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Onsager anisotropies in Heisenberg spin glasses

P. Nozières

Institut Laue Langevin, B.P. 156 X, 38042 Grenoble Cedex, France

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Résumé. — Un spin donné polarise son environnement : le champ moyen qu'il ressent peut être séparé en un champ de cavité d'Onsager, complété par une anisotropie locale due à l'orientation aléatoire des spins voisins (gelés à $T = 0$). Il peut alors exister plusieurs positions d'équilibre : partant d'un modèle d'Heisenberg, on rétablit un modèle d'Ising. L'influence d'une telle situation sur la susceptibility de spin et la chaleur spécifique est brièvement discutée, compte tenu de la nature quantique des spins.

Abstract. — Because a given spin polarizes its neighbourhood, the mean field it feels may be separated into an Onsager cavity field and a local anisotropy due to the random freezing of neighbours as $T \to 0$. Such a combination may produce several equilibrium positions, thus restoring an Ising picture out of a Heisenberg model. The effects on spin susceptibility and specific heat are briefly discussed, taking into account the quantum nature of spins.

At low temperature, the specific heat $C_v$ of a spin glass varies linearly with $T$, while the spin susceptibility $\chi$ is constant. In the mean field interpretation of Marshall [1] and Klein, Brout [2], one assumes a continuous distribution $P(H)$ of the local Weiss field : those spins for which $|H| \gtrless T$ are loose. For Ising spins, $P(0)$ if finite, leading to the required behaviour. On the other hand, for Heisenberg vector spins, a spin is loose only if the three components of $H$ vanish simultaneously. Then $P(H) \sim H^2$, leading to a specific heat $\sim T^3$ (the spin susceptibility remains constant because one can tilt a spin continuously in an external field). Such a behaviour has been confirmed in the extensive simulation work of Walker and Walstedt [3].

In this note, we show that a straightforward extension of the mean field concept restores two level structures in a random system of frozen Heisenberg spins. Basically, the environment creates a local anisotropy in spin space, allowing several equilibrium positions. Similar conclusions were reached by Villain [4], who studied a frustrated system of $(x, y)$ spins : he showed that the ground state involved canted configurations, reminiscent of vortices, with an arbitrary chirality. More recently, Ma [5] studied the behaviour of strongly coupled clusters. Because individual partners of such clusters feel different Weiss fields $H_i$, the resulting potential energy is anisotropic. Our purpose is to cast these ideas in a simple language similar in spirit to the Onsager reaction field [6].

We consider the standard RKKY model of spin glasses:

$$H = \frac{1}{2} \sum_{ij} J_{ij} S_i S_j.$$  

(1)
The oscillatory $J_{ij}$ has a random sign; its magnitude $\sim 1/R^3$ is proportional to the concentration $C$ of magnetic impurities. At low temperature, the spins $S_i$ are frozen in random directions (for our purpose, it does not matter whether the transition is sharp or not). Each spin feels an average Weiss field

$$H_{iw} = -J_{ij} \langle S_j \rangle .$$

At $T = 0$, $S_i$ points along $H_{iw}$. Let us now apply a small external field $B_i : S_i$ can only tilt. If $H_{iw}$ were fixed, the resulting transverse susceptibility tensor would be

$$\chi^\alpha_\beta = \frac{S}{H_{iw}} \left[ \delta^\alpha_\beta - \frac{H_{iw}^2 H_{iw}^\beta}{H_{iw}^2} \right].$$

Actually, $H_{iw}$ is modified by the response of neighbouring spins. The complete susceptibility tensor is given by the usual RPA equation

$$\chi^\alpha_\beta = \chi_i^{\alpha_\beta} \delta_{ij} - \chi_i^{\alpha_\beta} J_{ii} \chi_j^{\beta_\alpha} .$$

Note that (4) is exact for classical spins at $T = 0$ (as long as $B_i$ is small). Put another way, the mean field approach is exact if there are no fluctuations.

Formally, (4) may be solved by iteration. The local susceptibility is then given by

$$(\chi_i^{-1})^{\alpha_\beta} = (\chi_i^{1-1})^{\alpha_\beta} - \Sigma^{\alpha_\beta}_i$$

where the self energy $\Sigma_i$ excludes any return to the original site $i$. $\Sigma_i$ may be written as

$$\Sigma_i^{\alpha_\beta} = J_{ii} \chi_i^{\alpha_\beta} J_{ji}$$

where $\chi$ is the neighbourhood susceptibility tensor with a frozen spin $S_i$. In lowest order, $\chi$ may be replaced by $\nu$, yielding the approximate result

$$\Sigma_i^{\alpha_\beta} = J_{ii} \chi_i^{\alpha_\beta} J_{ji}$$

Note that $\Sigma_i$ is anisotropic because of the freezing of $S_i$ in specific directions. Such an anisotropy has nothing to do with the usual crystalline anisotropy. It is a pure exchange effect, due to spin freezing.

When calculating the macroscopic susceptibility $\chi$, we must do the configurational average over $J_{ij}$. In the present case where $\bar{J} = 0$, only the local susceptibility survives (non local terms $\chi_{ij}$ necessarily contain odd powers of $J_{ii}$ of $J_{ji}$). Thus in that case

$$\chi^{\alpha_\beta} = c\chi_i^{\alpha_\beta}$$

(8) would not be true if $\bar{J}$ were $\neq 0$: then the average magnetization would modify the susceptibility (standard exchange correction).

Let $z$ be the average number of neighbours of a given impurity. Then $H_{iw} \sim SJ\sqrt{z} \sim S/\nu_i$. The self energy $\Sigma_i$ is $\sim zJ^2 \nu_i \sim J\sqrt{z}$: it enhances the local susceptibility without changing its order of magnitude. The macroscopic susceptibility $\chi \sim c/(J\sqrt{z})$ is concentration independent, a well known result.

Let us now assume that $S_i$ departs from its equilibrium position $\langle S_i \rangle$. The change

$$\delta S_i = S_i - \langle S_i \rangle$$
is kept fixed (1). Such a rotation polarizes the neighbouring spins. If the coordinance $z$ is large, the resulting rotation $\delta S_j$ is small: it can be obtained in a linear approximation

$$\delta S_j^z = -\chi_{ij}^z J_{ij} \delta S_i^z$$

(9)

$\delta S_j$ in turn reacts on the mean field at site $i$, which becomes

$$H_i^a = H_{iw}^a - J_{ij} \delta S_j^a = H_{iw}^a + \Sigma_i \delta S_i^a$$

(10)

$H_i$ thus depends on $S_i$, as it would in an extended Hartree-Fock description. Since in a rotation the work done is $-H_i \cdot \delta S_i$, the resulting potential energy of the spin $S_i$ is

$$U = -H_{iw}^a \delta S_i^a - \frac{1}{2} \Sigma_i^{a\beta} \delta S_i^a \delta S_i^\beta .$$

(11)

The last term in (11) is the neighbourhood polarization energy. Equilibrium positions will correspond to a stationary $U$; it is easily verified that $S_i$ is then parallel to $H_i$, as it should.

We may rewrite (11) as:

$$H_i^a = H_{ic}^a + \Sigma_i^{a\beta} S_i^\beta$$

$$H_{ic}^a = H_{iw}^a - \Sigma_i^{a\beta} \langle S_i^\beta \rangle$$

(12)

$H_{ic}$ is the cavity field of Onsager, i.e. that part of $H_i$ which does not follow $S_i$. It is equal to the Weiss field $H_{iw}$ minus the reaction field $\Sigma \langle S_i \rangle = H_{ir}$. As pointed out by Cyrot [6], in a spin glass all three fields $H_{iw}$, $H_{ic}$, $H_{ir}$ are comparable, $\sim J S\sqrt{z}$. The correction is thus significant, in contrast to usual ferromagnets. The energy (11) may be written in the same way. Within an irrelevant constant, it becomes

$$U = -H_{ic}^a S_i^a - \frac{1}{2} \Sigma_i^{a\beta} S_i^a S_i^\beta .$$

(13)

The spin $S_i$ is thus subject to the local cavity field, $H_{ic}$, and to a local anisotropy, due to the anisotropy of $\chi$ at nearby sites.

The Onsager approximation amounts to treating the statistical equilibrium at temperature $T$ in the cavity field $H_{ic}$ instead of $H_{iw}$: this is the essence of the TAP approximation in spin glasses [6]. At very low temperature, it is no longer an approximation, since fluctuations are negligible. The self consistent mean field equations (12) and (13) are exact — except for the linearization in calculating the neighbourhood response.

We now examine the consequences of (13). At every site, $\Sigma_i^{a\beta}$ has a local easy magnetization axis (we choose it as the polar axis) against which the cavity field $H_{ic}$ will fight. If the transverse component $H_{ic}^z$ is not too large, there will exist two canted equilibrium positions: we recover the two level systems of Villain [4] and Ma [5]. In order for these two states to be degenerate, we need only one condition: the parallel component $H_{ic}^l$ (to the easy axis) must vanish. We thus return to the original Marshall picture: the number of spins with two equilibrium states within $T$ of each other is $\sim T$ — hence a linear specific heat. Note that the anisotropy is crucial: without it, there would be only one equilibrium position parallel to $H_{ic}$, and a loose spin would require $H_{ic}^z = H_{ic}^l = 0$.

(1) In three dimensions, one can rotate one spin without dragging the whole system along: an infinitesimal crystalline anisotropy is enough to block the spins at large distances. That would not be true in one dimension: then it takes a finite crystalline anisotropy to keep the perturbation localized (cf. Bloch walls).
For simplicity, let us assume that $\Sigma$ is uniaxial (not true in general). Only the eccentricity of $\Sigma$ is relevant. We thus write on each site

$$U = -\frac{\sigma}{2} S^2 \cos^2 \theta - H_\parallel S \cos \theta - H_\perp S \sin \theta$$

(14)

where $\theta$ is the angle between $S_i$ and the easy axis ($\sigma > 0$). Because the $v_j$ in (7) are oriented at random, the net anisotropy in $\Sigma_i$ should be $\sqrt{2}$ smaller than the trace. We thus expect $\sigma \sim J$; the coordinance should not be too large for the anisotropy to be significant. One shows easily that $U$ possesses two minima if

$$H_\perp^{2/3} + H_\parallel^{2/3} < (\sigma S)^{2/3}.$$  

(15)

When $H_\parallel = 0$, the two minima are degenerate; for small $H_\parallel$, their energy difference is

$$\Delta E = 2 S H_\parallel \cos \theta_m$$

(16)

where $\theta_m$ is the orientation of $S_i$ at equilibrium, given by

$$\sin \theta_m = \frac{H_\perp}{\sigma S}.$$  

(17)

For larger $H_\parallel$, the algebra is more messy. In figure 1, we sketch the behaviour of $\Delta E$ as a function of $H$ for different values of the angle $\alpha$ between $H$ and the easy axis. Note that the equilibrium positions of $S_i$ are not parallel to $H_\parallel$ — but of course they are parallel to the net field $H_i$.

In the more general biaxial case, the search for equilibrium is even more painful — but the qualitative conclusions are unchanged. In zero field, there exist two stable orientations of $S_i$ along the easy axis. They will persist in a finite region of $H$ space; the two minima will be degenerate if $H_\parallel = 0$.

![Fig. 1.](image)

Fig. 1. — The energy difference $\Delta E$ between the two equilibrium positions as a function of $H$ for different values of the angle $\alpha$ between $H$ and the easy axis. The dashed curve marks the limit of the two minima regions.

1. **Spin susceptibility.** — It contains two parts: one due to the small rotation of $S_i$ in its potential well under the influence of the applied field, the other due to the jump from one well to the other when $\Delta E$ is smaller than the resulting gain in magnetic energy, $-B.S_i$. The first part is given
by (5). We may estimate it by choosing a new set of local axes, with $z'$ along the equilibrium position of $S_i$, and $x', y'$ along the principal axes of $U$. Expanding $U$ near its minimum

$$U \sim \frac{\alpha}{2} S_x^2 + \frac{\beta}{2} S_y^2$$

we find at once

$$\chi_{xx} = \frac{1}{\alpha}, \quad \chi_{yy} = \frac{1}{\beta}, \quad \chi_{zz} = 0.$$  

The susceptibility is thus transverse and anisotropic. For those spins for which $H \ll \sigma S$, it is of order $1/\sigma$. If $H \gg \sigma S$, there is only one equilibrium position and $\chi \sim S/H$. When the coordinate $z$ is large, the latter contribution dominates.

The second contribution is similar to the Klein-Brout model. An external field $B_\parallel$ parallel to the easy axis flips all the spins for which $-B_\parallel < H_\parallel < 0$, by an amount $\Delta S = 25 \cos \theta_m$. The resulting susceptibility is comparable to the other term if $z$ is small. It becomes negligible for large $z$ since only a small fraction $\sim (\sigma S/H)^2$ of the spins feels an $H_\parallel$ small enough to guarantee two equilibrium positions.

Note that all the energies in the problem are of order $J$ : in the RKKY model, the susceptibility remains concentration independent, despite the complicated anisotropic behaviour.

2. Quantization and specific heat. — The above discussion was classical : it must be reconsidered for quantum spins. For spins $1/2$, for instance, there can be no anisotropy, since $(S_i)^2 = \frac{1}{4}$ : the whole discussion is irrelevant. For larger spins, anisotropy does exist — but it can only displace the $(2S + 1)$ quantum states. The concept of « equilibrium positions » is meaningless because of zero point motion : one should rather view $U(\theta)$ as a potential energy governing the motion of quantum rotators.

Let us assume that $U$ has two minima, as sketched on figure 2. The spin can tunnel from one to the other, and as a result the $(2S + 1)$ eigenstates will never be degenerate. The situation, however, simplifies if $S \gg 1$. The levels are then closely spaced, and one can use semi-classical approximations. Near the bottom of each well, $U$ may be expanded in the form (18). A standard Holstein-Primakoff expansion yields an harmonic oscillator set of levels, with frequency $\omega = \frac{S}{\hbar} \sqrt{\alpha \beta}$. If $S$ is large, $\hbar \omega \sim \frac{U}{S}$ is much smaller than the height $U$ of the potential barrier.

The two sets of levels in each potential well are coupled by tunnelling across the barrier — but the corresponding tunnelling amplitude $\Gamma$ is much smaller than $\hbar \omega$.

In the special case $H_\parallel = 0$ the two wells are perfectly symmetrical. Were it not for tunnelling, each harmonic oscillator state would be doubly degenerate. Tunnelling lifts that degeneracy by an amount $\pm \Gamma$-which however remains small when $S \gg 1$ ($\Gamma$ decreases exponentially with

Fig. 2. — The potential profile for a spin $S_i$ as a function of its orientation $\theta$. 

\[ \text{Fig. 2. — The potential profile for a spin $S_i$ as a function of its orientation $\theta$.} \]
the number of states in each well). If the temperature $T$ is $\gg T$, we can ignore that degeneracy: the spin behaves as a genuine two level system.

In calculating the entropy and specific heat, we should distinguish several temperature ranges.

(i) $T \gtrsim U$: the detailed shape of $U(\theta)$ is important — but anyhow this is outside the scope of the present discussion.

(ii) $\Gamma \ll T$, $\hbar \omega_0 \ll U$. Tunnelling is negligible; each well behaves as a separate harmonic oscillator. Let $\Delta E$ be the energy difference between the two minima: the probability of occupation of the two wells are in the ratio $\exp[-\Delta E/T]$. The entropy $S$ is a sum

\[ S = S_{\Delta E} + S_\omega \]

of the entropy $S_{\Delta E}$ of a two level system with splitting $\Delta E$ and the entropy $S_\omega$ of a single harmonic oscillator. When $\hbar \omega \gg T$, $S_\omega \sim \log (T/\hbar \omega)$ dominates, leading to the usual constant specific heat of a classical oscillator. When $\hbar \omega \ll T$, $S_\omega \rightarrow 0$: $S$ is equal to $\log 2$ if $\Delta E \ll T$, to $0$ if $\Delta E \gg T$.

(iii) $T \sim \Gamma$. Tunnelling cannot be neglected. The entropy goes to $0$ whatever $\Delta E$.

Following the Klein-Brout argument, a linear specific heat should obtain in the temperature range

\[ \Gamma \ll T \ll \hbar \omega_0, U. \]  \hspace{1cm} (19)

(A fraction $\sim T$ of the spins has $\Delta E < T$, each with an entropy $\log 2$.) Of course, only those spins for which $U$ has a double minimum will contribute (otherwise, the specific heat is $\sim T^3$). Note that $\Delta E \sim \sigma$ is proportional to the concentration. The specific heat is thus concentration independent, as expected.

In practice, the spin $S$ is never very large. $\Gamma$, $\hbar \omega_0$ and $U$ are comparable, so that the condition (19) can hardly be met. In order to salvage our classical picture, one should probably consider spin clusters, tightly linked together: one thus recovers the picture put forward by Ma [5]. Such a cluster has many states, and hopefully it can be treated as a classical object. Qualitatively, the above discussion remains valid. An entropy $\log 2$ results whenever the cluster has two local equilibrium configurations with the same energy. Since the resulting condition $\Delta E = 0$ is one dimensional, it should result in a linear specific heat.

Our brief discussion of quantization is not really conclusive. Putting it aside, we have shown that a straightforward classical mean field description, « à la Onsager », was sufficient to produce a local anisotropy, strictly due to exchange. The resulting two level systems are a step forward in understanding the linear specific heat of spin glasses. We thus complement the basic work of Cyrot [6], who focussed mostly on metastability and remanence.

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References


The TAP model was originally formulated for Ising spins. It was generalized to Heisenberg vector spins by Palmer, R. G., Pond, C. M., J. Phys. F 9 (1979) 1451 who showed that the distribution of local fields had a hole near $H = 0$. Their paper directly bears on the present work.

The Onsager approach has been explicitly applied to spin glasses by Cyrot, M., Phys. Rev. Lett. 43 (1979) 173, with special emphasis on its physical consequences (remanence, etc...). The present note is based on his work.