Random energy levels and low-temperature expansions for spin glasses

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In a previous paper (cond-mat/0106554) we showed the existence of two new zero-temperature exponents ($\lambda$ and $\theta'$) in two dimensional Gaussian spin glasses. Here we introduce a novel low-temperature expansion for spin glasses expressed in terms of the gap probability distributions for successive energy levels. After presenting the numerical evidence in favor of a random-energy levels scenario, we analyze the main consequences on the low-temperature equilibrium behavior. We find that the specific heat is anomalous at low-temperatures $c \sim T^\alpha$ with $\alpha = -d/\theta'$ which turns out to be linear for the case $\theta' = -d$.

Spin glasses are random systems where frustration plays a very important role. In a previous paper (hereafter referred as I) we have shown the importance of considering both small and large-scale excitations to properly understand the low-temperature behavior of spin glasses. The thermal exponent $\theta$, which determines the typical free energy cost to overturn a droplet of large size, scales like $L^\theta$ with $\theta = \theta' + d\lambda$. The exponent $\theta'$ gives the energy cost associated to the lowest excitation while the other exponent $\lambda$ has an entropic origin and accounts for the probability (proportional to $1/V^{\lambda}$) to find a large-scale lowest excitation.

In standard phenomenological approaches (domain-wall theory or the droplet model) the exponent $\lambda$ is not necessary because only typical excitations are considered for the low-temperature behavior. This case corresponds to $\lambda = 0$ or, equivalently, $\theta' = \theta$. Therefore, the main difference between our approach and the domain-wall approach is that the excitations we consider in our analysis are not typical at finite temperatures while those generated in domain-wall theory (by measuring the energy change in the ground state configuration after a twist of the boundary conditions, see I) are supposed to be typical. In our approach we infer the statistical properties of the typical excitations by looking at those excitations in the extreme tail of the energy gap distribution. The ultimate reason behind the validity of our approach is the random character of energy levels. Evidence in favor of a random energy levels scenario was already presented in I. In I, besides showing how the exact investigation of the lowest excitations may identify the two exponents, we also showed how the gap distribution does not depend on the size of the excitation, justifying a scenario of random-energy levels. Here we want to go further and check its validity by extending the analysis to second order excitations. Furthermore we want to show how we can use a novel low-temperature expansion for spin glasses and infer some results from that expansion by assuming random-energy levels. This expansion is useful to understand the low-temperature behavior of some quantities such as the specific heat or the spin-glass susceptibility.

Although the main results here and in I only considered 2D Gaussian spin glasses we have founded reasons to believe that the validity of our assumptions extends also to higher dimensions. To validate this new scenario beyond two dimensions we need systematic and powerful algorithms to look for low-lying excitations. Recent numerical developments promise a fast growth of this area and studies in 3D will be crucial.

The random-energy levels scenario is based on two assumptions. **Assumption A:** correlations between different energy gaps vanish in the $L \to \infty$ limit and **Assumption B:** Correlations between excitation volumes $v_i$ and gaps $E_i$ vanish in the $L \to \infty$ limit. These two assumptions are very natural. In a random system the ground state configuration is completely disordered. The fact that there are large-scale higher excitations indicates that there exist configurations very close in energy to the ground state energy but very far from each other in phase space. If the ground state configuration is suppressed from the set of allowed configurations the statistical properties of the new lowest gap $E_2 - E_1$ will remain the same to those of the original lowest gap $E_1$. Hence, any variable ($v$ or $E$) appears to be uncorrelated to the energy. Nevertheless, note that while energy levels are random, excitation volumes may be correlated among themselves. In a disordered system, the presence of random-energy levels extends to higher energy typical excitations supporting the core of the results presented in I. Obviously this is not true in an non-disordered system where the ground state may have a crystalline structure and typical excitations are not statistically represented by the lowest ones. The validity of this description in terms of a random-energy levels scenario is probably related to the stochastic stability property of disordered systems. If the system is stochastically stable then we can perturb it with a random Hamiltonian without changing the physical properties of the system (for instance, the value of the thermal exponent $\theta$). A slight perturbation of the original Hamiltonian corresponds to shift and mix the original distribution of energy levels. A good selection of the type of random perturbation and an appropriate tuning of its intensity might have the effect of making typical those lowest order excitations which originally were not. Because
the physical properties of the new perturbed system remain unchanged this implies that the statistical properties of lowest and typical excitations must be also the same.

To verify these assumptions we studied first and second excitations in the two dimensional Gaussian spin glass defined by

$$\mathcal{H} = - \sum_{i<j} J_{ij} \sigma_i \sigma_j ,$$

(1)

where the $\sigma_i$ are the spins ($\pm 1$) and the $J_{ij}$ are quenched random variables extracted from a Gaussian distribution with zero mean and unit variance. In I we found that two exponents $\lambda$ and $\theta'$ characterize the level spectrum. A question not addressed in detail was the issue of correlations. Using the transfer matrix method we have looked at first and second excitations for 2D spin glasses with periodic-periodic (PP), free-free (FF) and free-periodic (FP) boundary conditions. Second excitations are also cluster excitations, i.e. clusters of any two quantities for sample $s$. We define the second-excitation (with energy gap $E_2$) probability distribution $P^{(2)}(v,E_2) = g^{(2)}(v) \hat{P}_s^{(2)}(E_2)$ in analogous way as we did in I for first excitations. In figure 1 we show the probability to find a second excitation with volume $v g^{(2)}(v)$ for the PP case (the other cases are similar) showing the same functional shape to that found in the case of the lowest first excitations. Also in that figure we show the average gap for second excitations compared to the first-excitation gap as function of $L$ for PP and FF. We point out two important features: One the one hand, $g^{(2)}(v)$ follows the same functional form to the one describing first excitations with the same exponent $\lambda$ and tends to $g(v)$ in the large volume limit. It is also remarkable that the distributions $g(v)$ and $g^{(2)}(v)$ are nearly equal, except from a small discrepancy in the single-spin excitations weight. The reason for this difference comes from the excluded volume effect arising from the single-spin first excitation which leaves a smaller volume $V - 1$ available to the second excitation. For small systems this implies a net decrease of the probability of having one-spin excitations whereas, larger volume second excitations, are insensitive to this effect. Furthermore, this effect yields important $v_1 - v_2$ correlations. On the other hand, as was the case for for $\hat{P}_{v_1}(E_1)$, the energy distribution $\hat{P}_v^{(2)}(E_2)$ is independent of the size $v_2$ of the second excitation. As expected we have that $\hat{P}_v^{(2)}(E_2) = L^{-\theta''} \hat{P}_v^{(2)}(E_2/L^{\theta''})$. Within numerical precision $\theta'' = \theta'$ for a given size.

We now focus on the issue of the existence of correlations. Let us denote by $x_s, y_s$ any two quantities for sample $s$ and let us consider their corresponding correlation,

$$C_{x,y}(L) = \frac{x_s y_s - \overline{x_s} \overline{y_s}}{\sqrt{\overline{x_s^2} - \overline{x_s}^2} \sqrt{\overline{y_s^2} - \overline{y_s}^2}} .$$

(2)

We find that correlations between energies and volumes of the type $C_{v^{(i)},E^{(j)}(L)}$, whichever they are (first or second excitations, i.e. $i, j = 1, 2$) asymptotically vanish in the $L \to \infty$ limit (figure 2a). Correlations between the energies

FIG. 1. In plot a) we show the $g(q), g^{(2)}(q)$ for first (solid line) and second (dashed line) excitations for lattice sizes 4, 7 and 11 in the PP case. In plot b) we show, in a log-log scale, the average gap for the first and second excitations for the PP and FF cases. The full straight line corresponds to the power law $L^{-1.7}$.
of the levels deserve some comments. Since $E_2 > E_1$ there are trivial energy correlations. In this case it is convenient to consider correlations in taking $x = \Delta_1 = E_1$, $y = \Delta_2 = E_2 - E_1$. We see a slow but systematic decrease of $C_{\Delta_1, \Delta_2}(L)$ with $L$ suggesting there are no gap-gap correlations (figure 2b). Nevertheless correlations of the type $C_{v_1, v_2}(L)$ are much higher and, although they saturate and show a tendency to decrease later, we have no evidence that they indeed vanish in the $L \to \infty$ limit (figure 2c).

Based on the evidence in favor of a random-energy levels scenario we derive a novel low-temperature expansion for spin glasses. This expansion has been partially discussed in several papers but, to our knowledge, has never been worked out in detail. The systematic procedure to build this expansion is as follows. Consider a spin-glass system described by a Hamiltonian $H_J(\sigma)$ where $\sigma$ denotes the set of discrete spin variables and $J$ are the couplings that we take continuous in order to avoid accidental degeneracy of the ground state. Consider a given sample which we will denote by $(s)$ and let us denote its different excited levels by the index $r = 0, 1, 2, \ldots$ where $r = 0$ denotes the ground state configuration, $r = 1$ the first or lowest excitation, $r = 2$ the second excitation and so on.

The low-temperature expansion is done by fixing the "excited" level $r$ and keeping in the partition function all first $r$ levels plus the ground state configuration. The mathematical object in terms of which the expansion is written is the probability distribution $\mathcal{P}^{(1)}(E_1, E_2, \ldots, E_r, C(v_1, v_2, \ldots, v_r))$ where $E_i$ is the gap of the $i$th excitation and $C(v_1, v_2, \ldots, v_r)$ stands for a set of variables including all excitation volumes $v_i$ as well as some other volumes obtained by a given number of set operations (for instance, unions and intersections among the $v_i$). This set $C$ of volume variables may be quite complex and strongly depend on the observable we are expanding. For $r = 1$ the appropriate probability is $\mathcal{P}^{(1)}(E_1, v_1)$ as considered in 1. In practice, this procedure generates a low-temperature expansion in powers of $T$ up to order $T^2$. Including higher-order excitations in the partition function yields always higher order $T$ corrections so the expansion is well defined. As an example, let us see how the expansion works for the spin-glass susceptibility $\chi_{SG} = V(q^2)$ up to order $T^2$ ($q$ is the overlap between two replicas). In this case $r = 2$ and the probability is $\mathcal{P}^{(2)}(E_1, E_2, v_1, v_2, v)$ where $v = v_1 \cup v_2 - v_1 \cap v_2$, so $C(v_1, v_2)$ is the set of variables including each of the excitation volumes plus their total non-overlapping volume. This probability can be written as $\mathcal{P}^{(2)}(E_1, E_2, v_1, v_2, v) = g_{v_1, v_2, v} \tilde{P}^{(2)}(E_1, E_2)$ this last term being the conditioned probability for a given triplet $v_1, v_2, v$ to have energy gaps $E_1, E_2$. Therefore, if we keep only the first and second excitations in the Hamiltonian and we denote $x_i = \exp(-\beta E_i)$, we get

$$\chi_{SG} = V - \frac{8}{V} \sum_{v_1} v_1(V - v_1) \int_0^\infty dE_1 \int_{E_1}^\infty dE_2 \frac{x_1 \mathcal{P}^{(2)}(E_1, E_2)}{(1 + x_1 + x_2)^2} -$$

$$\frac{8}{V} \sum_{v_2} v_2(V - v_2) \int_0^\infty dE_1 \int_{E_1}^\infty dE_2 \frac{x_2 \mathcal{P}^{(2)}(E_1, E_2)}{(1 + x_1 + x_2)^2} -$$

$$\frac{8}{V} \sum_{v} v(V - v) \int_0^\infty dE_1 \int_{E_1}^\infty dE_2 \frac{x_1 x_2 \mathcal{P}^{(2)}(E_1, E_2)}{(1 + x_1 + x_2)^2},$$

(3)
where we have defined \( P^{(2)}_v(E_1, E_2) = \sum_{v_1'} \nu s \) except \( v \). \( P^{(2)}(E_1, E_2, v_1, v_2, v) \) where \( v_i \) stands for \( v_1, v_2 \) or \( v \). Expression \( \chi_{SG} \) can be worked out in the limit \( \beta \to \infty \) yielding, after some lengthy calculations,

\[
\chi_{SG} = V - \frac{4T}{V} \sum_{v_1} v_1 (V-v_1) P^{(1)}(0, v_1) - \frac{8 \log(2) T^2}{V} \sum_{v_1} v_1 (V-v_1) P^{(1)}(0, v_1) + \frac{4T^2}{V} \left( \log(6) \right)
\]

\[
\sum_{v_1} P^{(2)}_v(0, 0) v_1 (V-v_1) - 2 \log(3/2) \sum_{v_2} P^{(2)}_v(0, 0) v_2 (V-v_2) - \log(4/3) \sum_{v} P^{(2)}_v(0, 0) v (V-v) + \mathcal{O}(T^3)
\]  

(4)

where \( P^{(1)}(E_1, v_1) = \int_0^\infty d(E_2) P^{(2)}_v(E_1, E_2) \), \( P^{(1)}(E_1, v_1) = \frac{\partial P^{(1)}(E_1, v_1)}{\partial E_2} \), and these expressions appear evaluated at \( E_1 = 0 \) in \( \chi_{SG} \). In \( \chi_{SG} \) we recognize the linear contribution in \( T \) presented in \( I \). At first glance, this expansion looks too complicated to be useful. But as we will see below, it can be properly interpreted in a scenario of random-energy levels.

One of the most striking consequences of the random-energy levels scenario is that it can be used to predict the specific heat exponent. There has been a lot of work to understand the specific heat anomaly in structural glasses showing that, in good approximation, specific heat is linear in \( T \). This is usually explained by the fact that this kind of systems have a finite density of states at zero gap. Contrarily, in spin glasses the behavior of the specific heat at low-temperatures has not received much attention probably because the question (both from the numerical and experimental point of view) can hardly answered due to the difficulty to reach thermal equilibrium at low temperatures. Cheung and McMillan claimed that the specific heat in 2D should be linear in \( T \) while Fisher and Huse made some observations about the sample to sample fluctuations of the ground state energy and its relation to the low-temperature specific heat. The specific heat is given by the usual fluctuation-dissipation formula, \( c = \frac{\partial^2 E}{\partial T^2} \). Using the low-\( T \) expansion method discussed before we expand \( c \) up to any order in \( T \). The calculations are less laborious than for \( \chi_{SG} \) because the relevant probability functions \( P^{(r)}(E_1, E_2, \ldots, E_r) \) do not depend on the spectrum of excitation volumes. If we expand up to order \( T^2 \) then we must consider only the two lowest-lying excitations in the Hamiltonian. This yields the following expression for the specific heat,

\[
c(T, L) = \frac{\beta^2}{V} \int_0^\infty dx_1 \int_1^\infty dx_2 P^{(2)}(x_1, x_2) \left( \frac{x_1^2 \exp(-\beta x_1) + (x_1 - x_2)^2 \exp(-\beta (x_1 + x_2)) + x_2^2 \exp(-\beta x_2)}{1 + \exp(-\beta x_1) + \exp(-\beta x_2)} \right).
\]  

(5)

In the limit \( T \to 0 \) after some calculations we obtain,

\[
c(T, L) = \frac{\pi^2 T P^{(1)}(0)}{6V} + \frac{9 \zeta(3) T^2 P^{(1)}(0)}{2V} + \frac{0.77564T^2 P^{(2)}(0, 0)}{V}
\]  

(6)

where \( \zeta(s) = \sum_{k=1}^\infty k^{-s} \) is the Riemann function and \( P^{(1)}(E) = \frac{\partial P^{(1)}(E)}{\partial E} \). In general, it can be shown that the terms appearing in the expansion at order \( T^r \) are of the type, \( \nabla E_1, \ldots, E_r P^{(u)}(E_1, \ldots, E_u) \) evaluated at \( E_i = 0 \), \( \forall i \) with \( u + v = r \) (the symbol \( \nabla \) denotes all possible partial derivatives).

According to the assumption \( A \) of the random-energy levels scenario the \( r \)-point energy probability distribution factorizes, i.e. \( P^{(r)}(E_1, E_2, \ldots, E_r) = \prod_{i=1}^r P^{(1)}(E_i) \) where all the \( P^{(1)}(E_i) \) scale with the size of the system \( L \) with the same exponent \( \theta' \),

\[
P^{(1)}(E_i) = L^{-\theta'} \hat{P}_i \left( \frac{E_i}{L^{\sigma'}} \right)
\]  

(7)

and the dependence of the energy level \( i \) enters only through the scaling function \( \hat{P} \). The presence of the same exponent \( \theta' \) for all levels is also a consequence of the random-energy levels scenario. Therefore, at order \( T^r \) in the low-\( T \) expansion all terms scale like \( (TL^{-\theta'})^r / V \) thus leading (since \( \theta' < 0 \)) to an apparent divergent series. The whole series can then be resumed in a singular function \( \hat{c}(x) \), \( c(T, L) = \frac{\hat{c}(TL^{-\theta'})}{V} \) like in ordinary critical phenomena. In the scaling region \( T \to 0 \) and \( TL^{-\theta'} \) finite, we have a finite heat-capacity \( Vc(T, L) \). But if we take first the limit \( L \to \infty \) and afterwards \( T \to 0 \) the \( L \) dependence must disappear in the specific heat, therefore \( \hat{c}(x) \to x^{-\theta'} \) when \( x \to \infty \) yielding \( c(T \to 0) \sim T^{\alpha} \) with \( \alpha \) the specific heat exponent \( \alpha = -\frac{d}{\theta'} \). For Gaussian spin glasses in general dimensions there is a general argument (see \( I \)) supporting that \( \theta' = -d \), hence \( \alpha = 1 \). Nevertheless, in \( I \) we showed how both exponents \( \theta' \) and \( \lambda \) suffer from very strong finite-size corrections yielding effective values for the exponents \( \theta' \) and \( \alpha \) in the range of sizes \( L \leq 14 \): \( \theta'_\text{eff} = -1.7 \pm 0.1 \) and \( \alpha_{\text{eff}} \simeq 1.18 \pm 0.07 \). In figure 2 we show finite-temperature transfer matrix calculations for the 2D Gaussian spin glass in the same range of sizes \( L \leq 14 \) which nicely conform to this prediction (we tried the effective exponents \( \theta'_\text{eff} = -1.6, \alpha_{\text{eff}} = 1.25 \)). Only when the system reaches a temperature
such that \( TL^{-\theta'} \) is not too small (i.e. for pretty large sizes) we will obtain the right linear in \( T \) dependence. It is important to note that for finite systems \( c \) is always linear in \( T \) for low enough temperatures. Note that because \( \theta' < 0 \) the exponent \( \alpha \) is always positive. The calculation of the low-temperature specific heat exponent \( \alpha \) provides an indirect way to determine the gap exponent \( \theta' \). Preliminary investigations for the SK model\(^4\) show that the effective gap exponent \( d/\theta' \) is well compatible with 2 giving the well know result\(^2\) \( \alpha = 2 \).

We discuss now the behavior of the \( \chi_{SG} \) which is certainly more subtle. As observed in I, the linear term in \( T \) scales like \( VT L^{-\theta} \) but the first term of \( O(T^2) \) in expression (3) scales like \( VT^2 L^{-\theta - \theta'} \). The rest of quadratic terms would also scale like \( VT^2 L^{-\theta - \theta'} \) if the three distributions \( g_{v_1}, g_{v_2}, g_v \) \((v = v_1 \cup v_2 - v_1 \cap v_2)\) defined by \( P_v(E) = g_v \hat{P}_v(E) \) scale with the same exponent \( \lambda \). Indeed, we have seen that \( g_{v_1}, g_{v_2} \) are described by the same exponent \( \lambda \) and we also verified that the same is true for the \( g_v \). Therefore, to understand the character of the low-\( T \) expansion it is necessary to consider higher orders in \( T \) for \( \chi_{SG} \). The cubic term is more complex but can be also worked out. In this case, the third excitation must be included in the calculation and the \( T^3 \) gets contribution from the first, second and third excitations. The first and second excitation will yield terms of the type \( VT^3 L^{-\theta - 2\theta'} \) but the third excitation, since it can consist of two disconnected droplets, will yield terms of the type \( VT^3 L^{-\theta - \theta'} \). Therefore, at any order beyond the first one \((r = 1)\) there will be terms of the type \( VT^r L^{-\theta - \theta'} \) with \( u + v = r, r > 1; u, v \geq 0 \). Resummation of this divergent series yields, \( \chi_{SG}(T, L) = V \hat{\chi}(TL^{-\theta}, TL^{-\theta'}) \). There are two divergent length scales, but since \( \theta' \leq 0 \) \( (\theta = \theta' + d\lambda \text{ with } \lambda \geq 0) \) the leading scaling behavior is governed by the term \( TL^{-\theta} \). In renormalization group language this assertion implies that the leading behavior is determined by the fixed point which has largest correlation length exponent. In the region \( T \to 0, L \sim T^{1/\theta} \), the term \( TL^{-\theta'} \) diverges like \( L^{-\theta' - 1} \) and the scaling behavior of the susceptibility is given by, \( \chi_{SG}(T, L) = V \hat{\chi}(TL^{-\theta}, \infty) \). For \( L \gg T^{1/\theta} \) and \( T \to 0 \) this yields the usual low-\( T \) result\(^2\) \( \chi_{SG} \sim T^{-\gamma} \) with \( \gamma = -\frac{d}{\theta} \). Sub-leading corrections are then expected for \( \chi_{SG} \) because for a given temperature and finite \( L \), even if we keep \( TL^{-\theta} \) finite, the second argument of the scaling function \( \hat{\chi} \) systematically changes with \( L \). Only for sizes large enough such that \( TL^{-\theta} \gg 1 \) data would collapse. Note that these finite-size corrections can be important if \( \theta' \neq 0 \) (i.e. \( \lambda > 0 \)) as happens in 2D. This explains the corrections obtained for the susceptibility exponent \( \gamma \) obtained from Monte Carlo or finite-temperature transfer matrix methods\(^3\)\(^4\)\(^5\)\(^6\). Actually, in 1D (where \( \lambda = 0 \) and \( \theta = \theta' = -1 \) it can be shown that the scaling behavior for small sizes of the spin-glass susceptibility \( \chi_{SG}(T, L) = L \hat{\chi}(TL) \) is nearly perfect.

To summarize, we have shown the numerical evidence in support of random-energy levels and derived a low-temperature expansion for spin glasses by progressively including higher excitations into the partition function. The coefficients in this expansion can then be written in terms of a set of energy gap probability distributions and their derivatives evaluated at zero gap. In particular, we have obtained the specific heat exponent \( (c \sim T^{-\frac{d}{\theta}}) \) which is linear under the assumption \( \theta' = -d \) valid for Gaussian spin glasses in finite dimensions. It remains to be seen how 3d spin glasses fit to the new scenario and how to extend these ideas to \( \pm J \) spin glasses.

**Acknowledgments.** F.R. and M.S. are supported by the Spanish Ministerio de Ciencia y Tecnolog\‘ia, project PB97-0971 and grant AP98-36523875 respectively. M. P. and F. R. acknowledge support from the French-Spanish collaboration (Picasso program and Acciones Integradas HF1998-0097).
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