LETTER TO THE EDITOR

Cluster derivation of Parisi’s RSB solution for disordered systems

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Abstract. We propose a general scheme in which disordered systems are allowed to sacrifice energy equi-partitioning and separate into a hierarchy of ergodic sub-systems (clusters) with different characteristic time-scales and temperatures. The details of the break-up follow from the requirement of stationarity of the entropy of the slower cluster, at every level in the hierarchy. We apply our ideas to the Sherrington-Kirkpatrick model, and show how the Parisi solution can be derived quantitatively from plausible physical principles. Our approach gives new insight into the physics behind Parisi’s solution and its relations with other theories, numerical experiments, and short range models.

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The Parisi scheme [1] for replica symmetry breaking (RSB) has been one of the most celebrated tools in the description of the ‘glassy’ phase of disordered systems. It was initially proposed as the solution for the Sherrington-Kirkpatrick (SK) model [2] for spin glasses, but it has since then been successfully applied to a wide range of models. The physical interpretation of Parisi’s solution has been the subject of many discussions, and has generated notions such as hierarchies of disparate time-scales [3], effective temperatures [4], low entropy production [5] and nonequilibrium thermodynamics [6, 7]. Central is the idea of multiple temperatures, which are usually defined via the violation of fluctuation-dissipation relations; this often limits studies to very specific models where correlation- and response functions can be calculated explicitly. In this letter, in contrast, we present and derive a general scheme in which disordered systems are allowed to sacrifice full energy equi-partitioning by separating autonomously into a hierarchy of ergodic sub-systems with different characteristic time-scales; the statistics at every level (including effective temperatures) follow from the $\mathcal{H}$-theorem with constrained (i.e. stationary) entropy. When applied to the SK model, our scheme is found to yield the Parisi solution and to generate and connect the above concepts in a transparent way. Our assumptions are simple and natural, and all ingredients of our theory have a clear physical meaning. Our study proceeds in three distinct stages. First we show generally how and why multiple temperatures can arise in disordered systems. We then show how this generates replica theories with nested levels of replication, with dimensions reflecting ratios of temperatures. We apply our ideas to the ‘benchmark’ disordered system, the SK model, and derive Parisi’s solution. We close this letter with numerical evidence for the existence of multiple disparate
time-scales, a summary of the simple physical picture that naturally emerges from our scheme, and a discussion of the points which need further investigation.

To understand the origin of multiple temperatures in a system of stochastic variables \(\sigma = (\sigma_1,\ldots,\sigma_N)\) with Hamiltonian \(H(\sigma)\) and state probabilities (or densities) \(p(\sigma)\), we turn to Boltzmann’s \(H\)-function \(H = \text{Tr}_\sigma p(\sigma) \{ H(\sigma) + T \log p(\sigma) \}\), which decreases monotonically under standard Glauber or Langevin dynamics and is bounded from below by the free energy of the Boltzmann state. For the case where we have two groups of variables (fast vs. slow), i.e. \(\sigma = (\sigma_f,\sigma_s)\), we substitute \(p(\sigma_f,\sigma_s) = p(\sigma_f|\sigma_s)p(\sigma_s)\) and find

\[
H = \text{Tr}_\sigma p(\sigma_s) \{ H_{\text{eff}}(\sigma_s) + T \log p(\sigma_s) \} \tag{1}
\]

\[
H_{\text{eff}}(\sigma_s) = \text{Tr}_{\sigma_f} p(\sigma_f|\sigma_s) \{ H(\sigma_f,\sigma_s) + T \log p(\sigma_f|\sigma_s) \} \tag{2}
\]

In the case where \(\sigma_s\) and \(\sigma_f\) evolve on disparate time-scales, the minimisation of (1) will occur in stages. First, for every (fixed) \(\sigma_s\) the distribution \(p(\sigma_f|\sigma_s)\) of the fast variables will evolve such as to minimize (3), i.e. towards the Boltzmann state

\[
p(\sigma_f|\sigma_s) = Z_{\ell}^{-1}(\sigma_s) e^{-\beta H(\sigma_f,\sigma_s)} \quad Z_{\ell}(\sigma_s) = \text{Tr}_{\sigma_f} e^{-\beta H(\sigma_f,\sigma_s)} \tag{3}
\]

Finding multiple temperatures requires, in addition to disparate time-scales, stationarity of the entropy of the slow system (on the relevant ‘glassy’ time-scales). Now (3) is minimised subject to the constraint that the entropy \(S_s = -\text{Tr}_{\sigma_s} p(\sigma_s) \log p(\sigma_s)\) be kept constant, giving

\[
p(\sigma_s) = Z_{s}^{-1} e^{-\beta_{\text{eff}}(\sigma_s)} \quad Z_{s} = \text{Tr}_{\sigma_s} e^{-\beta_{\text{eff}}(\sigma_s)} \tag{4}
\]

i.e. a Boltzmann state for the slow variables, with the free energy of the fast ones acting as effective Hamiltonian, and at inverse temperature \(\tilde{\beta} = \tilde{m}\beta\). This leads to an \(\tilde{m}\)-dimensional replica theory, since combining (1)(2)(3) gives \(Z_s = \text{Tr}_{\sigma_s} [Z_{\ell}(\sigma_s)]^{\tilde{m}}\). The dimension \(\tilde{m}\) follows from demanding the prescribed value of the slow entropy: \(\tilde{m} \beta \tilde{m}^2 (\partial F_s / \partial \tilde{m}) = S_s\), with \(F_s = -\tilde{\beta}^{-1} \log Z_s\). For \(T > T\) the fast variables would start acting as a heat bath for the slow ones, so thermodynamic stability requires \(\tilde{m} \leq 1\). Note that \(\tilde{m} < 1\) implies that the contraining entropy must be larger than that of the Boltzmann state (indeed, a large characteristic time scale does not imply low entropy).

The above argument can be generalised to an arbitrary hierarchy. The variables \(\sigma_{\ell}\) at each level \(\ell\) are characterised by distinct time-scales and temperatures \(\{\tau_\ell, \beta_\ell\}\) (\(\ell = 0,1,\ldots,L\)); each level being adiabatically slower than the next, \(\tau_\ell \ll \tau_{\ell+1}\). This leads to replicating recursion relations for the partition sums at subsequent levels:

\[
Z_\ell = \text{Tr}_{\sigma_{\ell}} [Z_{\ell+1}]^{\tilde{m}_{\ell+1}} \quad (\ell < L)
\]

\[
Z_L = \text{Tr}_{\sigma_L} e^{-\beta_L H(\sigma)}
\]

with \(\tilde{m}_\ell = \beta_{\ell-1} / \beta_\ell \leq 1\), and \(\beta_L = \beta\). The replica dimensions \(\tilde{m}_\ell\) follow from the prescribed (stationary, but as yet unknown) values \(S_\ell\) of the level-\(\ell\) entropies, via \(\beta_{\ell+1} \tilde{m}_{\ell+1}^2 (\partial F_\ell / \partial \tilde{m}_{\ell+1}) = S_\ell\), with \(F_\ell = -\beta_{\ell}^{-1} \log Z_\ell\). Equivalently, using the specific nesting of the partition functions in (3) one shows that the \(\{\tilde{m}_\ell\}\) are uniquely determined by the identities

\[
\beta_{\ell+1} \tilde{m}_{\ell+1}^2 \frac{\partial}{\partial \tilde{m}_{\ell+1}} F_\ell = \Sigma_\ell \quad \Sigma_\ell = \langle \cdots \langle S_\ell \rangle \rangle_{\ell-1} \cdots \rangle_0 \tag{6}
\]
in which \( \langle \cdots \rangle \) denotes the average over the equilibrated level-\( r \) process. Due to the constrained minimisations underlying (5), the free energies \( F_\ell \) are generally not minimised; however, one can verify that \( F_0 \) still serves as a generator of observables:

\[
H(\{\sigma\}) \rightarrow H(\{\sigma\}) + \lambda \psi(\{\sigma\}) : \quad \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \lambda} F_0 = \langle \psi(\{\sigma\}) \rangle
\]

This generalises a formalism originally developed and applied for spin systems with slowly evolving bonds [9]. The construction reverts back to the conventional statistical mechanical picture if the constraining entropies \( S_k \) are identical to those of the full Boltzmann state: then the constraining forces vanish and \( \tilde{m}_\ell = 1 \) for all \( \ell \).

We now apply this scheme to the SK model [2], for which the Parisi solution was originally constructed, which describes \( N \) Ising spins with the conventional Hamiltonian \( H(\sigma) = -\sum_{i<j} J_{ij} \sigma_i \sigma_j \), but with suitably scaled independent random couplings \( J_{ij} \) (with average \( J_0/N \) and variance \( J/\sqrt{N} \)). We assume, following our previous arguments, that this system can be viewed as a hierarchy of \( L+1 \) levels of spins, each level \( \ell \) with distinct disparate time-scales and temperatures \( \{\tau_\ell, T_\ell\} \):

\[
\{1, \ldots, N\} = \bigcup_{\ell=0}^L I_\ell, \quad \sigma = (\sigma_0, \ldots, \sigma_L), \quad \sigma_\ell = \{\sigma_j | j \in I_\ell\}
\]

with \( |I_\ell| = \epsilon_\ell N \), and such that \( \tau_\ell \propto \tau_{\ell-1} \) for all \( \ell \) (thus larger values of \( \ell \) correspond to faster spins). The selection of time-scales for the spins is expected to depend on the realisation of the couplings, but here we will make the simplest approximation: the system can only choose the relative level sizes \( \{\epsilon_\ell\} \). A study of the autonomous selection of levels will be presented elsewhere [3]. We calculate the disorder-averaged free energy \( \overline{F}_0 \) (the general multi-level generator of observables) with the replica trick

\[
\overline{F}_0 = -\beta_0^{-1} \log \overline{Z}_0 = -\lim_{\tilde{n} \rightarrow 0} (\tilde{n} \beta_0)^{-1} \log \overline{Z}_0
\]

Together with the relations (3), this leads us to a nested set of \( \tilde{n} \prod_{\ell=1}^L \tilde{m}_\ell \) replicas. A spin at level \( \ell \) thus carries a set \( \{a\}_\ell = \{a_0, \ldots, a_\ell\} \) of replica indices, where \( a_0 \in \{1, \ldots, \tilde{n}\} \) reflects the disorder average, and with \( a_\ell \in \{1, \ldots, \tilde{m}_\ell\} \). As before \( \tilde{m}_\ell = \beta_{\ell-1}/\beta_\ell \leq 1 \). Following standard manipulations, the asymptotic free energy per spin \( f = \lim_{N \rightarrow \infty} \overline{F}_0/N \) is then found to be

\[
f = \lim_{\tilde{n} \rightarrow 0} \frac{1}{\tilde{n} \beta_0} \exp \left[ \frac{J^2 \beta^2}{4} \sum_{\{a\}_L, \{b\}_L} q_{\{a\}_L} \frac{L}{L} - \sum_{\ell=0}^{L} \epsilon_\ell \log K_\ell \right]
\]

Extremisation is to be carried out with respect to the order parameters \( q_{\{a\}_L} \), whose physical meaning is given by (with averages denoting the multi-temperature statistics):

\[
q_{\{a\}_L} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{\ell=0}^{L} \sum_{j \in I_\ell} \langle \sigma_j | a \rangle \langle \sigma_j | a \rangle
\]

With the new definitions \( m_\ell = \prod_{k=0}^\ell \tilde{m}_k = \beta_{\ell-1}/\beta_\ell \) we obtain \( \beta_0 \tilde{n} = \beta n \), and the connection with the original Parisi solution becomes clear. What remains is to assume full ergodicity within each level in the hierarchy of time-scales:

\[
q_{\{a\}_L} = q_{\ell}(\{a\}_L, \{b\}_L)
\]
where \( \ell(\{a\}_L, \{b\}_L) \) denotes the slowest level for which the two strings of replica coordinates \( \{a\}_L \) and \( \{b\}_L \) differ. Insertion of (13) into (10) gives

\[
f = \frac{\beta J^2}{2} \sum_{\ell=0}^{L} \left[ \frac{1}{2} m_{\ell+1} (q_{\ell+1}^2 - q_\ell^2) - \epsilon_\ell \sum_{r=\ell}^{L} m_{r+1} (q_r - q_r) \right] - \frac{1}{m_1 \beta} \sum_{\ell=0}^{L} \epsilon_\ell \int Dz_0 \log[N_\ell^{\uparrow}] \tag{14}
\]

where

\[
N_\ell^{\uparrow} = \begin{cases} 
\int Dz_r [N_r^{\downarrow+1}]^{\frac{m_r}{m_{r+1}}} & \text{for } r \leq \ell \\
2 \cosh(J \beta m_{\ell+1} \sum_{s=0}^{\ell} z_s \sqrt{q_s - q_{s+1}}) & \text{for } r = \ell + 1
\end{cases}
\tag{15}
\]

The physical meaning of \( q_\ell \) is

\[
q_\ell = \lim_{N \to \infty} \frac{1}{N} \sum_j \left\langle \ldots \left\langle \ldots \langle \langle \sigma_j \rangle_L \ldots \rangle_{\ell+1} \langle \sigma_\ell \rangle_{\ell} \ldots \right\rangle_0 \right\rangle
\tag{16}
\]

in which \( \langle \ldots \langle \ldots \ldots \rangle_0 \right\rangle \) denotes the disorder average. The physical saddle-point is the analytic continuation of the one which minimises \( f \) for positive integer values of \( \{\tilde{n}, \tilde{m}_\ell\} \). For such values, the minimum with respect to the \( \epsilon_\ell \) (with \( \sum_{\ell=0}^{L} \epsilon_\ell = 1 \)), in turn, is found to occur for \( \{\epsilon_\ell^* = 1, \epsilon_r^* = 0 \forall \ell < L\} \), i.e. in the thermodynamic limit the slow spins form a vanishing fraction of the system as a whole. We have now exactly recovered the \( L \)-th order Parisi solution. The values of the \( m_\ell \) follow from (6), which translates into

\[
\beta m_{\ell+1}^2 \frac{\partial}{\partial m_{\ell+1}} f = \Sigma_\ell/N \tag{17}
\]

The bounds \( 0 \leq \lim_{N \to \infty} \Sigma_\ell/N \leq \epsilon_\ell \log 2 \) subsequently dictate that, as \( \epsilon_\ell \to 0 \) for all \( \ell < L \), determining \( m_\ell \) via (17) simply reduces to extremising \( f \) with respect to \( m_\ell \), thus removing the need to know the values of the constraining entropies \( S_\ell \).

We have thus shown that the Parisi solution can be derived from simple physical principles, and can be interpreted as describing a system with an infinite hierarchy of time-scales where a vanishingly small fraction of slow spins act as effective symmetry-breaking disorder for the faster ones. The vanishing of the fraction of slow spins
indicates that the cumulative entropy of the slow spins is sub-extensive, and that the so-called complexity is zero. A block-size $m_{\ell}$ at level $\ell$ of the Parisi matrix is found to be the ratio of the effective temperature $T_{\ell}$ of that level and the ambient temperature $T$. Extremization of the free energy per spin with respect to $m_{\ell}$ is equivalent to saying that the average entropy of the spins at level $\ell - 1$ is stationary and sub-extensive. It follows from physical considerations (no heat flow in equilibrium) that $m_{\ell} \leq 1$ for all $\ell$. Ultra-metricity (see fig. 1) is a direct consequence of the existence of a hierarchy of time-scales. At each level $\ell$, the different descendants of a node represent different configurations of the $\sigma_{\ell+1}$, which share the same realisation of the disorder and of the slower spins.

Since our proposal relies fundamentally on the existence of clusters with widely separated characteristic time-scales, we sought to provide independent evidence for this assumption by measuring the distribution $\rho_{\text{sim}}(f, t)$ of the number of flips $f$ per spin at time $t$ in numerical simulations of the SK-model, see fig. 2. Upon assuming an independent characteristic time-scale $\tau_j$ for each spin $\sigma_j$, and a distribution $W(\tau)$ for these time-scales, one obtains a simple theoretical prediction for this distribution:

$$\rho_{\text{th}}(f, t|W) \simeq \int_0^\infty d\tau \ W(\tau) \left(\frac{t}{f}\right)^{1 - \frac{1}{\tau f}} \left(1 - \frac{1}{\tau f}\right)^{t-f}$$

(18)

Minimising the deviation $\sum_{f=0}^{\infty} [\rho_{\text{sim}}(f, t) - \rho_{\text{th}}(f, t|W)]^2$ with respect to the $W(\tau)$ yields an estimate of the most probable distribution of time-scales $W^*(\tau)$, see fig. 2 which clearly supports our assumptions. Both the number of peaks (in agreement with full RSB), and the separation between the peaks (in agreement with infinitely disparate time-scales) are found to grow with increasing system size and/or time, whereas the fraction of ‘slow’ spins appears to decrease with increasing system size.

In fig. 3 we sketch the qualitative picture emerging from our interpretation of the Parisi scheme. Most spins evolve at the fastest (microscopic) time-scale, at ambient temperature $T$; a small fraction evolves at (infinitely) slower time-scales, at higher effective temperatures. Cooling to a temperature $T_1 < T$, followed by heating back to $T$, will leave spins with $T_{\text{eff}} > T$ unchanged, explaining memory effects. Conversely, after heating to $T_2 > T$ and cooling back to $T$, the original states of spins with $T \leq T_{\text{eff}} \leq T_2$ will be erased, which may explain thermo-cycling experiments (for a recent review see e.g. [10]). We expect the qualitative features of our picture to survive in short range systems, where the time-scales need not be infinitely disparate due to activated processes. The origin of the slow time-scales of these clusters must lie in the latter being coupled much stronger internally, than (effectively) to the rest of the system. They could therefore be seen as a ‘soft’ version of the fully disconnected clusters which give rise to so-called Griffiths singularities in diluted systems [11]. In short range systems, the clusters would have to be spatially localized, in line with the droplet picture proposed by Fisher and Huse [12]. In such systems, each of the different levels would correspond to multiple localised spin clusters. The fact that the characteristic time-scale of a cluster increases with $T_{\text{eff}} - T$ explains why the effective age of a system at temperature $T$ is found to decrease upon spending time at $T_1 < T$, but to increase upon doing so at $T_2 > T$.

At a theoretical level, a more careful treatment of the selection of clusters is clearly needed (and is currently being carried out [8]), both for full- and 1-RSB models. This may allow us to calculate the complexity in such systems. Furthermore, it needs to be investigated whether slow clusters survive above the thermodynamic spin-glass
temperature $T_{sg}$. Our results also suggest further numerical experiments for both mean field and short range models, concentrating on quantities such as spin flip frequencies, avalanches, spatial correlations, and cluster persistency [13, 14, 15].

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[1] Parisi G 1979 Phys. Lett. 73A 203
[2] Sherrington D and Kirkpatrick S 1975 Phys. Rev. Lett. 35 1792
[3] Sompolinsky H 1981 Phys. Rev. Lett. 47 935
[4] Bonilla L L, Padilla F G and Ritort F 1998 Physica A 250 315
Figure 3. Qualitative sketch of the distribution $W(T_{\text{eff}})$ of (effective) temperatures (note: time-scales increase with $T_{\text{eff}}$) at ambient temperature $T$ (resp. $T_1$, $T_2$) in the spin glass phase.

[5] Cugliandolo L F and Kurchan J 1993 Phys. Rev. Lett. 71 173; 1997 Prog. Theor. Phys. Supp. 126 407
[6] Nieuwenhuizen T M 2000 Phys. Rev. E 61 267
[7] Franz S, Mézard M, Parisi G and Peliti L 1999 J. Stat. Phys. 97 459
[8] Coolen A C C and van Mourik J 2000 in progress
[9] Penney R W, Coolen A C C and Sherrington D 1993 J. Phys. A: Math. Gen. 26 3681
[10] Picco M, Ricci-Tersenghi F and Ritort F 2000 cond-mat/0005544 and references therein
[11] Griffiths R B 1969 Phys. Rev. Lett. 23 17
[12] Fisher D S and Huse D A 1986 Phys. Rev. Lett. 56 1601
[13] Takayama H and Yoshino H 1995 J. Phys. Soc. Jpn. 64 2766
[14] Barrat A and Zecchina R 1999 Phys. Rev. E 59 R1299
[15] Ricci-Tersenghi F and Zecchina R 2000 cond-mat/0004435