi_{DR}^2}-\frac{2}{\pi}\arctan\frac{\xi_{DR}}{z}\right]^{-1}, \quad (56)$$

and

$$\xi_{DR}=\mu_0^2[3(\mathbf{n}_i\cdot\mathbf{u}_{ij})(\mathbf{n}_j\cdot\mathbf{u}_{ij})+(qg_R-1)(\mathbf{n}_i\cdot\mathbf{n}_j)]^2 , \quad (57)$$

where A_{DRL} can be obtained from the expression of A_{DL} in which, as we mentioned in Sec. II, $\langle\phi\rangle$ is replaced by $\langle\psi\rangle$.

V. THE CAVITY DEPTH MODIFICATION

The correction function which was obtained in the preceding section gives a vanishing probability for zero local field. But this is not a necessary characteristic for the cavity. There exist different physical situations which modify substantially the cavity shape and depth. These contributions are usually connected to the local anisotropy. This fact has been taken into account in Ref. 8 to describe the metastable states of the nucleus. It was shown qualitatively that the nucleus field distribution, while it presents a cavity centered around zero field, nevertheless gives a nonzero probability for vanishing field. In other situations the cavity became so large that we can find vanishing probability for the field distribution below a finite H value.[17] We try in this section to obtain an analytic description for this effect, which can be used for the correction of the classical field distributions. For this purpose, because of the mathematical complexity of the problem, we take into consideration an extremely simple local anisotropy expression, which enters in the energy contribution as $K_i^*|\mu_i|^2$. In this case the total energy of the system can be written as [see Eq. (19)]

$$E=-\sum_{i=1}^{N}\mu_i\cdot\mathbf{H}_i , \quad (58)$$

with

$$\mathbf{H}_i=\sum_{\substack{j=1\\ j\neq i}}^{N}\mathbf{H}_{ij}-K_i^*\mu_i . \quad (59)$$

Using the same procedure as described in Sec. III, for the dipolar interaction we get

$$(H_i+K_i^*)(H_j+K_j^*) > \mu_0^2\left[3\frac{(\mathbf{n}_i\cdot\mathbf{u}_{ij})(\mathbf{n}_j\cdot\mathbf{u}_{ij})}{|\mathbf{r}_{ij}|^3}-\frac{\mathbf{n}_i\cdot\mathbf{n}_j}{|\mathbf{r}_{ij}|^3}\right]^2 , \quad (60)$$

where for simplification we have $K_i^*=K_j^*=K^*$. The correction can be obtained with the procedure described in Sec. IV. One obtains

$$C_0^*(H)=\prod_i\langle\Theta(H_i-\xi_D/(H+K^*)r^6+K^*)\rangle . \quad (61)$$

The $g(x)$ function, for example, in the double Lorentzian case becomes

$$g_L^*\left[\frac{\xi_D}{(H+K^*)r^6}-K^*\right]=\int_{x\Theta(x)}^{\infty}P_{0L}(\mathbf{H})d\mathbf{H} ,$$

$$x=\frac{\xi_D}{(H+K^*)r^6}-K^* . \quad (62)$$

In Eq. (62) the lower limit of the integral can be explained in the following way: Because P_{0L} depends only on $|\mathbf{H}|$ as an independent variable, the integral limits have been given for the field modulus. A modulus cannot have negative value, so if $x<0$ for the integral we must take into account zero lower limit. But if $x>0$, then in conformity with the restriction prescribed by Eq. (61), $|\mathbf{H}|$ can be taken only above x. From Eq. (62) we obtain

$$g_L^*(y)=1+\frac{2}{\pi}\frac{y}{1+y^2}-\frac{2}{\pi}\arctan y , \quad (63)$$

where $y=(x/A_{DL})\Theta(x/A_{DL})>0$. The property $0<g_L^*(y)<1$, as in the previously analyzed cases, guarantees that $\ln(g_L^*)^{-1}$ will be a positive function. Taking $z=A_{DL}(H+K^*)r^6$, we get the correction term as

$$C_0^*(H)=\exp\left[-(H+K^*)^{-1/2}\frac{B_{DL}^*}{(A_{DL})^{1/2}}\right] , \quad (64)$$

where

$$B_{DL}^*=\frac{n}{3}\int_0^{\pi}d\theta_i\int_0^{\pi}d\theta_j\sin\theta_j\int_0^{\infty}\frac{dz}{\sqrt{z}}\ln\left[1+\frac{2}{\pi}\frac{f(z)}{1+f^2(z)}-\frac{2}{\pi}\arctan f(z)\right]^{-1} , \quad (65)$$

and

$$f(z)=\left[\frac{\xi_D}{z}-\frac{K^*}{A_{DL}}\right]\Theta\left[\frac{\xi_D}{z}-\frac{K^*}{A_{DL}}\right] . \quad (66)$$

From Eq. (64) with $K^*>0$ results the fact that the cavity diminishes the probability density function $P_{0L}(\mathbf{H})$ around the origin, but at $H=0$ one has $C_0^*(H)>0$ so there is a finite nonzero probability to obtain a vanishing field at the sites. In the case in which $K^*<0$, $C_0^*(H)=0$ for $H<K^*$, so one reobtains a hole, a result similar to that predicted by Palmer and Pond.[17]

By using the presented procedure, a similar effect can be deduced for the RKKY, or the combined RKKY and dipolar cases, for double Lorentzian or Gaussian distributions. But these cases will not give qualitative new results, so we do not analyze them here in detail.

VI. DISCUSSIONS AND APPLICATIONS

In this paper we analyze the internal-field distribution functions for the dipolar and RKKY-dipolar couplings of vector spins distributed randomly in a nonmagnetic host. In Sec. II, we determined for these systems the internal field distribution in the most general case, taking into account totally random spin configurations. This assumption leads to the classical field distributions: a double Lorentzian if the interspin distances are nonrestricted and a Gaussian if they are restricted, conform with the central-limit theorem.

After this description, we took into consideration that because of the spin dynamics the spins are correlated with each other, so on the one hand the local spin configuration tries to minimize its energy contribution and on the other hand, because of the reciprocal spin connections, the total energy of the system tries to reach a local extremum point of the energy surface.

Without using a concrete description of the considered interactions, in Sec. III we gave a qualitative analytic formula for the correlation (or accommodation) between the spins, which was used to calculate the correction terms for the classical field-density-distribution functions. The correction terms cause a cavity to appear within the internal-field distribution, centered around $H=0$. Because of the cavity, $P(H)$ vanishes at $H=0$ and does not take its maximum value as in the classical cases. Furthermore, it is not necessary that $P(H)=0$ for $H=0$. If we take into consideration a simple local anisotropy, the cavity depth decreases, so we obtain a nonzero probability to get a vanishing field at impurity sites. This happens, for example, with the field-distribution function of the nucleus and can be interpreted as a consequence of the presence of metastable states within the system.[8] In some cases, the shape of the cavity is so modified that one can reobtain a hole predicted by Monte Carlo simulation.[17] Also an analytic description was given for this case, taking into account a simple anisotropy factor.

The possible applications are diverse and are connected to the probability density functions usage in different physical situations. In the Introduction we described this problem, so in this section we will analyze only one of them, from the relaxation domain.

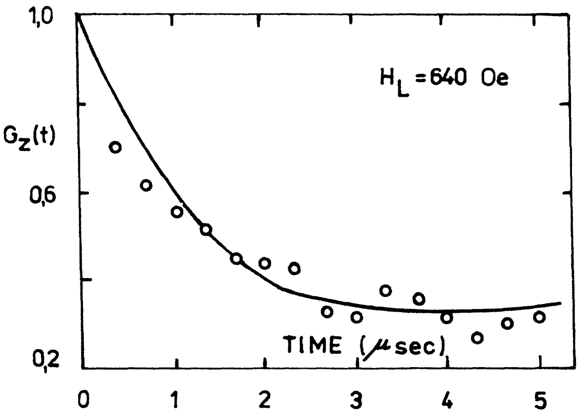

FIG. 1. $G_z(t)$ relaxation function for $H_L=640$ Oe. The solid line was obtained for $A_{DL}=30$ Oe and $B_{DL}=150$ Oe using Eq. (67).

The importance of μ^+ relaxation[22] to experimental methods[23] and the fact that it is determined by the internal dipolar field[4,24] is well known. Using the Kubo procedure,[25,26] we have calculated the relaxation function for a Cu—1% Mn spin-glass, in the case of a strong longitudinal external field ($H_L=640$ Oe). We analyzed this situation because the experimental data[27] has not been fitted well despite the fact that several different theories have been used.[4]

We write the longitudinal relaxation as

$$G_z(t)=\frac{1}{3}+\frac{8}{3\pi}A_{DL}K_L\int_0^\infty \frac{H^2dH}{[A_{DL}^2+(H-H_L)^2]^2}\cos[\gamma_\mu t(H-H_L)]\exp\left[-H^{-1/2}\frac{B_{DL}}{(A_{DL})^{1/2}}\right], \tag{67}$$

where γ_μ is the μ^+ gyromagnetic ratio.[22]

We mention that the correction term from the probability density function used in Eq. (67) is a specific way to take into consideration dynamic processes within the system. Furthermore, because of its origin, in the exponential correction factor did not enter the external magnetic field H_L. Despite the relative simplicity of the description, the fit agrees well with the experimental data[27] (see Fig. 1). We used $A_{DL}=30$ Oe which is in agreement with the experimental results for CuMn,[24,28] taking into account that in this case, because of the correction term, the width of the distribution function is diminished, and in fact it has been determined by A_{DL} and B_{DL} too. The fit is not sensitive to the variation of B_{DL} within 100 Oe—200 Oe. We took $B_{DL}=150$ Oe.

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