Replica trick with real replicas: A way to build in thermodynamic homogeneity

Václav Janiš and Lenka Zdeborová

Institute of Physics, Academy of Sciences of the Czech Republic,
Na Slovance 2, CZ-18221 Praha, Czech Republic

Abstract

We use real replicas to investigate stability of thermodynamic homogeneity of the free energy of the Sherrington-Kirkpatrick (SK) model of spin glasses. Within the replica trick with the replica symmetric ansatz we show that the averaged free energy at low temperatures is not thermodynamically homogeneous. The demand of minimization of the inhomogeneity of thermodynamic potentials leads in a natural way to the hierarchical solution of the Parisi type. Conditions for the global thermodynamic homogeneity are derived and evaluated for the SK and $p$-spin infinite range models.
I. INTRODUCTION

Thermodynamic potentials have to be state variables. It is so if they are thermodynamically homogeneous. Thermodynamic homogeneity means that the densities of thermodynamic potentials depend on the extensive variables only via their densities. This property is usually expressed as the Euler condition $\nu F(T, V, N, \ldots, X_i, \ldots) = F(T, \nu V, \nu N, \ldots, \nu X_i, \ldots)$, where $\nu$ is an arbitrary positive number and $X_i$ exhaust all extensive variables. It is straightforward to obtain from the Euler condition $f \equiv F/V = f(T, 1, N/V, \ldots, X_i/V, \ldots)$. This linear homogeneity condition leads to the existence of the thermodynamic limit independently of boundary conditions and the shape of the volume.

One of the authors recently argued that simple solutions (replica symmetric) of the SK model do not obey thermodynamic homogeneity [1]. Using the TAP approach a hierarchical solution equivalent to the Parisi replica-symmetry breaking (RSB) was derived from the demand of homogeneity, or better from minimizing the inhomogeneity of the averaged free energy.

In this paper we show that the same demand of thermodynamic homogeneity can be implemented into the replica trick for the SK and other mean-field models as scale invariance of the replica index.

II. REPLICA TRICK WITH REAL REPLICAS

The replica trick is used in systems with quenched randomness to overcome averaging of logarithm. The averaged free energy is defined in the replica trick as $\beta F_{av} = - \lim_{n \to 0} (\langle Z^n \rangle_{av} - 1)/n$. To investigate stability of thermodynamic homogeneity we replicate $\nu$ times the original spin space. The averaged free energy of such a replicated system is $\beta F_{\nu} = - \langle \ln Z^n \rangle_{av} / \nu = - \lim_{n \to 0} (\langle [Z^n]_{av} \rangle - 1)/n\nu$. If the limit $n \to 0$ leads to a thermodynamically homogeneous solution the resulting free energy $F_{\nu}$ should be independent of the parameter $\nu$. Hence thermodynamic homogeneity is equivalent to scale invariance of the replica representation, $n \to n\nu$.

We introduce two types of replica indices in the replica trick applied to a $\nu$ times replicated system. Real replicas we denote $a, b = 1, \ldots, \nu$ while $\alpha, \beta = 1, \ldots, n$ we use for the mathematical ones. After averaging over the random spin-spin interactions in the SK model
we obtain at the saddle-point

$$\beta f_{\nu} = \lim_{n \to 0} \frac{1}{n\nu} \left[ \frac{\beta^2 L_{n\nu}}{2} - \ln \text{Tr} \exp \left\{ \beta^2 \sum_{\alpha \leq \beta} \sum_{a \leq b} (Q_{ab})_{\alpha\beta} S_a^a S_b^b + \beta h \sum_{\alpha} \sum_{a} S_a^a \right\} \right].$$  \hspace{1cm} (1)

We denoted $L_{n\nu} = \sum_{\alpha \leq \beta} \sum_{a \leq b} (Q_{ab})_{\alpha\beta}^2 + n\nu/2$. Parameters \((Q_{ab})_{\alpha\beta} = \langle S_a^a S_b^b \rangle\) are determined from saddle point equations [2].

To proceed further with thermal averaging we have to determine symmetry of the matrix \((Q_{ab})_{\alpha\beta}\). We use the replica symmetric ansatz and distinguish only diagonal and off-diagonal elements. The super-diagonal elements are fixed, \((Q_{aa})_{\alpha\alpha} = 1\). Since the elements in the matrix of mathematical replicas are \(\nu \times \nu\) matrices, we can choose one parameter for the off-diagonal elements in the real-replica space even if the indices for the mathematical replicas are equal. We denote \((Q_{a\neq b})_{\alpha\alpha} = q_1\). In the spirit of the replica-symmetric ansatz we choose for the off-diagonal matrix elements in the space of mathematical replicas \((Q_{ab})_{\alpha\beta} = q_0\).

For convenience we denote \(\chi = q_1 - q_0, q = q_0\). It is now a straightforward task to perform averaging over the spin configurations in Eq. (1) using the above parameters. We arrive at

$$f_1(q, \chi; \nu) = -\frac{\beta}{4} (1 - q)^2 + \frac{\beta}{4} (\nu - 1) \chi (2q + \chi) + \frac{\beta}{2} \chi - \frac{1}{\beta \nu} \int_{-\infty}^{\infty} \mathcal{D} \eta \ln \int_{-\infty}^{\infty} \mathcal{D} \lambda \left\{ 2 \cosh \left[ \beta (h + \eta \sqrt{q} + \lambda \sqrt{\chi}) \right] \right\}^\nu.$$  \hspace{1cm} (2)

We used an abbreviation for the Gaussian differential \(\mathcal{D} \phi \equiv d\phi e^{-\phi^2/2}/\sqrt{2\pi}\).

The obtained free energy density depends formally on the scaling parameter \(\nu\). It is clear from the dependence of \(f_1\) on \(\nu\) in Eq. (2) that it actually depends on \(\nu\) if and only if \(\chi > 0\). We obtain easily from the saddle-point equations for \(q\) and \(\chi\) that this happens just below the de Almeida-Thouless instability line. Hence, the replica-symmetric solution becomes thermodynamically inhomogeneous (free energy does not obey the Euler condition) in the spin-glass phase. A thermodynamically inhomogeneous solution is physically unacceptable and has to be amended. The homogeneous free energy should be independent of \(\nu\). The dependence on this parameter is minimized in the saddle point where the free energy \(f_1\) does not depend on \(\nu\) at least locally. That is, we demand \(\partial f_1/\partial \nu = 0\). In the homogeneous state this equality becomes identity, but when we have an inhomogeneous solution this equation just determines an "equilibrium" scaling parameter \(\nu_{eq}\).

Comparing free energy [2] where parameters \(q, \chi\) and \(\nu\) are determined from the saddle-point equations with the Parisi RSB scheme we find equivalence with 1RSB solution [3].
The difference between these two constructions lies in their derivation and motivation. While Parisi arrives at 1RSB solution from the demand of maximality of the free energy, here we derived the saddle-point equations from the effort to restore thermodynamic homogeneity (minimize inhomogeneity). We believe that the latter construction has a more profound physical justification.

The local thermodynamic homogeneity achieved by free energy (2) is not enough to become a thermodynamically consistent solution. It would be if this newly won solution were independent of a new scaling (replicating) of the corresponding spin space. To check whether free energy (2) is homogeneous, i.e., independent of global scalings of the phase space, we write the number of real replicas as a product $\nu = \nu_1 \nu_2$, whereby e.g. $\nu_1$ be determined from stationarity equations resulting from Eq. (2). We then have two types of real replicas. The first one with indices $a, b = 1, \ldots, \nu_1$ determines the 1RSB solution, while the other with indices $a', b' = 1, \ldots, \nu_2$ serves to a replication of the phase space in which free energy $f_1$ was derived. Using again the replica-symmetric ansatz for averaging we obtain only three parameters that we denote $(Q^{a\neq b,a'})_{\alpha\alpha} = q + \chi_1, (Q^{ab,a'\neq b'})_{\alpha\alpha} = q + \chi_2, (Q^{ab,a'b'})_{\alpha\neq\beta} = q$. It is again a straightforward task to derive an explicit representation for the free energy in the $\nu_2$-times replicated spin space leading to Eq. (2). Not surprisingly we find that the resulting free energy formally corresponds to the Parisi 2RSB solution.

We can proceed with phase-space scalings in each higher hierarchical state with $q, \chi_1, \ldots, \chi_K$ and $\nu_1, \ldots, \nu_K$ as order parameters. We would end up with the Parisi full (infinite) RSB scheme. However, this is not the objective of this construction. We should produce at the end a solution that is globally thermodynamically homogeneous, the limit $n \to 0$ is scale independent.

III. GLOBAL THERMODYNAMIC HOMOGENEITY

Determining all the physical parameters $q, \chi_1, \ldots, \chi_K$ and the geometric ones $\nu_1, \ldots, \nu_K$ from the saddle-point equations of the $K$RSB free energy, we are left with the number of hierarchies $K$ as the only free parameter in this construction. This number will be fixed by reaching the global thermodynamic homogeneity. The solution becomes globally homogeneous when the free energy does not decay into a higher nontrivial hierarchy, i.e., when the number of parameters $\chi_1, \ldots, \chi_K$ does not increase when the phase space (replica
FIG. 1: Stability parameters \( \Lambda_1 \) and \( \Lambda_0 \) for a) SK model at \( T/J = 0.25 \) and b) 3-spin model at \( T/J = 0.4 \). Equilibrium \( \nu_{eq} \) is indicated showing that the 1RSB in the SK model is inhomogeneous, while in the \( p \)-spin model is globally homogeneous.

Having the 1RSB free energy \( \langle \rangle \) we have two possibilities how a 2RSB solution with \( \chi_1 > \chi_2 > 0 \) may arise. First, \( \chi \to \chi_2 \) and \( \chi_1 = \chi_2 \) becomes unstable. It happens if

\[
\Lambda_1 = 1 - \beta^2 \left\langle \left\langle \rho_\nu (1 - t^2)^2 \right\rangle_\eta \right\rangle < 0 ,
\]

where we denoted \( t \equiv \tanh \left[ \beta (\eta \sqrt{q} + \sqrt{X}) \right] \), \( \langle X(\lambda) \rangle_\lambda = \int_{-\infty}^\infty D\lambda \; X(\lambda) \) and \( \rho_\nu \equiv \cosh \left[ \beta (\eta \sqrt{q} + \sqrt{X}) \right]/\left\langle \cosh \left[ \beta (\eta \sqrt{q} + \sqrt{X}) \right] \right\rangle_\lambda \). Notice that condition (3a) is formally equivalent to the smallest replicon for 1RSB. Second, \( \chi \to \chi_1 \) and \( \chi_2 = 0 \) becomes unstable, which is the case if

\[
\Lambda_0 = 1 - \beta^2 \left\langle \left[ 1 - \langle \rho_\nu t^2 \rangle_\lambda + \nu \left( \langle \rho_\nu t^2 \rangle_\lambda - \langle \rho_\nu t^2 \rangle_\lambda \right)^2 \right] \right\rangle_\eta < 0 .
\]

Hence free energy \( \langle \rangle \) becomes thermodynamically homogeneous if both numbers \( \Lambda_1 \) and \( \Lambda_0 \) from Eqs. (3) are nonnegative for the equilibrium scaling parameter \( \nu_{eq} \). It is never the case in the SK model but it may happen above the Gardner temperature in the \( p \)-spin infinite-range model as illustrated in Fig. 1. In the \( p \)-spin model the stability parameters are only slightly modified \( \Lambda_1 = 1 - \beta^2 p(p - 1)q_1^{p-2}\langle \ldots \rangle_\eta/2 \), \( \Lambda_0 = 1 - \beta^2 p(p - 1)q_0^{p-2}\langle \ldots \rangle_\eta/2 \). For \( p = 2 \) it is the SK, for \( p > 2 \) there is always \( q_0 = 0 \) leading to \( \Lambda_0 = 1 \) [4].

To conclude, we demonstrated that the demand of thermodynamic homogeneity can be build in into the replica trick as scale invariance of the replica index \( n \). Successive scalings of the replica index lead to a formal dependence of the solution on the scaling parameter. The
replica symmetric solution depends on the scaling parameter virtually only in the spin glass phase and hence gets unstable. The RSB scheme of Parisi simultaneously with conditions for the global homogeneity (scale invariance) are then derived from successive scalings of the replica index by minimizing the incurred inhomogeneity (demanding local homogeneity or scale invariance).

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