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Origins, models and motivations

Abstract

We introduce the basic spin glass models, namely the Edwards– Anderson model on a finite-dimensional lattice with short-range interaction and the Sherrington–Kirkpatrick model on the complete graph. The quenched equilibrium state which is used to describe the thermodynamical properties of a general disordered system is defined, together with the concept of real replicas. The notion of meanfield for a spin glass model is discussed. Finally, the original computations for the Sherrington–Kirkpatrick model based on the replica method are presented – namely the replica symmetric solution and the Parisi replica symmetry breaking scheme.

1.1 The spin glass problem

Spin glass models have been considered in different scientific contexts, including experimental condensed matter physics, theoretical physics, mathematical statistical physics and, more recently, probability. They have also been used to solve problems in fields as diverse as theoretical computer science (combinatorial optimization, traveling salesman, Boolean satisfiability, number partitioning, random assignment, error correcting codes, etc.), biology (Hopfield model), population genetics (hierarchical coalescence), and the economy (modelization of financial markets). Thus spin glasses represent a true example of a multi-disciplinary topic.

The study of spin glasses began after experiments on magnetic alloys, for instance metals like Fe, Mn and Cr weakly diluted in metals such as Au, Ag and Cu. It was observed that their thermodynamical behavior was not compatible with the theory of ferromagnetism and showed peculiar dynamical out-of-equilibrium

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Cambridge University Press & Assessment 978-0-521-76334-9 — Perspectives on Spin Glasses Pierluigi Contucci, Cristian Giardinà Excerpt More Information

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properties such as aging and rejuvenation effects (for a recent account of spin glass dynamics and connection to experimental data see Cugliandolo and Kurchan (2008)). The experiments motivated the introduction of an Ising model with random interactions by Edwards and Anderson (1975). To simplify the model, and in the quest of a solvable model, a mean-field version was proposed by Sherrington and Kirkpatrick (1975). The mean-field theory was fully developed by G. Parisi, who proposed an ansatz to solve the problem exactly. Nowadays that theory is called *replica symmetry breaking* or *mean-field spin glass theory*. It revealed both unconventional physical properties and a very rich mathematical structure (Mézard *et al.* (1987)). In recent times some features of the theory have received a rigorous mathematical proof, in particular the computation of the free energy density in the thermodynamic limit due to Guerra (2003) and Talagrand (2006).

For the time being there is no consensus on the virtues of the mean-field Parisi solution in describing the behavior of magnetic alloys. While numerical simulations point to a mean-field behavior of the short-range Edwards–Anderson model on three-dimensional lattices, the mean-field picture has been questioned by the droplet-like picture in theoretical physics (Fisher and Huse (1988)) as well as by the metastate approach in mathematical physics (Newman and Stein (1996, 1998, 2002, 2003b); Newman (1997)).

Despite the lack of consensus about its relevance in condensed matter, in the last three decades the replica symmetry breaking theory has without doubt become a major paradigm in the theory of complex systems. It has been applied in the solution of many applied problems outside the realm of condensed matter physics, and the rich mathematical structure which has emerged from the Parisi solution of the Sherrington–Kirkpatrick (SK) model with non-rigorous techniques has attracted the interest of pure mathematicians and people working on rigorous results.

1.2 Random interactions, finite-dimensional models, mean-field models

The characteristic property of spin glass models is the presence of both positive ferromagnetic and negative antiferromagnetic interactions between the spins. While ferromagnetic couplings force the alignment of the spins in the low temperature phase, antiferromagnetic couplings prefer to anti-align the spins. When all bonds between spins cannot be satisfied, the model is generically said to be frustrated. For a precise definition of the concept of frustration one can look at the original paper by Toulouse (1977); the simplest example of a model containing apparent disorder – which can actually be removed by a gauge transform – is given in Mattis (1976).

Frustration can be realized in *deterministic* systems by properly choosing the couplings. An interesting class of deterministic systems with frustration and consequent glassy behavior is given by the so-called "sine model", introduced in

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Bouchaud and Mézard (1994); Marinari *et al.* (1994a, b) and further studied in Degli Esposti *et al.* (2001, 2003); Contucci *et al.* (2002).

However, the standard spin glass models have *random* interactions. Three distinct classes of models are usually considered:

- *finite-dimensional spin glasses* are defined on a *d*-dimensional lattice (with *d* an integer number) and typically have finite-range interactions among the spins;
- *mean-field spin glasses* are defined on the complete graph with interactions between all pairs (or *k*-tuples, for an integer number *k*) of spins;
- *spin glasses on random graphs* are defined on a random graph with interaction between the spins linked by an edge.

Random graphs constitute a very interesting subject per se. The simplest example is the Erdős–Rényi random graph with edges which are independently present with identical probability. More general random graphs, such as the configuration model or the preferential attachment model, also include dependence structures showing power law degree distribution and small-world effects (see for instance the lecture notes by van der Hofstad (2012)). Spin glasses on random graphs therefore have a double source of randomness, given by the spatial structure where the interaction takes place, and the sign and magnitude of the couplings between spins. They will not be investigated in this book; the interested reader may consult Mézard and Montanari (2009).

In this book we shall focus on the first two classes of spin glass models, showing whenever possible their differences and similarities. We now define the primary examples of each class.

Definition 1.1 (Edwards–Anderson Model) Consider a system in a box $\Lambda \subset \mathbb{Z}^d$ made of interacting spins $\sigma = {\sigma_i}_{i \in \Lambda}$ with $\sigma_i \in {-1, +1}$; the Edwards–Anderson model is defined by the Hamiltonian

$$H_{\Lambda}(\sigma, J) = -\sum_{||i-j||=1} J_{i,j}\sigma_i\sigma_j, \qquad (1.1)$$

where $|| \cdot ||$ denotes Euclidean distance and the couplings $J = \{J_{i,j}\}$ are independent random variables, all having the same distribution, which are assumed to be symmetric with

$$\mathbb{E}\left[J_{i,j}\right] = 0 \qquad \mathbb{E}\left[J_{i,j}^2\right] = 1 \tag{1.2}$$

where $\mathbb{E}[\cdot]$ denotes expectation. Note that the sum in the Hamiltonian is restricted to pairs of nearest-neighbor sites. A straightforward computation based on (1.2) and on independence gives, for the covariance of the Hamiltonian (a family of $2^{|\Lambda|}$

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centered random variables),

$$\mathbb{E}(H_{\Lambda}(\sigma, J)H_{\Lambda}(\tau, J)) = d|\Lambda|Q_{\Lambda}(\sigma, \tau),$$
(1.3)

where $Q_{\Lambda}(\sigma, \tau)$ is the *bond* overlap between two spin configurations σ and τ and is given by

$$Q_{\Lambda}(\sigma,\tau) = \frac{1}{d|\Lambda|} \sum_{||i-j||=1} \sigma_i \sigma_j \tau_i \tau_j.$$
(1.4)

In the case of standard Gaussian distributed interactions $\{J_{i,j}\}$, the previous formula for the covariance completely identifies the model and can be used as an alternative definition.

Remark 1.2 Boundary conditions do matter both in (1.1) and (1.4). This will be analyzed in Chapter 3.

Definition 1.3 (SK model) Consider a system of *N* spins $\sigma = {\sigma_i}_{i \in {1,...,N}}$ with $\sigma_i \in {-1, +1}$; the SK model is defined by the Hamiltonian

$$H_N(\sigma, J) = -\frac{1}{\sqrt{2N}} \sum_{i,j=1}^N J_{i,j} \sigma_i \sigma_j, \qquad (1.5)$$

where, for each couple $(i, j) \in \{1, ..., N\}^2$, the couplings $J = \{J_{i,j}\}$ are a family of independent identical random variables with symmetric distribution, and $\mathbb{E}[J_{i,j}] = 0$ and $\mathbb{E}[J_{i,j}^2] = 1$.

If the couplings $\{J_{i,j}\}$ have a standard Gaussian distribution, then an equivalent definition is that the energy levels of the SK model in the volume $\{1, ..., N\}$ are given by a family of 2^N centered Gaussian random variables with covariance

$$\mathbb{E}(H_N(\sigma, J)H_N(\tau, J)) = \frac{N}{2}q_N^2(\sigma, \tau), \qquad (1.6)$$

where $q_N(\sigma, \tau)$ is the *site* overlap between two spin configurations σ and τ and is given by

$$q_N(\sigma,\tau) = \frac{1}{N} \sum_{i=1}^N \sigma_i \tau_i.$$
(1.7)

In this book we will often work with a general spin glass model which includes (as special cases) both the Edwards–Anderson model and the SK model, as well as other finite-dimensional or mean-field models which will be defined later. If the couplings are chosen to have a Gaussian distribution then it is possible to use

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properties of Gaussian random variables (such as the integration by parts formula) which allow a few simplifications in the computations. The construction of such a model will be discussed in Chapter 2 where a general representation theorem for Gaussian Hamiltonians will be presented. The condition on the model parameters (means and variances of the couplings) for the thermodynamic limit to exist will be analyzed in Chapter 3. Here we limit ourselves to the following definition.

Definition 1.4 (General spin glass model) For a volume $\Lambda \subset \mathbb{Z}^d$ and spins $\sigma_i = \{-1, +1\}$ sitting on every site $i \in \Lambda$, the general spin glass model is defined by the Hamiltonian

$$H_{\Lambda}(\sigma, J) = -\sum_{X \subset \Lambda} J_X \sigma_X, \qquad (1.8)$$

where $\sigma_X = \prod_{i \in X} \sigma_i$ and the couplings $J = \{J_X\}_{X \in \Lambda}$ are independent random variables (with $J_{\emptyset} = 0$).

If those random variables are chosen to have a centered Gaussian distribution with variance $\mathbb{E}(J_X^2) = \Delta_X^2$, then an equivalent definition of the model is given by a family of $2^{|\Lambda|}$ centered Gaussian random variables $H_{\Lambda}(\sigma, J)$ with covariance

$$\mathbb{E}(H_{\Lambda}(\sigma, J)H_{\Lambda}(\tau, J)) = \mathcal{C}(\sigma, \tau) = |\Lambda|c_{\Lambda}(\sigma, \tau),$$
(1.9)

where $c_{\Lambda}(\sigma, \tau)$ is the *generalized* overlap between the two spin configurations σ and τ and is given by

$$c_{\Lambda}(\sigma,\tau) = \frac{1}{|\Lambda|} \sum_{X \subset \Lambda} \Delta_X^2 \sigma_X \tau_X.$$
(1.10)

Remark 1.5 By Schwartz' inequality, $|c_{\Lambda}(\sigma, \tau)| \leq c_{\Lambda}(\sigma, \sigma)$. A sufficient condition to guarantee existence of the thermodynamic limit is $\sup_{\Lambda} c_{\Lambda}(\sigma, \sigma) \leq \bar{c} < +\infty$ (see Section 3.2). Without loss of generality we will often assume that $c_{\Lambda}(\sigma, \sigma) = 1$.

Remark 1.6 The Edwards–Anderson model and the SK model correspond to special choices of the volume Λ and of the centered couplings J_X in the general spin glass model. Namely:

- 1. Definition 1.1 is recovered with the choice: $\Lambda \subset \mathbb{Z}^d$, and $\Delta_X = 1$ for X = (i, j) with $(i, j) \in \mathbb{Z}^d \times \mathbb{Z}^d$ and ||i j|| = 1, and $\Delta_X = 0$ otherwise.
- 2. Definition 1.3 is recovered with the choice: $\Lambda = \{1, ..., N\}$, and $\Delta_X = \frac{1}{\sqrt{2N}}$ for X = (i, j) with $(i, j) \in \{1, ..., N\}^2$, and $\Delta_X = 0$ otherwise.

Note however that the differences between finite-range interactions (constant variances Δ_X^2) and infinite-range interactions (variances Δ_X^2 depend on the volume)

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could imply substantial differences a priori on the thermodynamic properties in the large-volume limit.

1.3 Quenched measure and real replicas

The description of the thermodynamic properties of a disordered system with a random Hamiltonian requires the introduction of the *quenched state* notion. In spin glasses, the timescale of the spin variables' relaxation was observed to be much shorter than that of the interaction variables. This dynamical feature led physics to consider the interaction coefficient as *frozen* with respect to the spin ones. A proper mathematical formulation is then obtained by first averaging over the spin variables and computing the Boltzmann–Gibbs expectations, and then averaging over the disorder.

Definition 1.7 (Quenched expectation) For a random Hamiltonian of the form (1.8) on the volume Λ and a random (i.e. possibly depending on the *J*) function $f: \Sigma_{\Lambda} \to \mathbb{R}$ with $\Sigma_{\Lambda} = \{-1, +1\}^{|\Lambda|}$, the expectation with respect to the *random* Boltzmann–Gibbs measure at inverse temperature $\beta \ge 0$ is given by

$$\omega_{\Lambda,\beta}(f) = \frac{\sum_{\sigma \in \Sigma_{\Lambda}} f(\sigma) \exp\left[-\beta H_{\Lambda}(\sigma, J)\right]}{\sum_{\sigma \in \Sigma_{\Lambda}} \exp\left[-\beta H_{\Lambda}(\sigma, J)\right]}.$$
(1.11)

Averaging over the disorder, one obtains the quenched expectation, denoted by

$$\langle f \rangle_{\Lambda,\beta} = \mathbb{E} \left[\omega_{\Lambda,\beta}(f) \right].$$
 (1.12)

Remark 1.8 To alleviate the notation, we will not always write explicitly the volume- or temperature-dependence of either the random Boltzmann–Gibbs expectations or the quenched expectations.

Moreover, it is useful to distinguish between random thermodynamic observables and their quenched average. The fundamental thermodynamical quantity is the pressure (which gives up to a factor $1/\beta$ the negative of the free energy).

Definition 1.9 (Pressure) We define the random partition function

$$\mathcal{Z}_{\Lambda}(\beta) = \sum_{\sigma \in \Sigma_{\Lambda}} \exp\left[-\beta H_{\Lambda}(\sigma, J)\right], \qquad (1.13)$$

the random pressure

$$\mathcal{P}_{\Lambda}(\beta) = \log \mathcal{Z}_{\Lambda}(\beta) \tag{1.14}$$

and the quenched pressure

$$P_{\Lambda}(\beta) = \mathbb{E}\left[\mathcal{P}_{\Lambda}(\beta)\right]. \tag{1.15}$$

1.3 Quenched measure and real replicas

Remark 1.10 In the above definition we assume *free boundary conditions*. We will return to the choice of boundary conditions in Chapter 3, where we will show that they do not matter for the thermodynamic limit of the pressure and we will analyze the effect of them on the surface pressure in Section 3.8.

The generalized overlap in Eq. (1.10) is the main observable of spin glass theory. Indeed the standard thermodynamic quantities can be expressed in terms of the quenched expectation of the generalized overlaps among copies of the system, called *real replicas*, all subject to the same disorder. It is thus useful to introduce the product random Boltzmann–Gibbs state over real replicas and the corresponding quenched state.

Definition 1.11 (Real replicas) For a random Hamiltonian of the form (1.8) on the volume Λ and a random function $f: \Sigma_{\Lambda}^{R} \to \mathbb{R}$, the expectation with respect to the *R*-product random Boltzmann–Gibbs state (with *R* being an integer) is

$$\Omega_{\Lambda,\beta}(f) = \sum_{\{\sigma^{(1)},\dots,\sigma^{(R)}\}\in\Sigma_{\Lambda}^{R}} \frac{f(\sigma^{(1)},\dots,\sigma^{(R)})e^{-\beta[H_{\Lambda}(\sigma^{(1)},J)+\dots+H_{\Lambda}(\sigma^{(R)},J)]}}{[\mathcal{Z}_{\Lambda}(\beta)]^{R}}, \quad (1.16)$$

The quenched expectation is then

$$\langle f \rangle_{\Lambda,\beta} = \mathbb{E} \left[\Omega_{\Lambda,\beta}(f) \right].$$
 (1.17)

We now show how the concept of real replicas, which might seem artificial at first sight, naturally arises in the expression of the main thermodynamic quantities in the context of Gaussian spin glass models. Consider, for instance, the *internal energy* given by:

$$U_{\Lambda}(\beta) = -\frac{dP_{\Lambda}}{d\beta}(\beta) = \mathbb{E}(\omega_{\Lambda,\beta}(H_{\Lambda})).$$
(1.18)

Using the integration by parts formula for a set of centered Gaussian random variables $X = (X_1, ..., X_k)$ with covariances $a_{i,j} = \mathbb{E} [X_i X_j]$, namely

$$\mathbb{E}(X_i f(X)) = \sum_{j=1}^n a_{i,j} \mathbb{E}\left(\frac{\partial f}{\partial x_j}(X)\right), \qquad (1.19)$$

and assuming $c_{\Lambda}(\sigma, \sigma) = 1$, one obtains the following expression for the internal energy:

$$U_{\Lambda}(\beta) = -\beta |\Lambda| \langle 1 - c_{1,2} \rangle_{\Lambda,\beta}, \qquad (1.20)$$

with

$$\langle c_{1,2} \rangle_{\Lambda,\beta} = \mathbb{E} \left[\sum_{\{\sigma^{(1)}, \sigma^{(2)}\} \in \Sigma_{\Lambda}^{2}} c_{\Lambda}(\sigma^{(1)}, \sigma^{(2)}) \frac{e^{-\beta [H_{\Lambda}(\sigma^{(1)}, J) + H_{\Lambda}(\sigma^{(2)}, J)]}}{[\mathcal{Z}_{\Lambda}(\beta)]^{2}} \right].$$
(1.21)

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Another example is the specific heat

$$C_{\Lambda}(\beta) = -\beta^2 \frac{dU_{\Lambda}}{d\beta}(\beta) = \beta^2 \mathbb{E} \Big[\omega_{\Lambda,\beta} \Big(H_{\Lambda}^2 \Big) - \omega_{\Lambda,\beta}^2(H_{\Lambda}) \Big].$$
(1.22)

As for the internal energy, now using integration by parts twice, one obtains the following result:

$$C_{\Lambda}(\beta) = \beta^2 |\Lambda| \langle 1 - c_{1,2} \rangle_{\Lambda,\beta} - 2\beta^4 |\Lambda|^2 \langle c_{1,2}^2 - 4c_{1,2}c_{2,3} + 3c_{1,2}c_{3,4} \rangle_{\Lambda,\beta}, \quad (1.23)$$

with

$$\langle c_{1,2}c_{2,3} \rangle_{\Lambda,\beta} = \mathbb{E} \left[\sum_{\{\sigma^{(1)},\sigma^{(2)},\sigma^{(3)}\} \in \Sigma_{\Lambda}^{3}} c_{\Lambda}(\sigma^{(1)},\sigma^{(2)})c_{\Lambda}(\sigma^{(2)},\sigma^{(3)}) \right. \\ \left. \times \frac{e^{-\beta[H_{\Lambda}(\sigma^{(1)},J) + H_{\Lambda}(\sigma^{(2)},J) + H_{\Lambda}(\sigma^{(3)},J)]}}{[\mathcal{Z}_{\Lambda}(\beta)]^{3}} \right],$$
(1.24)

and an analogous expression (involving four replicas) for $(c_{1,2}c_{3,4})_{\Lambda,\beta}$.

In the previous formula we used the same bracket symbol as (1.17) in the lefthand sides of (1.21) and (1.24) where the observable f was a function of the spin configurations. The precise meaning of such a small abuse of notation is given by the following:

Definition 1.12 (Generalized overlaps random variables) For any integer $R \ge 1$ the formulas (1.21) and (1.24) and their generalization to arbitrary powers and an arbitrary number R of copies, define the family of random variables $\{c_{l,m}\}$ with $1 \le l < m \le R$ and their joint distribution $p_{lm}^{(\Lambda)}, p_{lm,l'm'}^{(\Lambda)}, \ldots$ via

$$\left\langle c_{1,2}^{k}\right\rangle _{\Lambda} = \int dx x^{k} p_{12}^{(\Lambda)}(x) \tag{1.25}$$

$$\langle c_{1,2}^k c_{2,3}^l \rangle_{\Lambda} = \int dx \int dy x^k y^l p_{12,23}^{(\Lambda)}(x,y)$$
 (1.26)

and similar. What the spin glass theory is interested in is the behavior of the former random variables in the thermodynamic limit whose distribution we will denote by $p_{12}(x)$, $p_{12,23}(x, y)$, etc.

Remark 1.13 We point out that the joint distribution of the overlap random variables is invariant under the action of the permutation group on the set $\{1, ..., R\}$. Denoting the symmetric random matrix with elements $\{c_{l,m}\}$ by *C* and assuming without loss of generality $c_{l,l} = 1$, the invariance under the permutation group is

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expressed by

$$PCP^{-1} \stackrel{\mathcal{D}}{=} C \qquad \text{for all } P,$$
 (1.27)

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where *P* is the matrix associated to a permutation of the set $\{1, 2, ..., R\}$. For example:

$$p_{12}(x) = p_{56}(x), \qquad p_{12,23}(x, y) = p_{13,35}(x, y).$$
 (1.28)

1.4 Definition of a mean-field spin glass

A spin glass model, such as the SK model, was given the name *mean-field* type for reasons of similarity with the Curie–Weiss model of ferromagnetism, in which the spins' interaction space is the complete graph of N vertices and the mutual interaction is invariant with respect to the permutation group. A similar property is also true for the SK model since the interaction space is still the complete graph and the interactions are invariant, in distribution, under the action of the permutation group. The apparent similarity between the two models goes much further and is manifest in the replica symmetric solution of the SK model, to the point that one could think of this model as a random version of the Curie–Weiss model. The similarity goes as follows.

The magnetization of the Curie-Weiss model, defined as

$$m = \lim_{N \to \infty} \omega_N^{(CW)} \left(\frac{1}{N} \sum_{i=1}^N \sigma_i \right)$$
(1.29)

where $\omega_N^{CW}(\cdot)$ denotes expectation with respect to the Boltzmann–Gibbs measure with Hamiltonian

$$H_N^{(CW)}(\sigma) = -\frac{1}{2N} \sum_{i,j=1}^N \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i, \qquad (1.30)$$

satisfies the equation (at positive inverse temperature β)

$$m = \tanh(\beta[h+m]). \tag{1.31}$$

This equation can also be obtained from the mean-field ferromagnetic model with Hamiltonian

$$H_N^{(MF)}(\sigma) = -\sum_{i=1}^N \sigma_i(h+M)$$
 (1.32)

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where M is a parameter representing the average field which is caused by all the other spins and which is required to satisfy the self-consistency equation

$$M = \omega_N^{(MF)} \left(\frac{1}{N} \sum_{i=1}^N \sigma_i \right), \qquad (1.33)$$

with $\omega_N^{(MF)}(\cdot)$ the expectation with respect to the Boltzmann–Gibbs measure with Hamiltonian (1.32). An immediate computation shows that the self-consistency equation (1.33) is equivalent to Eq. (1.31) with $M = m = \lim_{N \to \infty} \omega_N^{(CW)}(\sigma_i)$. Therefore, one usually says that the Curie–Weiss model is the mean-field theory of ferromagnetism.

Considering now the SK model, we will see in Section 1.6 that the original replica symmetric solution yields the following equation for the quenched expectation of the overlap:

$$q = \int d\mu(z) \tanh^2(\beta(h + \sqrt{q}z)), \qquad (1.34)$$

where $d\mu(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} dz$ and

$$q = \lim_{N \to \infty} \left\langle \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tau_i \right\rangle_N^{(SK)} = \lim_{N \to \infty} \mathbb{E} \left(\frac{1}{N} \sum_{i=1}^{N} \left[\omega_N^{(SK)}(\sigma_i) \right]^2 \right), \quad (1.35)$$

with $\langle \cdot \rangle_N^{(SK)}$ denoting the quenched expectation associated to the Hamiltonian

$$H_N^{(SK)}(\sigma) = -\frac{1}{\sqrt{2N}} \sum_{i,j=1}^N J_{i,j} \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i$$
(1.36)

and $\{J_{i,j}\}$ independent and identically distributed (i.i.d.) standard Gaussian random variables. Equation (1.34) can also be obtained from non-interacting spin models of the form

$$\tilde{H}_{N}^{(MF)}(\sigma) = -\sum_{i=1}^{N} \sigma_{i}(h+M_{i})$$
 (1.37)

where each spin σ_i , besides the external field *h*, feels the action of a centered Gaussian random field M_i with covariance

$$\mathbb{E}(M_i M_j) = \delta_{i,j} \bar{M}^2 \tag{1.38}$$

where \overline{M} is determined self-consistently by imposing that

$$\bar{M}^2 = \left\langle \frac{1}{N} \sum_{i=1}^N \sigma_i \tau_i \right\rangle_N^{(MF)}$$
(1.39)