Extended variational principle for the Sherrington-Kirkpatrick spin-glass model

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The recent proof by Guerra that the Parisi ansatz provides a lower bound on the free energy of the Sherrington-Kirkpatrick (SK) spin-glass model could have been taken as offering some support to the validity of the purported solution. In this work we present a broader variational principle, in which the lower bound as well as the actual value are expressed through an optimization procedure for which ultrametric/hierarchal structures form only a subset of the variational class. The validity of Parisi's ansatz for the SK model is still in question. The new variational principle may be of help in critical review of the issue.

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I. INTRODUCTION

The statistical mechanics of spin-glass models is characterized by the existence of a diverse collection of competing states, very slow relaxation of the quenched dynamics, and a rather involved picture of the equilibrium state.

A great deal of insight on the subject has been produced through the study of the Sherrington-Kirkpatrick (SK) model.[1] After some initial attempts, a solution was proposed by Parisi which has the requisite stability and many other attractive features.[2] Its development has yielded a plethora of applications of the method, in which a key structural assumption is a particular form of the replica symmetry breaking (i.e., the assumption of "ultrametricity," or the hierarchal structure, of the overlaps among the observed spin configurations).[3]

Yet to this day it was not established that this very appealing proposal does indeed provide the equilibrium structure of the SK model. A recent breakthrough is the proof by Guerra[4] that the free energy provided by Parisi's purported solution is a rigorous lower bound for the SK free energy.

More completely, the result of Guerra is that for any value of the order parameter, which within the assumed ansatz is a *function*, the Parisi functional provides a rigorous lower bound. Thus, this relation is also valid for the maximizer which yields the Parisi solution.

In this work we present a variational principle for the free energy of the SK model which makes no use of a Parisi-type order parameter, and which yields the result of Guerra as a particular implication. More explicitly, the new principle allows more varied bounds on the free energy, for which there is no need to assume a hierarchal organization of the Gibbs state (e.g., as expressed in the assumed ultrametricity of the overlaps[3]). Guerra's results follow when the variational principle is tested against the Derrida-Ruelle hierarchal probability cascade models (GREM).[5]

This leads us to a question which is not new: is the ultrametricity an inherent structure of the SK mean-field model, or is it only a simplifying assumption. The new variational principle may provide a tool for challenging tests of this issue.

II. THE MODEL

The SK model concerns Ising-type spins, $\sigma=(\sigma_1,\dots,\sigma_N)$, with an *a priori* equidistribution over the values $\{\pm 1\}$, and the random Hamiltonian

$$H_N(\sigma)=\frac{-1}{\sqrt{N}}\sum_{1\leq i<j\leq N} J_{ij}\sigma_i\sigma_j-h\sum_{i=1}^{N}\sigma_i, \tag{1}$$

where $\{J_{ij}\}$ are independent normal Gaussian variables.

Our analysis applies to a more general class of Hamiltonians which includes all the even "p-spin" models.[6,7] Namely,

$$H_N(\sigma)=-K_N(\sigma)-h\sum_{i=1}^{N}\sigma_i \tag{2}$$

with

$$K_N(\sigma)=\sqrt{\frac{N}{2}}\sum_{r=1}^{\infty}\frac{a_r}{N^{r/2}}\sum_{i_1,\dots,i_r=1}^{N} J_{i_1,\dots,i_r}\sigma_{i_1}\cdots\sigma_{i_r}, \tag{3}$$

where all the $\{J_{i_1,\dots,i_r}\}$ are independent normal Gaussian variables (for convenience, the tensor is not assumed here to be symmetric), and $\Sigma_{r=1}^{\infty}|a_r|^2=1$. As in Ref. 7, our argument requires that the function $f(q)=\Sigma_{r=1}^{\infty}|a_r|^2q^r$ be convex on $[-1,1]$.

One may note that $K_N(\sigma)$ form a family of centered Gaussian variables with the covariance

$$\mathbb{E}[K_N(\sigma)K_N(\sigma')]=\frac{N}{2}f(q_{\sigma,\sigma'}), \tag{4}$$

which depends on the spin-spin overlap: $q_{\sigma,\sigma'}=1/N\Sigma_j\sigma_j\sigma_j'$. The standard SK model corresponds to $f(q)=q^2$.

The partition function Z, the quenched free energy F, and what we shall call here the pressure P, are defined as

$$Z_N(\beta,h)=\sum_{\sigma_1,\dots,\sigma_N=\pm 1} e^{-\beta H_N(\sigma)}, \tag{5}$$

$$P_N(\beta,h)=\frac{1}{N}\mathbb{E}[\ln Z_N(\beta,h)]=-\beta F_N(\beta,h), \tag{6}$$

where $\mathbb{E}(-)$ is an average over the random couplings $\{J_{ij}\}$. The thermodynamic limit for the free energy, i.e., the existence of $\lim_{N\to\infty}P_N(\beta,h)=P(\beta,h)$, was recently established by Guerra-Toninelli[8] through a much-awaited argument.

III. THE VARIATIONAL PRINCIPLE

Our variational expression for $P(\beta,h)$ employs a setup which may at first appear strange, but is natural from the cavity perspective, when one considers the change in the total free energy caused by the addition of M spins to a much larger system of size N. The expression for Z_{N+M}/Z_N simplifies in the limit $N\to\infty$, at fixed M. In the following idealized definition one may regard the symbol α as representing the configuration of the bulk. The discreteness seen in the definition $(\Sigma\xi_\alpha)$ is just for the convenience of the formulation of the variational bounds, and not an assumption on the Gibbs state, though such an assumption may well be true. (A more general formulation is possible, but not much is lost by restricting attention to the "ROSt" defined below.)

Definition (random overlap structures). A *random overlap structure* (ROSt) consists of a probability space $\{\Omega,\mu(d\omega)\}$ where for each ω there is associated a system of weights $\{\xi_\alpha(\omega)\}$ and an "overlap kernel" $\{\tilde{q}_{\alpha,\alpha'}(\omega)\}$ such that, for each $\omega\in\Omega$,

(i) $\Sigma_\alpha\xi_\alpha(\omega)<\infty$; (ii) the quadratic form corresponding to $\{\tilde{q}_{\alpha,\alpha'}\}$ is positive definite; (iii) $\tilde{q}_{\alpha,\alpha}=1$, for each α, and hence (by the Schwarz inequality) also $|\tilde{q}_{\alpha,\alpha'}|\leq 1$ for all pairs $\{\alpha,\alpha'\}$.

An important class of ROSt's is provided by the Derrida-Ruelle probability cascade model which is formulated in Ref. 5 (called there GREM).

Without additional assumptions, one may associate to the points in any ROSt two independent families of centered Gaussian variables $\{\eta_{j,\alpha}\}_{j=1,2,\ldots}$ and $\{\kappa_\alpha\}$ with covariances (conditioned on the random configuration of weights and overlaps)

$$\mathbb{E}(\eta_{j,\alpha}\eta_{j',\alpha'}|\tilde{q}_{\alpha,\alpha'})=\tfrac{1}{2}\delta_{j,j'}f'(\tilde{q}_{\alpha,\alpha'}), \tag{7}$$

$$\mathbb{E}(\kappa_\alpha\kappa_{\alpha'}|\tilde{q}_{\alpha,\alpha'})=\tilde{q}_{\alpha,\alpha'}f'(\tilde{q}_{\alpha,\alpha'})-f(\tilde{q}_{\alpha,\alpha'}). \tag{8}$$

The existence of such processes requires positive definiteness of the joint covariance, but that is evident from the following explicit construction in the case that the α's are N vectors, with $q_{\alpha,\alpha'}=\frac{1}{N}\Sigma_j\alpha_j,\alpha'_j$:

$$\eta_{j,\alpha}=\sqrt{\frac{N}{2}}\sum_r\frac{\sqrt{r}a_r}{N^{r/2}}\sum\tilde{J}_{j,i_1,\ldots,i_{r-1}}\alpha_{i_1}\cdots\alpha_{i_{r-1}}, \tag{9}$$

where the second sum is over $i_1,\ldots,i_{r-1}$ which range from 1 to N, and

$$\kappa_\alpha=\sum_r\frac{\sqrt{r-1}a_r}{N^{r/2}}\sum_{i_1,\ldots,i_r=1}^{N}\hat{J}_{i_1,\ldots,i_r}\alpha_{i_1}\cdots\alpha_{i_r}. \tag{10}$$

We shall now denote by $\mathbb{E}(\cdot)$ the combined average, which corresponds to integrating over three sources of randomness: the SK random couplings $\{J_{ij}\}$, the random overlap structure described by the measure $\mu(d\omega)$, and the Gaussian variables $\{\kappa_\alpha\}$ and $\{\eta_{j,\alpha}\}$.

Guided by the cavity picture, we associate with each ROSt the following quantity:

$$G_M(\beta,h;\mu)=\frac{1}{M}\mathbb{E}\left[\ln\left(\frac{\sum_{\alpha,\sigma}\xi_\alpha\exp\left(\beta\sum_{j=1}^{M}(\eta_{j,\alpha}+h)\sigma_j\right)}{\sum_\alpha\xi_\alpha\exp(\beta\sqrt{M/2}\kappa_\alpha)}\right)\right], \tag{11}$$

where $\sigma=(\sigma_1,\ldots,\sigma_M)$

Our main result is the following:

Theorem 1. (i). For any finite M,

$$P_M(\beta,h)\leq\inf_{(\Omega,\mu)}G_M(\beta,h;\mu)\leq P_U(\beta,h), \tag{12}$$

where the infimum is over ROSt's and $P_U(\beta,h)$ denotes the free energy $\times(-\beta)$ obtained through the Parisi "ultrametric" (or "hierarchal") ansatz. (ii). The infinite volume limit of the free energy satisfies

$$P(\beta,h)=\lim_{M\to\infty}\inf_{(\Omega,\mu)}G_M(\beta,h;\mu). \tag{13}$$

Proof. These results can be seen as consisting of two separate parts: lower and upper bounds, which are derived by different arguments.

(i). The upper bound: The left inequality in Eq. (12) employs an interpolation argument which is akin to that used in the analysis of Guerra,[4] but which here is formulated in broader terms without invoking the ultrametric ansatz. The second inequality in Eq. (12) holds since the Parisi calculation represents the restriction of the variation to the subset of hierarchal ROSt's.

To derive the first inequality let us introduce a family of Hamiltonians for a mixed system of M spins $\sigma=(\sigma_1,\ldots,\sigma_M)$ and the ROSt variables α, with a parameter $0\leq t\leq 1$:

$$-H_M(\sigma,\alpha;t)=\sqrt{1-t}\left(K_M(\sigma)+\sqrt{\frac{M}{2}}\kappa_\alpha\right)+\sqrt{t}\sum_{j=1}^{M}\eta_{j,\alpha}\sigma_j+h\sum_{j=1}^{M}\sigma_j, \tag{14}$$

and let

$$R_M(\beta,h;t)=\frac{1}{M}\mathbb{E}\left[\ln\left(\frac{\sum_{\alpha,\sigma}\xi_\alpha e^{-\beta H_M(\sigma,\alpha;t)}}{\sum_\alpha\xi_\alpha e^{\beta\sqrt{M/2}\kappa_\alpha}}\right)\right]. \tag{15}$$

Then

$$R_M(\beta,h;0)=P_M(\beta,h), \tag{16}$$

$$R_M(\beta,h;1)=G_M(\beta,h;\mu), \tag{17}$$

and we shall show that $\frac{d}{dt}R_M(\beta,h;t)\geqslant 0$.

We use the following notation for replica averages over pairs of spin and ROSt variables. For any $X=X(\sigma,\alpha)$ and $Y=Y(\sigma,\alpha;\sigma',\alpha')$:

$$\mathbb{E}_t^{(1)}(X)=\mathbb{E}\left(\sum_{\alpha,\sigma} w(\sigma,\alpha;t)X\right),$$

$$\mathbb{E}_t^{(2)}(Y)=\mathbb{E}\left(\sum_{\alpha,\sigma}\sum_{\alpha',\sigma'} w(\sigma,\alpha;t)w(\sigma',\alpha';t)Y\right) \tag{18}$$

with the "Gibbs weights"

$$w(\sigma,\alpha;t)=\xi_\alpha e^{-\beta H_M(\sigma,\alpha;t)}/\sum_{\alpha,\sigma}\xi_\alpha e^{-\beta H_M(\sigma,\alpha;t)}. \tag{19}$$

We now have

$$\frac{d}{dt}R_M(\beta,h;t)=-\frac{\beta}{M}\mathbb{E}_t^{(1)}\left(\frac{d}{dt}H_M(\sigma,\alpha;t)\right). \tag{20}$$

The term $\frac{d}{dt}H_M(\sigma,\alpha;t)$ includes Gaussian variables, and one may apply to it the generalized Wick's formula (Gaussian integration by parts) for correlated Gaussian variables, $X_1,\ldots,X_n$:

$$\mathbf{Av}[X_1\psi(X_1,\ldots,X_n)] =\sum_{j=1}^{n}\mathbf{Av}(X_1X_j)\mathbf{Av}\left(\frac{\partial\psi(X_1,\ldots,X_n)}{\partial X_j}\right). \tag{21}$$

The result is (after an elementary calculation)

$$-\frac{\beta}{M}\mathbb{E}_t^{(1)}\left(\frac{d}{dt}H_M(\sigma,\alpha;t)\right)=\frac{\beta^2}{4}\mathbb{E}_t^{(2)}(\varphi) \tag{22}$$

with

$$\varphi(\sigma,\alpha;\sigma',\alpha')=[f(q_{\sigma,\sigma'})-f(\tilde{q}_{\alpha,\alpha'})] -(q_{\sigma,\sigma'}-\tilde{q}_{\alpha,\alpha'})f'(\tilde{q}_{\alpha,\alpha'}). \tag{23}$$

Therefore,

$$\frac{d}{dt}R_M(\beta,h;t) =\frac{\beta^2}{4}\mathbb{E}_t^{(2)}([f(q_{\sigma,\sigma'})-f(\tilde{q}_{\alpha,\alpha'})] -(q_{\sigma,\sigma'}-\tilde{q}_{\alpha,\alpha'})f'(\tilde{q}_{\alpha,\alpha'}))\geqslant 0. \tag{24}$$

The last inequality, which is crucial for us, follows from the assumed convexity of *f*. For the SK model, the above expression simplifies to $(\beta^2/4)\ \mathbb{E}_t^{(2)}[(q_{\sigma,\sigma'}-\tilde{q}_{\alpha,\alpha'})^2]$.

Putting the positivity of the derivative together with Eqs. (16) and (17) clearly implies the first bound in Eq. (12).

As was noted earlier, a particular class of random overlap structures is provided by the Derrida-Ruelle probability cascade models (GREM) of Ref. 5, which are parametrized by a monotone function $x:[0,1]\to[0,1]$. These models have two nice features: (i) the distribution of $\{\xi_\alpha\}$ is invariant, except for a deterministic scaling factor, under the multiplication by random factors as in Eq. (11) [consequently the value of $G_M(\ldots,\mu_{x(\cdot)})$ for such ROSt does not depend on M]; (ii) quantities like $G_M(\ldots,\mu_{x(\cdot)})$ can be expressed as the boundary values of the solution of a certain differential equation, which depends on $x(\cdot)$. Evaluated for such models $G_M(\ldots,\mu_{x(\cdot)})$ reproduces the Parisi functional for each value of the order parameter $x(\cdot)$. The Parisi solution is obtained by optimizing (taking the inf) over the order parameter $x(\cdot)$. This relation gives rise to the second inequality in Eq. (12).

(ii) To prove Eq. (13) we need to supplement the first inequality in Eq. (12) by an opposite bound.

Our analysis is streamlined by continuity arguments, which are enabled by the following basic estimate (proven by two elementary applications of the Jensen inequality).

Lemma 2. Let $Z(H)$ denote the partition function for a system with the Hamiltonian $H(\sigma)$, and let $U(\sigma)$ be, for each σ, a centered Gaussian variable which is independent of H. Then

$$0\leqslant\mathbb{E}\left(\ln\frac{Z(H+U)}{Z(H)}\right)\leqslant\frac{1}{2}\mathbb{E}(U^2). \tag{25}$$

Using the above, it suffices to derive our result for interactions with the sum over *r*, in Eq. (3), truncated at some finite value.

A convenient tool is provided by the superadditivity of $Q_N\equiv NP_N$, which was established in the work of Guerra-Toninelli[8] and its extensions.[7,9] The statement is that for the systems discussed here (and in fact a broader class) for each $M,N\in\mathbb{N}$,

$$Q_{M+N}(\beta,h)\geqslant Q_M(\beta,h)+Q_N(\beta,h). \tag{26}$$

The superadditivity was used in Ref. 8 to establish the existence of the limit $\lim_{N\to\infty}P_N$. However, it has a further implication based on the following useful fact.

Lemma 3. For any superadditive sequence $\{Q_N\}$ satisfying Eq. (26) the following limits exist and satisfy

$$\lim_{N\to\infty}Q_N/N=\lim_{M\to\infty}\liminf_{N\to\infty}[Q_{M+N}-Q_N]/M. \tag{27}$$

For our purposes, this yields.

$$\lim_{N\to\infty}P_N=\lim_{M\to\infty}\liminf_{N\to\infty}\frac{1}{M}\mathbb{E}\left(\ln\frac{Z_{N+M}}{Z_N}\right). \tag{28}$$

We now claim, based on an argument employing the cavity picture, that for any *M*,

$$\liminf_{N\to\infty}\frac{1}{M}\mathbb{E}\left(\ln\frac{Z_{N+M}}{Z_N}\right)\geqslant\inf_{(\Omega,\mu)}G_M(\beta,h;\mu), \tag{29}$$

which would clearly imply Eq. (13). The reason for this inequality is that when a block of M spins is added to a much larger "reservoir" of N spins, the change in the free energy is exactly in the form of Eq. (11)—except for corrections whose total contribution to G_M is of order $O(M/N)$. [The spin-spin couplings within the smaller block and the subleading terms from the change $N \mapsto (N+M)$ in Eq. (3).] Thus, the larger block of spins acts as a ROSt.

To see that in detail, let us split the system of $M+N$ spins into $\sigma = (\tilde{\sigma}, \alpha)$, with $\tilde{\sigma} = (\sigma_1, \ldots, \sigma_M)$ and $\alpha = (\sigma_{M+1}, \ldots, \sigma_{M+N})$. With this notation, the interaction decomposes into

$$K_{M+N}(\sigma) = \tilde{K}_N(\alpha) + \sum_{j=1}^{M} \tilde{\eta}_{j,\alpha} \sigma_j + U(\tilde{\sigma}, \alpha), \tag{30}$$

where: (i) $\{\tilde{K}_N(\alpha)\}$ consists of the terms of $K_{M+N}(\sigma)$ which involve only spins in the larger block, (ii) the second summand includes all the terms which involve exactly one spin in the smaller block, and (iii) U consists of the remaining terms of $K_{M+N}(\sigma)$, including the spin-spin interactions within the smaller block.

One should note that $\{\tilde{K}_N(\alpha)\} \neq \{K_N(\alpha)\}$ since, as a consequence of the addition of the smaller block, the terms in $\{\tilde{K}_N(\alpha)\}$ are weighted by powers of $(N+M)$ rather than N, as presented in Eq. (3). By the law of addition of independent Gaussian variables, $\{K_N(\alpha)\}$ [which are of higher variance than $\{\tilde{K}_N(\alpha)\}$] have the same distribution as the sum of independent variables

$$\left\{ \tilde{K}_N(\alpha) + \sqrt{\frac{M}{2}} \kappa_\alpha \right\}, \tag{31}$$

where $\{\kappa_\alpha\}$ are centered Gaussian variables independent of $\tilde{K}_N(\alpha)$. Up to factors $[1 + O(M/N)]$, the covariances of $\{\tilde{\eta}_{j,\alpha}\}$ and $\{\kappa_\alpha\}$ satisfy Eqs. (7) and (8), respectively, and

$$\frac{1}{M} \mathbb{E}[U(\tilde{\sigma}, \alpha)^2] \leq C \frac{M}{N}. \tag{32}$$

Taking

$$\xi_\alpha := \exp\left[\beta \left(\tilde{K}_N(\alpha) + h \sum_{i=1}^{N} \alpha_i \right) \right], \tag{33}$$

we find that Eq. (29) follows by directly substituting the above into Eq. (11) [using Eqs. (25) and (32)].

IV. DISCUSSION

At first glance, the recent result of Ref. 4 may be read as offering some support to the widely shared belief that the Parisi ansatz has indeed provided the solution of the SK model. However, we showed here that the Guerra bound is part of a broader variational principle in which no reference is made to the key assumption of Ref. 2 that in the limit $N \to \infty$ the SK Gibbs state develops a hierarchal organization. The reasons for such an organization, which is equivalently expressed in terms of "ultrametricity" in the overlaps $q_{\sigma,\sigma'}$, are not *a priori* obvious. (A step, approaching the issue from a dynamical perspective, was taken in Ref. 10, but this result has yet to be extended to the interactive cavity evolution.) Our result (12) raises the possibility that perhaps some other organizing principles may lead to even lower upper-bounds. This reinstates the question whether the ultrametricity assumption, which has enabled the calculation of Ref. 2, is correct in the context of the SK-type models.

It should be emphasized, however, that the question is not whether the SK model exhibits replica symmetry breaking at low temperatures. That, as well as many other aspects of the accepted picture, are supported by both intuition and by rigorous results.[11–16] The question concerns the validity of a solution-facilitating ansatz about the hierarchal form of the replica symmetry breaking. The interest in this question is enhanced by the fact that this assumption yields a computational tool with many other applications.[3]

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[1] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975).
[2] G. Parisi, J. Phys. A **13**, 1101 (1980).
[3] M. Mezard, G. Parisi, and M. Virasoro, *Spin Glass Theory and Beyond*, World Scientific Lecture Notes in Physics Vol. 9 (World Scientific, Teaneck, NJ, 1987).
[4] F. Guerra, Commun. Math. Phys. **233**, 1 (2003).
[5] D. Ruelle, Commun. Math. Phys. **108**, 225 (1987).
[6] B. Derrida, Phys. Rev. B **24**, 2613 (1981).
[7] F. Guerra and F. Toninelli, Markov Proc. Rel. Fields **9**, 195 (2003).
[8] F. Guerra and F. Toninelli, Commun. Math. Phys. **230**, 71 (2002).
[9] P. Contucci, M. Degli Esposti, C. Giardina, and S. Graffi, Commun. Math. Phys. **236**, 55 (2003).
[10] A. Ruzmaikina and M. Aizenman (unpublished).
[11] M. Aizenman, J. Lebowitz, and D. Ruelle, Commun. Math. Phys. **112**, 3 (1987).
[12] J. Fröhlich and B. Zegarlinski, Commun. Math. Phys. **112**, 553 (1987).
[13] L.A. Pastur and M.V. Shcherbina, J. Stat. Phys. **62**, 1 (1991).
[14] F.L. Toninelli, Europhys. Lett. **60**, 764 (2002).
[15] M. Talagrand, *Spin Glasses: A Challenge for Mathematicians* (Springer-Verlag, Berlin, 2003).
[16] C. Newman and D. Stein, cond-mat/0301202.