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STATISTICAL MECHANICS ON THE SPIN GLASS PHASE

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We propose a statistical theory of spin glasses, which have degenerate local minimum states. In order to study how the relevant system changes from one local minimum state to another, we introduce here two kinds of symmetry breaking fields: quenched and annealed symmetry breaking fields for short and long time scales, respectively, on the basis of the concept of the real replica proposed by one of the present authors. We give a general frame-work to calculate the spin glass order parameter and its response for each kind of symmetry breaking field.

§1. Introduction

The purpose of the present paper is to present a unified picture of spin glass. There have been proposed many theories of spin glass, which may be classified roughly into two groups, namely Edwards-Anderson replica-type and Mattis-type (i.e., generalized antiferromagnetic phase or ROP). Spin glass phase transitions may also be interpreted experimentally (or using the Monte Carlo simulation) in two ways, namely as equilibrium and non-equilibrium phase transitions. In this confusing situation, we try to understand the spin glass phase transition in a unified way, from the view-point that it is an intrinsically non-equilibrium phenomenon. Our picture of a spin glass is the following. There exists a certain characteristic time t_c of the spin glass and an equilibrium phase transition is observed in an experimental time scale less than t_c (i.e., $t \ll t_c$), while a non-equilibrium (or quasi-equilibrium) phase transition is observed for the time scale $t \gg t_c$. Our key-point is to propose explicit formulations to describe the above situations by introducing the concepts of a) annealed symmetry breaking field and b) quenched symmetry breaking field. The former is closely related to the replica theory and it corresponds to the region of long-time scale ($t \gg t_c$), while the latter discribes the short-time behavior.

§2. Annealed Symmetry Breaking Field

In this section we introduce an annealed symmetry breaking field h_s by

$$F_A^{(n)} = -k_B T < \log \mathrm{Tr} \exp\{-\beta \sum_{\alpha=1}^{n} \mathcal{H}(s_j^{\alpha}) + h_s \sum_{j=1}^{N} \sum_{\alpha,\beta}^{n,\alpha\neq\beta} s_j^{\alpha} s_j^{\beta}\}>_{av} \qquad (2.1)$$

for the real n-replica, which was first introduced by one of the present authors[1] Here $\mathcal{H}(\alpha)$ denotes the Hamiltonian of the n-th replicon, s_j denotes the Ising spin at site j and n is an integner not less than two. The notation <...> denotes the average over the random distribution of the exchange coupling. It should be noted that the limit $n \to 0$ is not taken anywhere in arguments, which is one of the essential points of our real n-replica method [1]. This concept of the real replica method has been extensively applied by Sherrington [2] and by Kasai, Okiji and Syozi [3]. These applications have been discussed in annealed real n-replica systems. The above free energy $F_A^{(n)}$ corresponds to the quenched real n-replica with an annealed symmetry breaking field. However, the fundamental ideas of both formulations are essentially the same in the sense that they were both introduced in order to define the spin-glass order parameter without using the trick $n \to 0$ of the Edwards-Anderson replica method.[4] The quenched real two-replica method was extensively used by Blandin, Gabay, Garel and De Dominicis.[5,6]

Now the spin-glass order parameter $q_{(n)}$ corresponding to the formulation (2.1) is defined by

$$q_{(n)} = \lim_{h_s\to+0} \lim_{N\to\infty} N^{-1} < \sum_{j=1}^{N} \sum_{\alpha,\beta}^{n,\alpha\neq\beta} <s_j^{(\alpha)} s_j^{(\beta)}>>_{av} \tag{2.2}$$

The corresponding Landau quasi free energy $F_A^{(n)}(q_{(n)})$ for a fixed spin-glass order parameter $q_{(n)}$ is defined by

$$F_A^{(n)}(q_{(n)}) = -k_BT<\log \mathrm{Tr}\, \delta(\sum_{j=1}^{N} \sum_{\alpha,\beta}^{n,\alpha\neq\beta} s_j^{(\alpha)} s_j^{(\beta)} -Nq)\exp\{-\beta \sum_{\alpha=1}^{n} {}^{(\alpha)}(s_j^{(\alpha)})\} \tag{2.3}$$

This free energy can be expanded formally as

$$F_A^{(n)}(q_{(n)}) = F_A^{(n)}(0) + c^{(n)}(T)q_{(n)}^2 + d^{(n)}(T)q_{(n)}^3 + e^{(n)}(T)q_{(n)}^4 + \cdots \tag{2.4}$$

by using the Suzuki[7]-Brout[8]-Nakano[9] method, where all the coefficients $c^{(n)}(T)$, $d^{(n)}(T)$, $e^{(n)}(T)$,... are expressed microscopically with the use of cumulants[10] $<\cdots>_c$. For example, we have

$$c^{(n)}(T) = \frac{1}{2} Nk_BT\{<<(\sum_{j=1}^{N} \sum_{\alpha,\beta}^{n,\alpha\neq\beta} s_j^{(\alpha)} s_j^{(\beta)})^2>_c>_{av}\}^{-1} \tag{2.5}$$

The spin-glass order parameter $q_{(n)}$ can be determined by <u>minimizing</u> the free energy $F_A^{(n)}(q_{(n)})$ (not maximizing as in the Edwards-Anderson replica method). This is one of the great merits of our real replica method, as was pointed out in Ref. 1.

Here it should be noted that the coefficient $d^{(2)}(T)$ in (2.4) always vanishes from the symmetry property of the two real replica, as was pointed out in Ref. 1. Therefore, the symmetry of $F_A^{(2)}(q)$ is quite different from $F_A^{(n)}(q)$ for $n\geq 3$. That is, $F_A^{(2)}(q)$ is an even function of q, while $F^{(n)}(q)$ for $n\geq 3$ are not. Then one might be worried about the arbitrariness of our theory. In fact, if we apply[1] the Landau type argument to the present problem, we obtain the temperature dependence of $q^{(2)}$ quite different[1] from $q^{(n)}$ for $n \geq 3$, even in the mean field theory. However, it is sufficient that all $q^{(n)}$ yield the same critical point and essentially the same physical picture of the spin-glass phase transition. In fact we can easily show this consistency of the definitions of various order parameters $\{q_{(n)}\}$.

For this purpose we apply the Landau type argument to the free energy $F_A^{(n)}(q)-h_sq$, namely by minimizing it we obtain

$$2c^{(n)}(T)q_{(n)} + 3d^{(n)}(T)q_{(n)}^2 + 4e^{(n)}(T)q_{(n)}^3 +\cdots = h_s \ . \tag{2.6}$$

Therefore, the response of $q_{(n)}$ is given by the spin-glass susceptibility $\chi_{sg}^{(n)}$ as

$$q_{(n)} = \chi_{sg}^{(n)} h_s \quad ; \quad \chi_{sg}^{(n)} = 1/[2c^{(n)}(T)]. \tag{2.7}$$

If we use the microscopic expression (2.5), we arrive at

$$\chi_{sg}^{(n)} = \beta N^{-1}<< \sum_{j=1}^{N} \sum_{\alpha,\beta=1}^{n,\alpha\neq\beta} s_j^{(\alpha)} s_j^{(\beta)}>_c^2>_{av} \ . \tag{2.8}$$

Of course, this formula can be obtained directly from the differentiation of (2.1).

For simplicity, we now consider the case $T > T_{sg}$ for the symmetric distribution $P(-J_{ij}) = P(J_{ij})$. Then, from the local gauge invariance, we obtain

$$\chi_{sg}^{(n)} = \frac{n(n-1)}{2N} \beta \sum_{i,j}^{N} \langle\langle s_i s_j \rangle^2\rangle_{av} \quad . \tag{2.9}$$

Therefore, all $\chi_{sg}^{(n)}$ have the same singularity, which is expressed by the correlation in the origianl system (say $\alpha = 1$). That is, all $q_{(n)}$ yield the same critical point and the same response to the symmetry breaking field h_s, although $q^{(n)}$ themselves behave quite differently for $n = 2$ and for $n \geq 3$ as is easily seen from (2.6).

Now we discuss the nonlinear suceptibility [1] χ_2 defined by

$$m = \chi_0 h + \chi_2 h^3 + \cdots \tag{2.10}$$

for the magnetization m. It is well-known [11] that

$$\chi_0 = \beta(1-q^{(2)}) \tag{2.11}$$

and

$$\chi_2 = \frac{1}{6N} \beta^3 \langle\langle M^4 \rangle_c\rangle_{av} = \frac{1}{6N} \beta^3 \langle\langle M^4\rangle - 3\langle M^2\rangle^2\rangle_{av} \, , \tag{2.12}$$

where $M \equiv \sum_j s_j$. If the system has again the local gauge invariance for the symmetric distribution of J_{ij}, then we obtain

$$\chi_2 = -N\beta^3 \sum_{i,j} \langle\langle s_i s_j \rangle^2\rangle_{av} = -\frac{2\beta^2}{n(n-1)} \chi_{sg}^{(n)} \quad . \tag{2.13}$$

above the spin-glass transition point T_{sg} and consequently it diverges negatively at $T = T_{sg}+0$, and also we have [12]

$$\begin{aligned} \chi_2 = & -\beta^3 N^{-1} \sum_{ij} \langle(\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle)^2\rangle_{av} \\ & + 2\beta^3 N^{-1} \sum_{ij} \langle\langle s_i\rangle\langle s_j\rangle(\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle)\rangle_{av} + (\text{lower terms}) . \end{aligned} \tag{2.14}$$

for $T < T_{sg}$. For the Mattis model [12], χ_2 diverges positively [13] just below T_{sg}. In general frustrated spin systems, the first tems in (2.14) is expected to be more dominant than the second term and consequently we may expect the negative divergence [14 ∿ 18] of χ_2. More explicitly, we may assume the following scaling relations

$$C_1(R) \equiv \langle(\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle)^2\rangle_{av} \simeq R^{-\hat{\eta}_s} f_1(R/\xi) \tag{2.15}$$

$$C_2(R) \equiv \langle\langle s_i\rangle\langle s_j\rangle(\langle s_i\rangle\langle s_j\rangle - \langle s_i\rangle\langle s_j\rangle)\rangle_{av} \simeq R^{-\hat{\eta}_s} f_2(R/\xi) \quad . \tag{2.16}$$

Therefore, we obtain

$$\int C_1(R) d^d R \simeq \int x^{-\hat{\eta}_s} f_1(x)\, d^d x \cdot \xi^{d-\hat{\eta}_s} \tag{2.17}$$

and

$$\int C_2(R) d^d R \simeq \int x^{-\hat{\eta}_s} f_2(x)\, d^d x \cdot \xi^{d-\hat{\eta}_s} \quad . \tag{2.18}$$

Thus, the first and second terms in (2.14) give the same singularity under our scaling assumptions (2.15) and (2.16). Consequently the quantity $f \equiv (2c_2 - c_1)$ determines the sign of the divergence of χ_2, where

$$c_j \equiv \int x^{-\hat{\eta}_s} f_j(x)\, d^d x. \tag{2.19}$$

In non-frustrated systems, the quantity $\langle s_i\rangle\langle s_j\rangle$ in the second term in (2.14) gives a large contribution to χ_2, because it is essentially the square of the spontaneous magnetization. As the frustration increases, it becomes smaller and smaller. Therefore, as the frustration increases, the sign of the divergence of χ_2 changes abruptly at a certain point of "the degree of frustration", if it is appropriately defined. Thus, we may call f the frustration parameter. We may say that the system is intrinsic spin-glass, if $f < 0$, and that the system is essentially spin-glass of Mattis-type, if $f > 0$. In this sense, the sign of the divergence of the nonlinear susceptibility χ_2 below the transition point is essentially important.

An application of the above formulation to the SK model [19] will be discussed later.

§3. Quenched Symmetry Breaking Field

In this section we introduce a quenched symmetry breaking field h_s by [17]

$$F_Q = -k_BT < \sum_{\{s_i\}} P(\{s_i\}\ \beta',h')\log \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}(\sigma)+R\sum_{s_i}\sigma_i s_i}>_{av} \tag{3.1}$$

where $\mathcal{H}(\sigma)$ is the hamiltonian of the system,

$$\mathcal{H}(\sigma) = -\sum_{ij} J_{ij}\sigma_i\sigma_j - H\sum_i \sigma_i \quad , \tag{3.2}$$

and $P(\{s_j\},\beta',h')$ denotes the probability distribution function of quenched symmetry breaking field. Usually, it is given by the canonical distribution corresponding to the same Hamiltonian $\mathcal{H}(s)$. The order parameter of the spin-glass is defined by

$$q = \lim_{h_s\to+0}\ \lim_{N\to\infty} <<<\sigma_j>_\beta\ s_j>_{\beta'}>_{av} \quad , \tag{3.3}$$

where $<\sigma_j>_\beta$ is the canonical average of σ_j at the inverse temperature β. When $\beta' = \beta$, q is reduced to $q^{(2)}$ in the annealed symmetry breaking field. The quasi free energy $F_Q(q)$ for q fixed is given by

$$F_Q(q) = -k_BT< \sum_{\{s_i\}} P(\{s_i\},\beta',h')\log \sum_{\{\sigma_i\}} \delta(\sum_i s_i\sigma_i - Nq)e^{-\beta\mathcal{H}(\sigma)}>_{av} \quad . \tag{3.4}$$

This can be expanded again as

$$F_Q(q) = F_Q(0) + cq^2 + dq^4 + \cdots \quad , \tag{3.5}$$

which is an even function of q. Therefore, the spontaneous order parameter $q_0(T)$ is given by the solution $2cq_0 + 4dq_0^3 + \cdots = 0$, i.e., $q_0 = (-c/2d)^{1/2} \sim (T_c-T)^{1/2}$ in the mean field theory. The response of q is given by $q = \chi_{sg}^Q h_s$, where

$$\chi_{sg}^Q = \frac{1}{N}\sum_{i,j}^{N} <<s_i\ s_j>_{\beta'}<\sigma_i\sigma_j>_\beta>_{av} \quad . \tag{3.6}$$

If we take the limit $\beta' = \infty (T' = 0)$, then χ_{sg}^Q is reduced to Binder's definition [20] of the spin-glass susceptibility. The nonlinear susceptibility χ_2 is also defined by (2.12).

Now we may expect the following quite interesting situation that χ_{sg}^Q diverges at a certain temperature T_0 for a fixed large value of β', say $\beta' = \infty$, although $\chi_{sg}^{(n)}$ (or χ_2) do not diverge at finite temperatures. If possible, it corresponds to a quasi (or non-equilibrium) phase transition, because our formulation of the quenched symmetry breaking field describes the short-time behavior of the spin glass, as was mentioned in §1. That is, the possible singularity of χ_{sg}^Q describes the transient phase transition, namely the freezing of spins in some local minimum state for short-time scale. In this sense, our formulation yields the statistical mechanics of the spin-glass phase.

§4. Classifications of Spin Glasses

It may be convenient to classify spin glass phases according to our formulations as follows.

i) 1st classification: There may be two types of spin glasses, namely A-type in which $\chi_{sg}^A \to \infty$ (and also $\chi_{sg}^Q \to \infty$) at $T = T_{sg}$ and Q-type in which $\chi_{sg}^Q \to \infty$ at $T = T_{sg}$ but χ_{sg}^A = finite. For example, the Mattis model [12] and the SK model [19] belong to A-type, and the Cayley tree Ising spin glass belong to Q-type near T_c at which χ_{sg}^Q diverges but χ_{sg}^A is finite. This situation clarifies the difference between the glass-like phase [21] and ROP [22].

ii) 2nd classification: As is discussed in §2, there are two types of divergence of χ_2, namely positive or divergence for $T \to T_{sg}-0$. Spin glass with positive divergence (i.e., $f > 0$) is of Mattis type, and we call it "weakly frustrated (or non-frustrated) spin glass". Spin glass with negative divergence is intrinsically frustrated spin glass and we may call it Edward-Anderson-Sherrington-Kirkpatrick (EASK) type. A typical example of EASK type is the SK model.

iii) 3rd classification: One may also classify spin glasses according to whether there exists a permanent local moment or not. If it exists, it can be a well-defined order parameter to describe the spin glass phase, as in the SK model and in the Mattis model. If it does not exist, then it is quite difficult to define the order parameter even in the case of the existence of a phase transition and the transition point is defined only by the divergence of χ_2. This case may be quite similar to the Kosterlitz-Thouless transition of the two-dimensional planar model. There is another situation in which there occurs no phase transition at all in the sense of equilibrium phase transition, but a transient spin glass phase may appear as in the two-dimensional $\pm J$ model.

If we combine the above three classification methods, then we may have some clear vision for various different kinds of phenomena in random spin systems.

§5. Discussions

In the present paper, we have got around the difficulty that the minimization of the Landau type free energy gives always a positive divergence of the nonlinear susceptibility [17]. That is, we have used the microscopic expression (2.14) of the nonlinear susceptibility χ_2 rather than the phenomenological relation between χ_2 and χ_{sg} as in [17].

We have also applied our two formulations to the SK model and we have obtained a sharp saturation of the magnetic susceptibility in a certain region of strength of the magnetic field. This sharp saturation is characteristic of spin glasses. Details will be reported elsewhere [23].

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