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Large Deviations for Ising Spin Glasses with Constrained Disorder

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We consider a d-dimensional Ising spin glass and construct lower bounds for the mean free energy density which, in general, improve the classical lower bounds given by the annealed free energy density. The bounds are achieved by introducing generalized finite-volume free energy densities. The large-deviations aspects of the problem are displayed and examples discussed.

KEY WORDS: Spin glasses; large deviations.

1. INTRODUCTION

It is well known that the computation of the free energy density of a disordered system is a difficult problem even in simple one-dimensional models.

Assuming that the free energy density $f(\beta)$ of the considered system has the self-averaging property, the problem itself reduces to the evaluation of its mean value $\mathbb{E}[f(\beta)]$ with respect to the probability distribution of the underlying randomness. For mean-field spin-glass systems this task is generally accomplished by means of the replica trick, which has greatly contributed to the physical understanding of the glassy-phase properties.[(5)] Unfortunately, the replica trick cannot be usefully adapted to study Ising spin glasses on a lattice.

In this paper we follow a quite different approach to disordered systems which has been recently proposed in ref. 13 and applied to different

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models (in refs. 6 and 7 to one-dimensional models and in ref. 8 to a model with short-range $J = \pm 1$ interactions competing with long-range positive interactions). The method consists in an improvement of the annealed approximation of the mean free energy density. The starting point is the introduction of generalized finite-volume partition functions depending on some Lagrangian multipliers μ associated with intensive variables of the disorder. Examples of these variables are the concentration of negative bonds in ferromagnetic Ising models with impurities and the frustration in Ising spin glasses. The idea is to take first the expectation of these generalized partition functions in order to estimate the mean free energy density and then optimize the result by a proper choice of the Lagrangian multipliers. In this way it is possible to constrain the disorder to minimize the difference between the mean free energy density and its annealed approximations. The method, for the special case of single-plaquette frustration, was proposed in ref. 9, and, in another special context, in ref. 10. A similar approach, based on the use of a microcanonical ensemble, can be found in ref. 11.

The paper is organized as follows.

In Section 2 we introduce the Ising spin-glass model on the d-dimensional lattice $\mathbb{Z}^d$. We first report some known rigorous results, then we prove a theorem which ensures the existence of the momentum generating function associated with the partition function. This result is used to state some large-deviations properties of the model and to give an alternative proof of the existence of the mean free energy density for a large class of distributions of the random couplings $\{J_{ij}\}$.

In Section 3 we introduce a generalized class of partition functions $Z_\Lambda(\beta, \mu)$ and the associated finite-volume free energy densities $f_\Lambda(\beta, \mu)$. We then discuss the associated large-deviation problem and we show that the generalized free energy densities coincide with the ordinary free energy densities $f_\Lambda(\beta)$ only in the thermodynamic limit. Finally we show how to improve concretely the annealed lower bound by computing the infinite-volume limit of $-(1/\beta\,|\Lambda|) \ln \mathbb{E}[Z_\Lambda(\beta, \mu)]$ and by taking the supremum with respect to the Lagrange multipliers μ (Theorem 3.3).

In Section 4 we discuss in detail some applications to d-dimensional Ising spin glasses in order to illustrate the approximation strategy proposed in the paper. We consider three cases: (a) Gaussian couplings; (b) dichotomic couplings in two dimensions, where we consider intensive variables of the disorder of the type proposed in ref. 9; and (c) dichotomic couplings in three dimensions, where we extend the approach used in the previous point. In all these cases we improve the annealed estimates for the free energy and ground-state energy of Ising spin glasses with nearest-neighbor interactions.

2. LARGE DEVIATIONS

We consider an Ising spin-glass system on the d-dimensional lattice $\mathbb{Z}^d$ with nearest-neighbor interactions. The Hamiltonian which defines the model is

$$H_\Lambda(\sigma) = - \sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j \tag{2.1}$$

where Λ is a finite subset of $\mathbb{Z}^d$ with cardinality $|\Lambda|$ and $\langle i,j \rangle$ denotes nearest-neighbor sites i, j in Λ. The $\{J_{ij} \mid i,j \in \mathbb{Z}^d\}$ are random couplings and the $\{\sigma_i \mid i \in \mathbb{Z}^d\}$ are spin variables which can take values $+1$ or -1. In the following the couplings J_{ij} will be chosen to be i.i.d. random variables, and averages with respect to their probability distribution will be indicated by $\mathbb{E}[\cdot]$.

The associated partition function is obtained as a sum over all the configurations of $\sigma = \{\sigma_i \mid i \in \Lambda\}$,

$$Z_\Lambda(\beta) = \sum_{\{\sigma\}} \exp[-\beta H_\Lambda(\sigma)] \tag{2.2}$$

where $\beta > 0$ is the inverse of the temperature. The free energy density is then defined by the following limit:

$$f(\beta) = - \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{\beta\,|\Lambda|} \ln[Z_\Lambda(\beta)] \tag{2.3}$$

The thermodynamic limit (2.3), performed in the sense of Van Hove, was shown to exist with probability one for very general coupling distributions by different authors.[16,14,3,4] Their proofs are not limited to nearest-neighbor couplings, but they extend to the case of generic short-range interactions. Moreover, the same authors rigorously proved the self-averaging property: the free energy density $f(\beta)$ equals the mean free energy density $\mathbb{E}[f(\beta)]$ almost surely.

In this section we are interested in the large-deviations properties of the model. We refer to refs. 1, 15, and 14 for some already established results on disordered systems and in particular on spin glasses.

Let us consider a sequence $\{\Lambda_N\}$ of regular cubes of increasing size such that $\Lambda_N \subset \Lambda_{N+1} \nearrow \mathbb{Z}^d$, and the associated sequences of random variables $\{\ln Z_{\Lambda_N}\}$. We then define the logarithm of the moment generating function (divided by $|\Lambda_N|$)

$$\phi_N(t) \equiv \frac{1}{|\Lambda_N|} \ln \mathbb{E}[(Z_{\Lambda_N})^t] \tag{2.4}$$

It is well known that if

$$\phi(t) \equiv \lim_{N\to\infty} \phi_N(t) \tag{2.5}$$

exists finite for all $t \in \mathbb{R}$, then the large-deviation upper bound

$$\limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \ln Q_N(K) \leqslant -\inf_{z\in K} I(z) \tag{2.6}$$

is satisfied for each closed set $K \subset \mathbb{R}$, where Q_N is the distribution of the random variable $-\beta f_N(\beta) \equiv (1/|\Lambda_N|) \ln(Z_{\Lambda_N})$ on $\mathbb{R}$. The random variable $f_N(\beta)$ is the finite-volume free energy density and $I(z)$ is the rate function given by the Legendre–Fenchel transform[2]

$$I(z) \equiv \sup_{t\in\mathbb{R}} [tz - \phi(t)] \tag{2.7}$$

In the physical literature the logarithm of the moment generating function and its Legendre–Fenchel transform have been widely studied in different contexts (for example in the so-called multifractal approach[17]). We will prove the following result, which, as remarked, implies (2.6):

Theorem 2.1. Assume there is a function λ: $\mathbb{R}^+ \to \mathbb{R}^+$ such that one has $\exp[-\lambda(u)] \leqslant \mathbb{E}[\exp(-u\,|J_{ij}|)$ and $\mathbb{E}[\exp(+u\,|J_{ij}|)] \leqslant \exp[+\lambda(u)]$; then the function ϕ defined in (2.5) exists finite on $\mathbb{R}$.

Proof. Subdivide the cube Λ_N into subcubes $\{\Lambda^i_M \mid i=1,..., k^d\}$ of cardinality $|\Lambda^i_M| \equiv M \equiv m^d$ for all i so that $|\Lambda_N| = (km)^d = k^d M$. To any subcube of such decomposition is associated the partition function $Z^i \equiv Z_{\Lambda^i_M}$. From definitions (2.1) and (2.2) it is easy to state the following inequalities:

$$\left(\prod_{i=1}^{k^d} Z^i\right) \exp\left(\beta \sum_{\langle i,j\rangle'} -|J_{ij}|\right) \leqslant Z_{\Lambda_N} \leqslant \left(\prod_{i=1}^{k^d} Z^i\right) \exp\left(\beta \sum_{\langle i,j\rangle'} +|J_{ij}|\right) \tag{2.8}$$

where the sum runs over all the couples of first-neighbor sites $\langle i,j\rangle'$ with i and j in different subcubes. Since the couplings J_{ij} are independent random variables, we have from (2.8)

$$\begin{aligned}
&\frac{1}{|\Lambda_N|} \sum_{i=1}^{k^d} \ln \mathbb{E}[(Z^i)^t] + \frac{1}{|\Lambda_N|} \sum_{\langle i,j\rangle'} \ln \mathbb{E}[\exp(-\beta|t|\cdot|J_{ij}|)] \\
&\quad \leqslant \frac{1}{|\Lambda_N|} \ln \mathbb{E}[(Z_{\Lambda_N})^t] \\
&\quad \leqslant \frac{1}{|\Lambda_N|} \sum_{i=1}^{k^d} \ln \mathbb{E}[(Z^i)^t] + \frac{1}{|\Lambda_N|} \sum_{\langle i,j\rangle'} \ln \mathbb{E}[\exp(+\beta|t|\cdot|J_{ij}|)]
\end{aligned} \tag{2.9}$$

Moreover, since the couplings J_{ij} are identically distributed, we have $\mathbb{E}[(Z^i)^t] = \mathbb{E}[(Z^1)^t]$. This implies

$$\frac{1}{|\Lambda_N|} \sum_{i=1}^{k^d} \ln \mathbb{E}[(Z^i)^t] = \frac{k^d}{|\Lambda_N|} \ln \mathbb{E}[(Z^1)^t] = \frac{1}{M} \ln \mathbb{E}[(Z^1)^t] \qquad (2.10)$$

The total number of couples of first-neighbor sites $\langle i, j \rangle'$ with i and j in different subcubes is estimated from above by $dk^d m^{d-1}$. Therefore, using our hypotheses and inequality (2.9), we get

$$\left| \frac{1}{|\Lambda_N|} \ln \mathbb{E}[(Z_{\Lambda_N})^t] - \frac{1}{M} \ln \mathbb{E}[(Z^1)^t] \right| \leqslant \frac{dk^d m^{d-1}}{|\Lambda_N|} \lambda(|t| \, \beta) = \frac{d}{m} \lambda(|t| \, \beta) \qquad (2.11)$$

i.e., with the notations of (2.4),

$$\left| \phi_N(t) - \frac{1}{M} \ln \mathbb{E}[(Z^1)^t] \right| \leqslant \frac{c}{m} \qquad (2.12)$$

where $c = c(\beta, t, d) > 0$. The above estimate now implies

$$0 \leqslant \limsup_{N \to \infty} \phi_N(t) - \liminf_{N \to \infty} \phi_N(t) \leqslant \frac{2c}{m} \qquad (2.13)$$

for all m. The result follows. ▮

Remark 2.1. There is a well-known argument (e.g., ref. 12) which ensures that the existence of the limit for the sequence $\{\phi_N\}$ attached to the geometrical sequence of cubes $\{\Lambda_N\}$ implies the existence of the thermodynamic limit for $\{\phi_\Lambda\}$ ($\Lambda \nearrow \mathbb{Z}^d$ in the sense of van Hove).

Remark 2.2. The result of the Theorem 2.1 remains true, up to small technical modifications, for short-range interaction systems.

Remark 2.3. The hypothesis on the J_{ij} contained in the theorem defines a large class of distributions which includes all distributions with finite support and the Gaussian distribution.

Before concluding this section, we give an alternative proof of the existence of the mean free energy density.

Theorem 2.2. Assume the hypothesis of Theorem 2.1 and moreover assume $\lambda(u) = \mathcal{O}(u)$ as $u \to 0$; then the derivative of $\phi(t)$ at $t = 0$ exists and equals $-\beta \mathbb{E}[f(\beta)]$.

Proof. By (2.11) and the hypothesis on λ we have

$$\left|\frac{\phi_N(t)}{t} - \frac{1}{Mt} \ln \mathbb{E}[(Z^1)^t]\right| \leqslant \frac{c}{m} \tag{2.14}$$

with $c = c(\beta, d) > 0$ and $|t|$ small enough. Letting $N \to \infty$ (as before, M is kept fixed), by Theorem 2.1 we have that (2.14) also holds with $\phi(t)$ replacing $\phi_N(t)$.

By a first-order Taylor expansion of the exponential and logarithmic functions we obtain

$$\ln \mathbb{E}[(Z^1)^t)] = [t + o(t)]\, \mathbb{E}[\ln(Z^1)] \tag{2.15}$$

for $|t|$ sufficiently small.

Therefore

$$\left|\frac{\phi(t)}{t} - \left(\frac{1}{M} + \frac{o(t)}{t}\right) \ln \mathbb{E}[(Z^1)]\right| \leqslant \frac{c}{m} \tag{2.16}$$

which implies

$$0 \leqslant \limsup_{t \to \infty} \frac{\phi(t)}{t} - \liminf_{t \to \infty} \frac{\phi(t)}{t} \leqslant \frac{2c}{m} \tag{2.17}$$

for all m. Since $\phi(0) = 0$, the differentiability of ϕ at $t = 0$ follows. Now we take in (2.16) the limit for $t \to 0$ and we get

$$\left|\phi'(0) - \mathbb{E}\left[\frac{1}{M} \ln(Z_{\Lambda_M^1})\right]\right| \leqslant \frac{c}{m} \tag{2.18}$$

(in order to stress the dependence on M, we avoided here the use of the short notation Z^1). Then for $m = M^{1/d} \to \infty$ we obtain the result. ∎

Remark 2.4. Since $\phi(t)$ is a convex function vanishing at the origin, one has $\mathbb{E}[f(\beta)] \geqslant -(1/\beta)\, \phi(t)/t$ for any positive t. In particular one has the well-known lower bound

$$\mathbb{E}[f(\beta)] \geqslant f_a(\beta) \equiv -\frac{1}{\beta} \phi(1) \tag{2.19}$$

The function $f_a(\beta)$ is the annealed approximation of the free energy density.

3. GENERALIZED THERMODYNAMIC POTENTIALS

In this section we consider again an Ising spin-glass system on the d-dimensional lattice $\mathbb{Z}^d$ with first-neighbor interaction. The random couplings $\{J_{ij}\}$ are assumed to satisfy the condition of Theorem 2.1.

Let $\alpha: \mathbb{R} \to \mathbb{R}$ be a function such that the $\{\alpha(J_{ij})\}$ are i.i.d. random variables which satisfy $\mathbb{E}[\alpha(J_{ij})] = 0$. We then define a generalized class of finite-volume partition functions:

$$Z_\Lambda(\beta, \mu) \equiv \sum_{\{\sigma\}} \exp[-\beta H_\Lambda(\sigma) + \mu A_\Lambda] \tag{3.1}$$

where

$$A_\Lambda \equiv \sum_{\langle i,j \rangle} \alpha(J_{ij}) \tag{3.2}$$

As before, Λ is a finite subset of $\mathbb{Z}^d$ with cardinality $|\Lambda|$ and $\langle i,j \rangle$ denotes nearest-neighbor sites i, j in Λ. The real variable μ has to be seen as a Lagrangian multiplier and, obviously, $Z_\Lambda(\beta, 0) = Z_\Lambda(\beta)$ (the partition function defined in the previous section); moreover, we have the following result.

Proposition 3.1. For any real μ the following equality holds:

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} -\frac{1}{\beta\, |\Lambda|} \mathbb{E}[\ln\{Z_\Lambda(\beta, \mu)\}] = \mathbb{E}[f(\beta)] \tag{3.3}$$

Proof. Equation (3.1) can be rewritten as

$$Z_\Lambda(\beta, \mu) = Z_\Lambda(\beta) \exp(\mu A_\Lambda) \tag{3.4}$$

Substituting in (3.3) and taking into account that $\mathbb{E}[A_\Lambda] = 0$, the proof follows. ∎

Proposition 3.2. Assume that the i.i.d. random variables $\{\alpha(J_{ij})\}$ satisfy the condition $\mathbb{E}[|\alpha(J_{ij})|] < \infty$; then the following limit holds almost surely:

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} -\frac{1}{\beta\, |\Lambda|} \ln[Z_\Lambda(\beta, \mu)] = f(\beta) \tag{3.5}$$

Proof. It is sufficient to remark that the strong law of large numbers implies

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} -\frac{1}{\beta\, |\Lambda|} A_\Lambda = \lim_{\Lambda \nearrow \mathbb{Z}^d} -\frac{1}{\beta\, |\Lambda|} \sum_{\langle i,j \rangle} \alpha(J_{ij}) = 0 \tag{3.6}$$

almost surely. ∎

We consider now, as before, a sequence $\{\Lambda_N\}$ of regular cubes of increasing size such that $\Lambda_N \subset \Lambda_{N+1} \nearrow \mathbb{Z}^d$. We then define a class of finite-volume generalized free energe densities

$$f_N(\beta, \mu) \equiv -\frac{1}{\beta\,|\Lambda_N|} \ln[Z_{\Lambda_N}(\beta, \mu)] \tag{3.7}$$

We have the obvious equality

$$f_N(\beta, 0) = f_N(\beta) \tag{3.8}$$

where $f_N(\beta)$ is the free energy density defined in the previous section. It should be remarked that all the above generalized free energy densities, by virtue of Propositions 3.1 and 3.2, are equivalent to ordinary free energy density in the thermodynamic limit. The finite-volume fluctuations, on the contrary, depend on μ.

We are now interested in giving estimates on the large deviations of the $f_N(\beta, \mu)$; moreover, we are also interested in improving the annealed lower bound on the free energy of Remark 2.4. Define

$$\phi_N^\mu(t) \equiv \frac{1}{|\Lambda_N|} \ln \mathbb{E}[\{Z_{\Lambda_N}(\beta, \mu)\}^t] \tag{3.9}$$

The following theorem shows that under suitable conditions the function

$$\phi^\mu(t) \equiv \lim_{N \to \infty} \phi_N^\mu(t) \tag{3.10}$$

exists finite for all $t \in \mathbb{R}$.

Theorem 3.1. Let ε be a real number for which there is a function λ^ε: $\mathbb{R}^+ \to \mathbb{R}^+$ such that the following inequalities hold:

$$\exp[-\lambda^\varepsilon(u)] \leqslant \mathbb{E}[\exp\{-u\,|J_{ij}| + \varepsilon u \alpha(J_{ij})\}]$$

$$\mathbb{E}[\exp\{+u\,|J_{ij}| + \varepsilon u \alpha(J_{ij})\}] \leqslant \exp[+\lambda^\varepsilon(u)]$$

Then for $\mu = \varepsilon\beta$ the function ϕ^μ defined in (3.10) exists finite on $\mathbb{R}$.

Proof. The proof is a trivial modification of the proof of Theorem 2.1. ∎

Theorem 3.2. Assume the hypothesis of Theorem 3.1 and moreover assume that $\lambda^\varepsilon(u) = \mathcal{O}(u)$ as $u \to 0$; then the derivative of $\phi^\mu(t)$ at $t = 0$ exists and equals $-\beta\mathbb{E}[f(\beta)]$.

Proof. The proof is the same as in Theorem 2.2. ▌

The existence of the function $\phi^{\mu}(t)$ for any real t [notice that $\phi^{0}(t) = \phi(t)$, where $\phi(t)$ is defined in the previous section] allows us to estimate the large deviations of the variables $f(\beta, \mu)$. In fact, the following large-deviation upper bound is satisfied:

$$\limsup_{|\Lambda_N| \to \infty} \frac{1}{N} \ln Q_N^{\mu}(K) \leqslant - \inf_{z \in K} I^{\mu}(z) \tag{3.11}$$

for each closed set $K \subset \mathbb{R}$, where Q_N^{μ} is the distribution of $-\beta f_N(\beta, \mu)$ on $\mathbb{R}$. The random variable $f_N(\beta, \mu)$ is the finite-volume generalized free energy density and $I^{\mu}(z)$ is the rate function given by the Legendre–Fenchel transform

$$I^{\mu}(z) \equiv \sup_{t \in \mathbb{R}} [tz - \phi^{\mu}(t)] \tag{3.12}$$

We can give to our results the following interpretation: the multiplicative term $\exp(\mu A_{\Lambda})$ [A_{Λ} is defined in (3.2)] has the effect of a constraint on the disorder which modifies the distribution of the finite-volume free energy.

We now use the above results to improve the annealed estimate of $\mathbb{E}[f(\beta)]$. Let us define the constrained annealed approximation of the free energy density

$$g(\beta) \equiv \sup_{\mu \in \Gamma} \left[-\frac{1}{\beta} \phi^{\mu}(1) \right] \tag{3.13}$$

where Γ is the subset of $\mathbb{R}$ consisting of the numbers μ for which $\phi^{\mu}(1)$ exists. Then we have the following result.

Theorem 3.3. Suppose Γ includes the origin; then the following inequalities hold:

$$\mathbb{E}[f(\beta)] \geqslant g(\beta) \geqslant f_a(\beta) \tag{3.14}$$

where $f_a(\beta) \equiv -(1/\beta)\, \phi^{0}(1)$ is the annealed approximation of the free energy density introduced in Remark 2.4.

Proof. Since $\phi^{\mu}(t)$ is a convex function of t, vanishing at $t = 0$, one has $\mathbb{E}[f(\beta)] \geqslant -(1/\beta)\, \phi^{\mu}(t)/t$ for any $t \in \mathbb{R}^{+}$ and $\mu \in \mathbb{R}$. In particular, one has $\mathbb{E}[f(\beta)] \geqslant -(1/\beta)\ \phi^{\mu}(1)$. From this inequality it immediately follows that

$$\mathbb{E}[f(\beta)] \geqslant \sup_{\mu \in \Gamma} \left[-\frac{1}{\beta} \phi^{\mu}(1) \right] \equiv g(\beta) \tag{3.15}$$

On the other hand, by definition, one has

$$g(\beta) \equiv \sup_{\mu \in \Gamma} \left[-\frac{1}{\beta} \phi^{\mu}(1) \right] \geqslant -\frac{1}{\beta} \phi^{0}(1) \equiv f_a(\beta) \tag{3.16}$$

which complete the proof. ∎

Remark 3.1. Notice that if the $\{J_{ij}\}$ have distribution of the type described in Remark 2.3, then Theorem 2.1 holds and Γ includes the origin.

Remark 3.2. It is in general possible to extend the previous results to the case of short-range interactions and to the case where the function α depends not only on the variable J_{ij}, but also on the variables $J_{i'j'}$ with $i'j'$ in a short range around ij.

Remark 3.3. The results can be also easily extended to the case where a vectorial function α and a vectorial Lagrangian multiplier μ are considered. In this case the exponent μA will be the scalar product $\mu A = \mu_1 A_1 + \mu_2 A_2 + \cdots + \mu_n A_n$. The function $g(\beta)$ will be obtained by taking the supremum with respect to all the components of μ.

Theorem 3.3 defines a variational method which enables one in many cases to compute explicitly the constrained annealed approximation of the free energy $g(\beta)$. The value of the $g(\beta)$ obviously depends on the function $\alpha(J_{ij})$ which appears in the exponent of the generalized partition functions. The choice of α cannot be optimized by *a priori* strategies. This choice will be done case for case by taking into account both the feasibility of calculations and the fact that the larger the number of components of the vectors μ and α, the better the estimates.

4. SPIN GLASSES IN TWO AND MORE DIMENSIONS: EXAMPLES AND NUMERICAL RESULTS

In this section we will discuss some applications of the approximation strategy discussed in Section 3. We will consider nearest-neighbor spin glasses in dimension d with $d \geqslant 2$, the case $d = 1$ being exactly solvable. Nevertheless, it is useful to state some facts about the one-dimensional Ising spin glass (see also ref. 14) which are useful for comparison with Ising spin glasses of higher dimensionality.

The partition function of the one-dimensional Ising spin glass is

$$Z_N = \sum_{\{\sigma\}} \prod_i \exp(\beta J_i \sigma_i \sigma_{i+1}) = 2^N \prod_i \cosh(\beta J_i) \tag{4.1}$$

Since the variables J_i are i.i.d., we immediately obtain

$$\phi(t) = \lim_{N \to \infty} \frac{1}{N} \ln \mathbb{E}[(Z_N)^t] = t \ln 2 + \ln\{\mathbb{E}[(\cosh\{\beta J_i\})^t]\} \tag{4.2}$$

were J_i is any one of the couplings. From (2.3) it is straightforward to compute the free energy density $\mathbb{E}[f(\beta)]$ for a given distribution of the couplings:

$$\mathbb{E}[f(\beta)] = -\frac{1}{\beta} \ln 2 - \frac{1}{\beta} \mathbb{E}[\ln \cosh(\beta J_i)] \tag{4.3}$$

Let us recall that Eq. (2.7) gives the rate function $I(z)$ as a Legendre–Fenchel transform of $\phi(t)$ computed in (4.2). For distributions of the coupling variables J_i for which the expectation in (4.2) is differentiable for all real t, the following inequality holds:

$$\liminf_{N \to \infty} \frac{1}{N} \ln Q_N(G) \geqslant -\inf_{z \in G} I(z) \tag{4.4}$$

for each open set G in $\mathbb{R}$. This inequality is the large-deviation lower bound for Ising spin glasses in one dimension and cannot be easily extended to higher dimensions. The large-deviation upper bound, on the contrary, is stated in Section 2 for Ising spin glasses of arbitrary dimension.

4.1. Gaussian Couplings

Let us consider a d-dimensional spin glass with i.i.d. couplings J_{ij} distributed according to a normal Gaussian ($\mathbb{E}[J_{ij}] = 0$ and $\mathbb{E}[J_{ij}^2] = 1$). We first compute the annealed approximation of the free energy density and then a constrained annealed approximation obtained by means of a function A_N of the type introduced in Section 3. The partition function is

$$Z_N = \sum_{\{\sigma\}} \prod_{\langle ij \rangle} \exp(\beta J_{ij} \sigma_i \sigma_j) \tag{4.5}$$

(here and in the following we denote Z_{A_N} by Z_N and A_{A_N} by A_N). It is easy to compute the expectation $\mathbb{E}[Z_N]$ since the product in (4.5) is a product of independent variables. From this expectation one immediately obtains the annealed free energy density

$$f_a(\beta) = -\frac{1}{\beta}\ln 2 - \frac{d\beta}{2} \tag{4.6}$$

where d is the dimension of the lattice. We see that, also in the one-dimensional case, this approximation is very bad for low temperatures. In fact, the function $f_a(\beta)$ decreases linearly (negative entropy!) for large β while $f(\beta)$ approaches a constant. Nevertheless, this result can be used, following ref. 9, to estimate the ground-state energy of the quenched model as

$$E_0 \geqslant \sup_\beta f_a(\beta) = -(2d\ln 2)^{1/2} \tag{4.7}$$

This estimate is simply based on the observation that the entropy must be positive for the quenched mode and therefore

$$E_0 = \mathbb{E}[f(\beta=\infty)] = \sup \mathbb{E}[f(\beta)] \geqslant \sup f_a(\beta)$$

Both (4.6) and (4.7) can be improved by using the constrained annealed approximations of the free energy. Our choice of A_N is of the type

$$A_N = \sum_{\langle i,j\rangle} \alpha(J_{ij}) \tag{4.8}$$

with the variable α depending on a single coupling J_{ij}. The simplest trial for α is to assume that it is linear with respect to the coupling. A direct computations shows that this choice would not lead to an improvement of the annealed estimate. Indeed, it is possible to show that odd functions α do not allow an improvement of the estimate of the free energy.[6] Our choice is

$$\alpha(J_{ij}) = \ln\{\cosh(\beta J_{ij})\} - \mathbb{E}[\ln\{\cosh(\beta J_{ij})\}] \tag{4.9}$$

α is an even function with vanishing average. The reason for this particular choice will be more evident later. The generalized partition function is

$$Z_N(\beta,\mu) = \sum_{\{\sigma\}} \prod_{\langle ij\rangle} \exp[\beta J_{ij}\sigma_i\sigma_j + \mu\alpha(J_{ij})] \tag{4.10}$$

Also in this case we can compute

$$-\frac{1}{\beta\,|\Lambda_N|}\ln \mathbb{E}[Z_N(\beta,\mu)] \tag{4.11}$$

The supremum with respect to μ of the above expression gives constrained free energy density

$$g(\beta) = -\frac{1}{\beta}\ln 2 - \frac{d}{\beta}\,\mathbb{E}[\ln\cosh(\beta J_{ij})] \tag{4.12}$$

where J_{ij} is any one of the couplings distributed according to a normal Gaussian. This is a better approximation than $f_a(\beta)$; in fact, we have a strict inequality $g(\beta) > f_a(\beta)$. Moreover, for large β, $g(\beta)$ approaches a constant. This is a qualitative behavior which is at variance with the *wrong* behavior of $f_a(\beta)$. Finally, in one dimension, $g(\beta)$ is the correct free energy density $f(\beta)$ in (4.3). The expression (4.9) is, in fact, an *ad hoc* choice to obtain the correct result at least in one dimension.

Also in this case it is possible to estimate the ground-state energy of the quenched model as

$$E_0 \geqslant \sup_\beta g(\beta) \tag{4.13}$$

which improves the result (4.7). For example, for $d=3$ the inequality (4.7) gives $E_0 \geqslant -2.04$, while the inequality (4.13) gives $E_0 \geqslant -1.82$. The functions $f_a(\beta)$ and $g(\beta)$ are plotted for $d=3$ in Fig. 1.

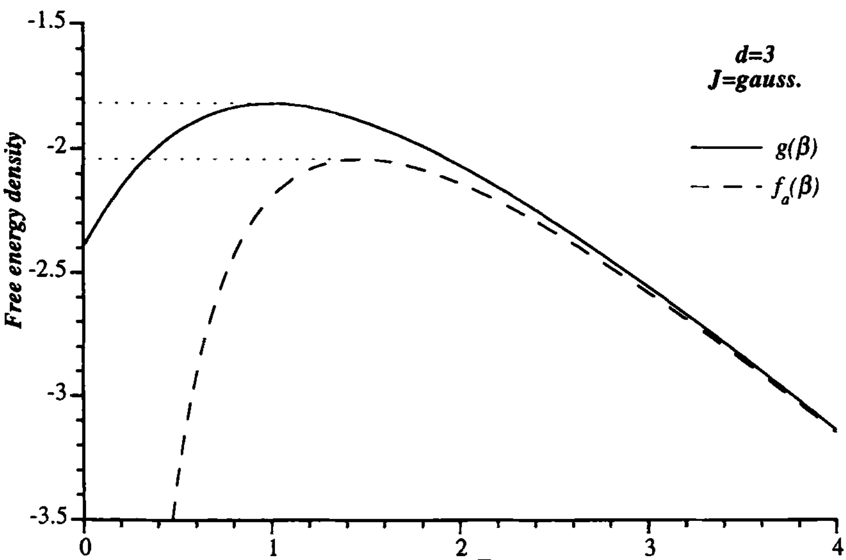

Fig. 1. Gaussian couplings: the annealed (– –) and constrained (—) free energy densities in $d=3$ versus $T=1/\beta$. The maximum of the two functions ($\cdots$) estimate the quenched ground-state energy.

4.2. Dichotomic Couplings in Two Dimensions

Let us now consider a d-dimensional spin glass with i.i.d. couplings J_{ij} which assume two possible values ± 1 with probability 1/2. The annealed approximation of the free energy density is

$$f_a(\beta) = -\frac{1}{\beta}\ln 2 - \frac{d}{\beta}\ln\cosh(\beta) \tag{4.14}$$

We remark that this annealed approximation gives the correct free energy density (4.3) in one dimension. This is at variance with the Gaussian case, where the correct free energy in one dimension is recovered only after that the Lagrangian multiplier is introduced. One would be tempted to improve this result using an intensive variable A_N of the type in (4.8) with α depending on a single coupling J_{ij}. Unfortunately, a direct calculation shows that no improvement is possible following this choice. To improve this result it is necessary to make a choice of variables α depending on more than a single coupling. A possibility (first proposed in ref. 9) is to introduce variables α associated with the single square plaquette frustration. With this choice the intensive variable A_N is

$$\sum_p \tilde{J}_p \tag{4.15}$$

where the $\tilde{J}_p$ are the products of the four couplings of each plaquette. The sums run over all plaquettes of the d-dimensional spin glass ($d \geqslant 2$) or on a part of them. The associated generalized partition function is

$$Z_N(\beta, \mu) = \sum_{\{\sigma\}} \exp\left(\sum_{\langle ij\rangle} \beta J_{ij}\sigma_i\sigma_j + \sum_p \mu\tilde{J}_p\right) \tag{4.16}$$

We now take the average of this generalized partition function. Taking into account that the couplings are dichotomic with equal probability, we can perform the transformation $J_{ij} \to J_{ij}\sigma_i\sigma_j$ which leaves unchanged the $\tilde{J}_p$ ($\tilde{J}_p \to \tilde{J}_p$). The averaged partition function is

$$\mathbb{E}[Z_N(\beta, \mu)] = 2^{|A_N|}\mathbb{E}\left[\exp\left(\sum_{\langle ij\rangle} \beta J_{ij} + \sum_p \mu\tilde{J}_p\right)\right] \tag{4.17}$$

This expression (which is meaningful for any dimension $d \geqslant 2$) cannot be computed exactly if the sum goes over all plaquettes. However, the above expression remains meaningful if the sum is restricted on a subset of the plaquettes. Our proposal is to consider the $d = 2$ case and restrict ourselves to one-half of the plaquettes, to be chosen in order that they do not share couplings (say, the white plaquettes of a chessboard). With this choice the above expectation contains a sum over products of $\mathcal{N}_N$ independent variables (corresponding to the $\mathcal{N}_N$ white plaquettes in Λ_N) and can be rewritten as

$$\mathbb{E}[Z_N(\beta, \mu)] = 2^{|\Lambda_N|}\mathbb{E}[\exp\{\beta(J_1 + J_2 + J_3 + J_4) + \mu J_1 J_2 J_3 J_4\}]^{\mathcal{N}_N} \tag{4.18}$$

where J_1, J_2, J_3, and J_4 are the couplings of one of the plaquettes and equal ± 1 with probability 1/2. This expectation is easily computed and, after having taken the thermodynamic limit [taking into account that $\lim_{N\to\infty}(\mathcal{N}_N/|\Lambda_N|) = 1/2$] and maximizing with respect to μ, one obtains

$$g(\beta) = -\frac{3}{4\beta}\ln 2 - \frac{1}{4\beta}\ln\cosh 2\beta - \frac{1}{4\beta}\ln[(\cosh 2\beta)^2 + 1] \tag{4.19}$$

This $d = 2$ constrained annealed free energy improves the annealed estimate (4.14). The functions $f_a(\beta)$ in (4.14) and $g(\beta)$ in (4.20) are plotted for $d = 2$ in Fig. 2. We see that, at variance with the annealed case, the entropy remains positive when the temperature approaches zero and the improvement is therefore relevant. The ground-state energy estimate is

$$E_0 \geqslant \sup_\beta g(\beta) \geqslant g(\beta = \infty) = -1.5 \tag{4.20}$$

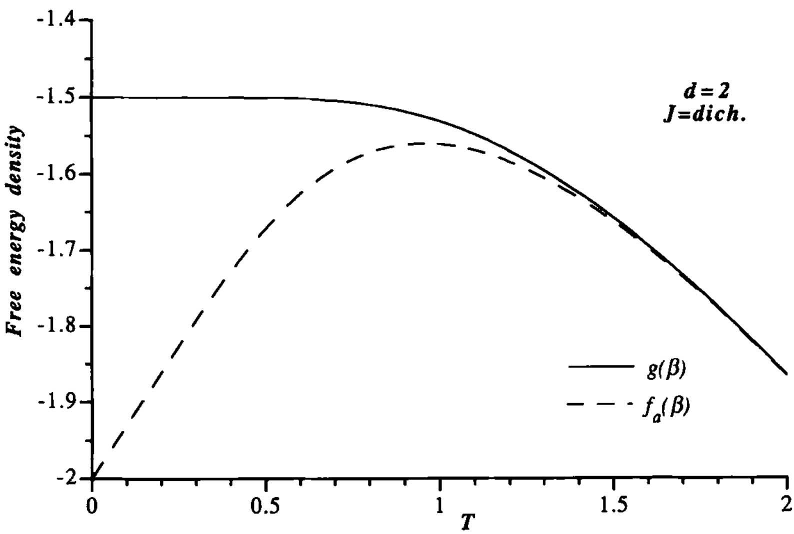

Fig. 2. Dichotomic couplings: the annealed (– –) and constrained (—) free energy densities in $d = 2$ versus $T = 1/\beta$.

The analogous $d=2$ estimate obtained from $f_a(\beta)$ in (4.14) gives $E_0 \geqslant -1.56$. These results can be usefully compared with the numerical or finite-volume estimate $E_0 = -1.404 \pm 0.002$.[18]

It is not immediately evident that our approach can be repeated in any dimension $d>2$, i.e., that it is possible to find a way of grouping the couplings in independent elementary plaquettes. In three dimensions, after some reasoning and some experiments, one becomes convinced that this is in fact possible. The only difference is that the number of plaquettes is 3/2 larger than in the $d=2$ case. These considerations lead to the expression for the $d=3$ constrained free energy density:

$$g(\beta) = -\frac{5}{8\beta}\ln 2 - \frac{3}{8\beta}\ln\cosh 2\beta - \frac{3}{8\beta}\ln[(\cosh 2\beta)^2 + 1] \qquad (4.21)$$

which is shown in Fig. 3. In this case the estimate (4.21) is rather unsatisfactory, since $g(\beta)$ is unphysical at low temperature because the entropy becomes negative. The ground-state energy is estimated by the supremum of (4.21) as $E_0 \geqslant -1.939$.

However, we shall see in the next subsection that this bound for the $d=3$ case can be improved by choosing a more clever strategy.

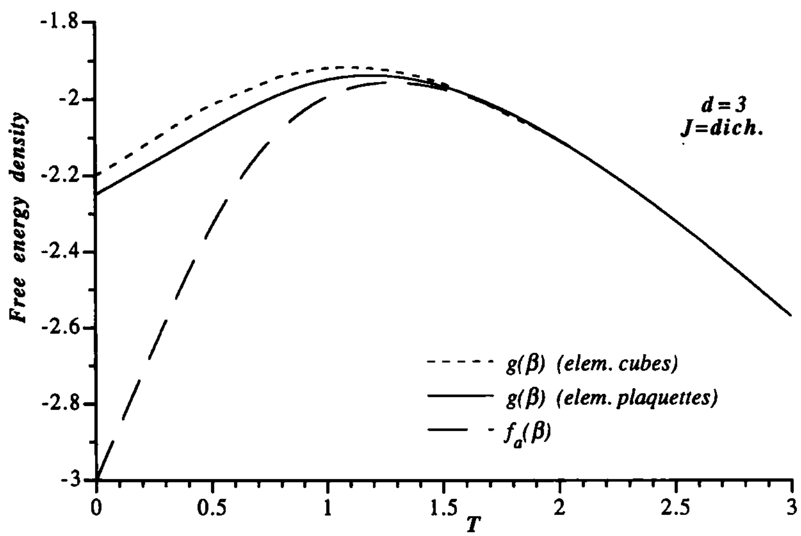

Fig. 3. Dichotomic couplings: the annealed (– –) and two constrained free energy densities in $d=3$ versus $T=1/\beta$. These constraints are related, respectively, to square plaquettes (—) and to unitary cubes (- - -).

4.3. Dichotomic Couplings in Three Dimensions

In this subsection we consider again a finite cube Λ_N in $\mathbb{Z}^3$ and dichotomic couplings $J_{ij} = \pm 1$ (with probability 1/2) between nearest neighbors.

Let $\mathscr{E}(\Lambda_N)$ denote the set of all the edges of Λ_N. An edge of Λ_N will be called internal if at least one of its vertices is an internal point of Λ_N (a point being internal if its nearest neighbors are all in Λ_N). We select a subset $E_N \subset \mathscr{E}(\Lambda_N)$ in the following way. Each internal edge of Λ_N belongs to E_N. Moreover, E_N also contains boundary edges (i.e., edges of Λ_N which are not internal) in such a way that it must be possible to write E_N as the union of the edges of $\mathcal{N}_N$ unitary cubes with vertices in Λ_N having no common edge. We shall consider only couplings related to edges of E_N. Notice that this decomposition of E_N into cubes generalizes the $d=2$ chess-board-type selection of plaquettes used in the previous subsection. We introduce in the notation of the couplings a new index (k) specifing the unitary cube to which they belong: $J_{ij}^{(k)}$ means that the coupling J_{ij} belongs to the kth unitary cube $(k = 1,..., \mathcal{N}_N)$.

Our goal is to compute an annealed average of the partition function Z_N with constraints over all the possible quantities of the kind

$$A_s = \sum_{k=1}^{\mathcal{N}_N} \prod_{L_s} J_{ij}^{(k)} \tag{4.22}$$

with $\mathbb{E}[A_s] = 0$, where L_s is a closed loop inside a unitary cube. As a consequence, $\prod_{L_s} J_{ij}^{(k)}$ can be thought of as the frustration computed along the closed loop L_s of the kth cube. Therefore the average of the generalized partition function is

$$\mathbb{E}\left[Z_N \exp\left(\sum_s \mu_s A_s\right)\right] = \sum_{\{\sigma\}} \mathbb{E}\left[\exp\left(\beta \sum_{\langle ij\rangle} J_{ij}^{(k)}\sigma_i\sigma_j + \sum_s \mu_s A_s\right)\right] \tag{4.23}$$

Recalling (4.22) and the trick used in Section 4.2, i.e., the transformation $J_{ij} \to J_{ij}\sigma_i\sigma_j$, we can factorize the right-hand side of the previous relation among the cubes, so that one has

$$\mathbb{E}\left[Z_N \exp\left(\sum_s \mu_s A_s\right)\right] = \left\{\mathbb{E}\left[Z_{\text{cube}} \exp\left(\sum_s \mu_s \prod_{L_s} J_{ij}\right)\right]\right\}^{\mathcal{N}_N} \tag{4.24}$$

where now $\{J_{ij}\}$ are the 12 couplings of a single unitary cube in the lattice, and Z_{cube} is the partition function of this cube.

The resulting constrained annealed free energy densities is

$$g(\beta) = -\frac{1}{\beta}\left(\lim_{N\to\infty}\frac{\mathcal{N}_N}{|\Lambda_N|}\right)\ln\left\{\min_{\{\mu_s\}}\mathbb{E}\left[Z_{\text{cube}}\exp\left(\sum_s \mu_s \prod_{L_s} J_{ij}\right)\right]\right\} \tag{4.25}$$

A moment of reflection shows that $\lim_{N\to\infty}(\mathcal{N}_N/|\Lambda_N|) = 1/4$. We have therefore changed our problem into the computation of a quantity limited to a single unitary cube of the lattice.

Let us consider five faces of the unitary cube, numbered from 1 to 5. Moreover, we introduce the frustrations $\{\tilde{J}_i\}$ related to these squares, that is, the products of the four couplings of each face.

Any generic closed loop L_s inside the cube can be thought of as the contour of an appropriate subset of these five faces, and the frustration along the loop L_s can be expressed as

$$\prod_{L_s} J_{ij} = \prod_{i=1}^{5} \tilde{J}_i^{s_i} \tag{4.26}$$

where $s_i \in \{0, 1\}$ indicates if the ith face belongs ($s_i = 1$) or not ($s_i = 0$) to the subset that built up the loop L_s. The relation between the $\{s_i\}$ and the index s can be established by

$$s = \sum_{i=1}^{5} s_i 2^i \tag{4.27}$$

As a consequence, we have 31 different closed loops inside the cube (indeed the topologically different loops are only 8). The case $s = 0$ means no loop.

The five frustrations $\{\tilde{J}_i\}$ turn out to be a set of independent dichotomic random variables ($\tilde{J}_i = \pm 1$ with probability 1/2) that can fully describe the system of a single unitary cube. In fact the partition function Z_{cube} reads

$$Z_{\text{cube}} = 2^8[\cosh(\beta)]^{12} \sum_{s=0}^{31} [\tanh(\beta)]^{l_s} \prod_{i=1}^{5} \tilde{J}_i^{s_i} \tag{4.28}$$

where l_s is the length of the loop L_s. Indeed, by virtue of the dichotomic nature of the variables $\{\tilde{J}_i\}$, Z_{cube} can be written as

$$Z_{\text{cube}} = \exp\left(\sum_{s=0}^{31} a_s \prod_{i=1}^{5} \tilde{J}_i^{s_i}\right) \tag{4.29}$$

where the coefficients $\{a_s\}$ are defined by

$$a_k = \mathbb{E}\left[\left(\prod_{i=1}^{5} \tilde{J}_i^{k_i}\right) \ln Z_{\text{cube}}\right] \tag{4.30}$$

with $k=\sum_{i=1}^{5} k_i 2^i$. As a consequence, the nontrivial part of (4.25) becomes

$$\min_{\{\mu_s\}} \mathbb{E}\left[Z_{\text{cube}} \exp\left(\sum_s \mu_s \prod_{L_s} J_{ij}\right)\right] = \min_{\{\mu_s\}} \mathbb{E}\left[\exp\left\{a_0 + \sum_{s=0}^{31} (a_s+\mu_s) \prod_{i=1}^{5} \mathcal{J}_i^{s_i}\right\}\right] \tag{4.31}$$

A moment of reflection shows that the minimum is reached for

$$\mu_s = -a_s \qquad \forall s \in \{1,..., 31\} \tag{4.32}$$

so that

$$\min_{\{\mu_s\}} \mathbb{E}\left[Z_{\text{cube}} \exp\left(\sum_s \mu_s \prod_{L_s} J_{ij}\right)\right] = \exp(a_0) = \exp(\mathbb{E}[\ln Z_{\text{cube}}]) \tag{4.33}$$

Coming back to $g(\beta)$, one obtains

$$g(\beta) = -\frac{1}{4\beta} \mathbb{E}[\ln Z_{\text{cube}}] = 2\, \mathbb{E}[f_{\text{cube}}(\beta)] \tag{4.34}$$

where $\mathbb{E}[f_{\text{cube}}(\beta)]$ is the quenched free energy density of a random system formed by a single unitary cube of the lattice, which has a long expression, but can be exactly computed. This permits us to recover $g(\beta)$, the annealed free energy density of the whole three-dimensional spin glass with constraints on the frustrations inside the unitary cubes, which is shown in Fig. 3. Indeed, this new quantity is unphysical, too, at low temperature (negative entropy), but its supremum with respect to β gives a better estimate of the ground-state energy density: $E_0 \geqslant -1.917$.

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