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A Spherical Bound for the Sherrington-Kirkpatrick Model

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Abstract. — We prove existence of a phase transition for the Sherrington-Kirkpatrick model at $\beta = 1$: making use of the domination by the spherical model, we derive a bound for the pressure as well as for the ground state energy.

1. Introduction. The Sherrington-Kirkpatrick (SK) model consists of a set of N binary spins $\sigma_i \in \{-1, +1\}$ with Hamiltonian

$$H_N(\sigma) = -\frac{1}{\sqrt{N}} \sum_{1 \leq i < j \leq N} J_{ij} \sigma_i \sigma_j - \frac{1}{\sqrt{2N}} \sum_{1 \leq i \leq N} J_{ii} \sigma_i^2 \quad (1.1)$$

where the couplings J_{ij} are independent Gaussian random variables with mean zero and unit variance. Compared with the original definition [SK] we have added the second summand in (1.1) which does not depend on σ in the binary case and does not change the results below. The partition function at inverse temperature β and the pressure of the model are the random variables

$$Z_N^{\text{SK}} = \mathbb{E}_\sigma \exp \{-\beta H_N(\sigma)\}, \quad p_N^{\text{SK}} = \frac{1}{N} \log Z_N^{\text{SK}} \quad (1.2)$$

depending on the J_{ij} 's; in (1.2) we have used the notation $\mathbb{E}_\sigma = 2^{-N} \sum_{\sigma \in \{-1, +1\}^N}$ to denote the average over the spin configurations, and we keep the symbol \mathbb{E} for expectations over the couplings J_{ij} .

Among the few mathematical results for this model it is known that, at high temperature, the “quenched” and “annealed” behaviors coincide:

$$p_N^{\text{SK}} \xrightarrow{N \rightarrow \infty} \frac{\beta^2}{4} = \lim_{N \rightarrow \infty} \frac{1}{N} \log \mathbb{E} Z_N^{\text{SK}}. \quad (1.3)$$

Convergence in probability and in L_p , $1 \leq p < \infty$, follows from the fluctuations results of [ALR] or [CN], and convergence with probability one follows using in addition the

concentration property proved in [T] from general considerations, or in [BGP] more directly. On the other hand, the convergence (1.3) cannot hold for large β since the entropy per spin is at most $\log 2$ for binary spins.

In this note we show that the convergence in (1.3) only happens when $\beta \leq 1$ and hence phase transition takes place at $\beta_c = 1$. For this we prove below a (weak) bound for the limit points of p_N^{SK} , which is a self-averaging quantity [PS]. This bound implies another one for the ground state energy.

These bounds reflect the domination of the SK model by the spherical model, where the uniform probability measure E_σ on the N -dimensional hypercube $\{-1, +1\}^N$ is replaced with the uniform probability measure E_η on the sphere

$$\{\eta \in \mathbb{R}^N ; |\eta|^2 := \sum_{i=1}^N \eta_i^2 = N\} .$$

The partition function and pressure of this second model

$$Z_N^{\text{S}} = E_\eta \exp \{-\beta H_N(\eta)\} , \quad p_N^{\text{S}} = \frac{1}{N} \log Z_N^{\text{S}} \quad (1.4)$$

depend only on the eigenvalues of the quadratic form H_N . Spherical models, introduced by Berlin and Kac [BK], are completely solvable in many instances. They are commonly analysed via the method of steepest descent, or more simply via the mean-spherical approximation (i.e., as Gaussian models where the spherical constraint is satisfied in the mean). The asymptotics of (1.4) are studied in [KTJ] and in [Th], but for completeness of this note, we give below a quick derivation of the bound.

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2. Spherical bound and consequences.

The $N \times N$ symmetric matrix M , with coefficients $M_{ij} = \frac{1}{2\sqrt{N}} J_{ij}$ if $i < j$ and $M_{ii} = \frac{1}{\sqrt{2N}} J_{ii}$, has a.s. simple eigenvalues $\lambda_1 < \lambda_2 < \dots < \lambda_N$ with normalized eigenvectors $\phi_1 = (\phi_{1,j})_{j \leq N}, \dots, \phi_N$. Since the distribution of M is invariant under orthogonal transformations, the diagonal matrix Λ of the eigenvalues $\lambda_1, \dots, \lambda_N$ is independent of the orthogonal matrix $\phi = (\phi_1, \dots, \phi_N)$, and we may clearly choose the frame ϕ such that it is uniformly distributed on the set $O(N)$ of orthogonal matrices; in particular one has for any positive measurable function F

$$\mathbb{E}\{F(M)|\Lambda\} = \mathbb{E}_\phi F(\phi\Lambda\phi^t) , \quad \mathbb{P}\text{-a.s.} \quad (2.1)$$

with \mathbb{E}_ϕ the expectation in ϕ uniformly distributed on $O(N)$. This implies that the spherical model dominates the SK model: more precisely, for any fixed binary spin σ , the distribution of the scalar products $(\sigma, \phi_i)_{i \leq N}$ under \mathbb{E}_ϕ is the uniform measure E_η on the sphere, and then

$$\mathbb{E}\{Z_N^{\text{SK}}|\Lambda\} = Z_N^{\text{S}} . \quad \mathbb{P}\text{-a.s.} \quad (2.2)$$

On the other hand, by Wigner's semicircle law, the empirical measure of eigenvalues converges weakly [G]

$$\frac{1}{N} \sum_{k=1}^N \delta_{\lambda_k} \xrightarrow{N \rightarrow \infty} w(\lambda) d\lambda := \frac{2}{\pi} (1 - \lambda^2)^{\frac{1}{2}} \mathbb{1}_{[-1,1]}(\lambda) d\lambda \quad \mathbb{P}\text{-a.s.} \quad (2.3.a)$$

and moreover the maximal and minimal eigenvalues do not deviate [BY]

$$\lim_{N \rightarrow \infty} \lambda_N = - \lim_{N \rightarrow \infty} \lambda_1 = 1. \quad \mathbb{P}\text{-a.s.} \quad (2.3.b)$$

Let us now state our main result which implies non-analyticity of the pressure at $\beta = 1$.

Proposition: a) For all $\beta \geq 1$,

$$\limsup_{N \rightarrow \infty} p_N^{\text{SK}} \leq \beta - \frac{1}{2} \log \beta - \frac{3}{4}. \quad \mathbb{P}\text{-a.s.}$$

b) In particular, $\limsup_{N \rightarrow \infty} p_N^{\text{SK}} < \beta^2/4$ \mathbb{P} -a.s. when $\beta > 1$, though the limit (1.3) holds when $0 \leq \beta \leq 1$.

In fact the bound in a) is equal to the limit of p_N^{S} [Th]. For $\beta > 1$ but close to 1, the bound is larger than the Sherrington-Kirkpatrick solution for the pressure of the SK model, and then it does not prove absence of self-averaging of the Edwards-Anderson order parameter [PS] for these values of β .

Proof. We will prove that

$$\limsup_{N \rightarrow \infty} p_N^{\text{SK}} \leq \inf_{s > \beta} \left\{ s - \frac{1}{2} - \frac{1}{2} \int \log 2(s - \beta\lambda) w(\lambda) d\lambda \right\} \quad \mathbb{P}\text{-a.s.} \quad (2.4)$$

Then, noticing that the function between braces in (2.4) is convex in s , and using the identities

$$\int (s - \beta\lambda)^{-1} w(\lambda) d\lambda = 2\beta^{-2} \left[s - (s^2 - \beta^2)^{\frac{1}{2}} \right] \quad (2.5.a)$$

$$\int \log (s - \beta\lambda) w(\lambda) d\lambda = \beta^{-2} s \left[s - (s^2 - \beta^2)^{\frac{1}{2}} \right] + \log \left(\left[s + (s^2 - \beta^2)^{\frac{1}{2}} \right] / 2 \right) - 1/2 \quad (2.5.b)$$

valid for $s > \beta$, it can be checked that the bound in (2.4) is achieved for $\beta < 1$ at the saddle-point $s = (\beta^2 + 1)/2$ and is equal to $\beta^2/4$, but corresponds to $s = \beta$ when $\beta \geq 1$ and is equal to $\beta - \frac{1}{2} \log \beta - \frac{3}{4}$.

We now prove (2.4). Let $s > s_0 > \beta$; and assume that $\beta\lambda_N \leq s_0$. Then,

$$a_N := \int_{\mathbb{R}^N} \exp \{ \beta \zeta^t \Lambda \zeta - s |\zeta|^2 \} d\zeta = \exp \left\{ \frac{N}{2} \log 2\pi - \frac{1}{2} \log \det 2(s\mathbf{I} - \beta\Lambda) \right\}. \quad (2.6)$$

For $\epsilon \in]0, 1[$, let $v_{N,\epsilon}$ be the Euclidean volume of $\{ \zeta \in \mathbb{R}^N, |\zeta|^2/N \in [1 - \epsilon, 1] \}$. The uniform probability measure on this domain makes the vectors $\eta = \sqrt{N}(\zeta_i/|\zeta|)_{i \leq N}$

and $|\zeta|^2/N$ independent, the first one with distribution \mathbb{E}_η and the second one with mean $m_{N,\epsilon} \in [1-\epsilon, 1]$. Therefore, we have

$$\begin{aligned} a_N &\geq \int \exp \frac{|\zeta|^2}{N} \{\beta\eta^t \Lambda \eta - sN\} \mathbb{1}_{N^{-1}|\zeta|^2 \in [1-\epsilon, 1]} d\zeta v_{N,\epsilon}^{-1} \cdot v_{N,\epsilon} \\ &\geq v_{N,\epsilon} \cdot \mathbb{E}_\eta \exp m_{N,\epsilon} \{\beta\eta^t \Lambda \eta - sN\} \end{aligned}$$

from Jensen inequality for \mathbb{E}_η . Since $s > s_0 \geq \beta\lambda_N$, the last term in braces is negative, the function $m \mapsto \mathbb{E}_\eta \exp m \{\beta\eta^t \Lambda \eta - sN\}$ is decreasing and

$$a_N \geq v_{N,\epsilon} \mathbb{E}_\eta \exp \{\beta\eta^t \Lambda \eta - sN\} = V_{N,\epsilon} \exp \{-Ns\} Z_N^S.$$

Combining (2.6) and the estimate

$$\begin{aligned} v_{N,\epsilon} &= \pi^{N/2} \Gamma(1+N/2)^{-1} N^{N/2} [1 - \exp \frac{N}{2} \log(1-\epsilon)] \\ &= \exp \frac{N}{2} \{\log 2\pi + 1 + \mathcal{O}_\epsilon(1)\} \end{aligned}$$

with some (deterministic) sequence $\mathcal{O}_\epsilon(1)$ going to zero, we obtain finally for $\beta\lambda_N \leq s_0$

$$p_N^S \leq s - \frac{1}{2} - \frac{1}{2N} \sum_{i=1}^N \log 2(s - \beta\lambda_k) + \mathcal{O}_\epsilon(1). \quad (2.7)$$

Letting $b = s - \frac{1}{2} - \frac{1}{2} \int \log 2(s - \beta\lambda) w(\lambda) d\lambda$ we define the following set A_N of couplings $A_N = \{\lambda_N \leq s_0/\beta, \lambda_1 > -2, s - \frac{1}{2} - \frac{1}{2N} \sum_{i=1}^N \log 2(s - \beta\lambda_k) < b + \epsilon\}$. We have

$$\begin{aligned} \mathbb{E} Z_N^{\text{SK}} \mathbb{1}_{A_N} &= \mathbb{E} \mathbb{1}_{A_N} \mathbb{E}(Z_N^{\text{SK}} | \Lambda) \\ &= \mathbb{E} \mathbb{1}_{A_N} Z_N^S \quad (\text{from (2.2)}) \\ &\leq \exp N(b+2\epsilon) \quad \text{for large } N \quad (\text{from (2.7)}), \end{aligned}$$

$$\mathbb{P}(\{p_N^{\text{SK}} \geq b+3\epsilon\} \cap A_N) \leq \exp -N\epsilon$$

and the Borel-Cantelli lemma implies that $\mathbb{P}(\limsup_{N \rightarrow \infty} \{p_N^{\text{SK}} \geq b+3\epsilon\} \cap A_N) = 0$. On the other hand we know from (2.3.a and b) that $\mathbb{P}(\liminf_{N \rightarrow \infty} A_N) = 1$, therefore $\mathbb{P}(\limsup_{N \rightarrow \infty} \{p_N^{\text{SK}} \geq b+3\epsilon\}) = 0$ for all $\epsilon > 0$. We have finally $\limsup_{N \rightarrow \infty} p_N^{\text{SK}} \leq b$ \mathbb{P} -a.s., which shows (2.4).

The statement b) is an obvious consequence of a), except for $\lim_N p_N^{\text{SK}} = \beta^2/4$ if $\beta = 1$; but this follows from convexity of p_N^{SK} in β , from (1.3) and a) for $\beta = 1$. See also [Gu] for the case $\beta = 1$. \blacksquare

Simple entropy considerations yield an improvement of the proposition, which in turn reflects as a bound on the ground state energy (per site)

$$\mathcal{E}_N = \max_{\sigma} \left\{ \frac{-1}{N} H_N(\sigma) \right\} .$$

Following [ALR] note that, since the entropy rate does not exceed $\log 2$, the function $(p_N^{\text{SK}}(\beta) + \log 2)/\beta$ is non-increasing. Hence if some asymptotic upper bound $\bar{p}(\beta)$ for the pressure $p_N^{\text{SK}}(\beta)$ has its tangent line at some $\beta_0 > 0$ which intersect the vertical axis at height $-\log 2$, then this tangent is itself an asymptotic upper bound for $\beta \geq \beta_0$, and its slope is an asymptotic upper bound for \mathcal{E}_N . Taking here $\bar{p}(\beta) = \beta^2/4$ for $\beta \leq 1$ and $\bar{p}(\beta) = \beta - \frac{1}{2} \log \beta - \frac{3}{4}$ for $\beta > 1$ we obtain the following.

Corollary: \mathbb{P} -a.s., $\limsup_{N \rightarrow \infty} \mathcal{E}_N \leq 1 - e^{\frac{1}{2}}/8 = 0.79390 \dots$

and

$$\limsup_{N \rightarrow \infty} p_N^{\text{SK}} \leq (1 - e^{\frac{1}{2}}/8) - \log 2, \quad \beta \geq 4e^{-\frac{1}{2}} .$$

This bound on \mathcal{E}_N numerically improves the bound 0.83 in [ALR], and is slightly better than the bound $(2/\pi)^{1/2} = 0.798 \dots$ given in [S] with the use of Slepian's lemma. We recall that the asymptotic value for the ground state energy predicted from numerical studies is 0.76 (see [MPV], p. 2).

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