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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 timescales 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 timescales [3], effective temperatures [4], low entropy production [5] and non-equilibrium 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 timescales; 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 the 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 timescales, 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 $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$ with Hamiltonian $H(\boldsymbol{\sigma})$ and state probabilities (or densities) $p(\boldsymbol{\sigma})$, we turn to Boltzmann's $\mathcal{H}$-function $\mathcal{H} = \mathrm{Tr}_{\boldsymbol{\sigma}}\, p(\boldsymbol{\sigma})\{H(\boldsymbol{\sigma}) + T \log p(\boldsymbol{\sigma})\}$, 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 versus slow), i.e. $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_{\mathrm{f}}, \boldsymbol{\sigma}_{\mathrm{s}})$, we substitute $p(\boldsymbol{\sigma}_{\mathrm{f}}, \boldsymbol{\sigma}_{\mathrm{s}}) = p(\boldsymbol{\sigma}_{\mathrm{f}}|\boldsymbol{\sigma}_{\mathrm{s}})p(\boldsymbol{\sigma}_{\mathrm{s}})$ and find

$$\mathcal{H} = \mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{s}}}\; p(\boldsymbol{\sigma}_{\mathrm{s}})\{H_{\mathrm{eff}}(\boldsymbol{\sigma}_{\mathrm{s}}) + T \log p(\boldsymbol{\sigma}_{\mathrm{s}})\} \tag{1}$$

$$H_{\mathrm{eff}}(\boldsymbol{\sigma}_{\mathrm{s}}) = \mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{f}}}\; p(\boldsymbol{\sigma}_{\mathrm{f}}|\boldsymbol{\sigma}_{\mathrm{s}})\{H(\boldsymbol{\sigma}_{\mathrm{f}}, \boldsymbol{\sigma}_{\mathrm{s}}) + T \log p(\boldsymbol{\sigma}_{\mathrm{f}}|\boldsymbol{\sigma}_{\mathrm{s}})\}. \tag{2}$$

In the case where $\boldsymbol{\sigma}_{\mathrm{s}}$ and $\boldsymbol{\sigma}_{\mathrm{f}}$ evolve on disparate timescales, the minimization of (1) will occur in stages. First, for every (fixed) $\boldsymbol{\sigma}_{\mathrm{s}}$ the distribution $p(\boldsymbol{\sigma}_{\mathrm{f}}|\boldsymbol{\sigma}_{\mathrm{s}})$ of the fast variables will evolve such as to minimize (2), i.e. towards the Boltzmann state

$$p(\boldsymbol{\sigma}_{\mathrm{f}}|\boldsymbol{\sigma}_{\mathrm{s}}) = \mathcal{Z}_{\mathrm{f}}^{-1}(\boldsymbol{\sigma}_{\mathrm{s}})\, \mathrm{e}^{-\beta H(\boldsymbol{\sigma}_{\mathrm{f}}, \boldsymbol{\sigma}_{\mathrm{s}})} \qquad \mathcal{Z}_{\mathrm{f}}(\boldsymbol{\sigma}_{\mathrm{s}}) = \mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{f}}}\; \mathrm{e}^{-\beta H(\boldsymbol{\sigma}_{\mathrm{f}}, \boldsymbol{\sigma}_{\mathrm{s}})}. \tag{3}$$

Finding multiple temperatures requires, in addition to disparate timescales, stationarity of the entropy of the slow system (on the relevant 'glassy' timescales). Now (1) is minimized subject to the constraint that the entropy $S_{\mathrm{s}} = -\,\mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{s}}}\; p(\boldsymbol{\sigma}_{\mathrm{s}}) \log p(\boldsymbol{\sigma}_{\mathrm{s}})$ be kept constant, giving

$$p(\boldsymbol{\sigma}_{\mathrm{s}}) = \mathcal{Z}_{\mathrm{s}}^{-1} \mathrm{e}^{-\tilde{\beta} H_{\mathrm{eff}}(\boldsymbol{\sigma}_{\mathrm{s}})} \qquad \mathcal{Z}_{\mathrm{s}} = \mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{s}}}\; \mathrm{e}^{-\tilde{\beta} H_{\mathrm{eff}}(\boldsymbol{\sigma}_{\mathrm{s}})} \tag{4}$$

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 (2)–(4) gives $\mathcal{Z}_{\mathrm{s}} = \mathrm{Tr}_{\boldsymbol{\sigma}_{\mathrm{s}}}[\mathcal{Z}_{\mathrm{f}}(\boldsymbol{\sigma}_{\mathrm{s}})]^{\tilde{m}}$. The dimension $\tilde{m}$ follows from demanding the prescribed value of the slow entropy: $\beta\tilde{m}^2(\partial\mathcal{F}_{\mathrm{s}}/\partial\tilde{m}) = S_{\mathrm{s}}$, with $\mathcal{F}_{\mathrm{s}} = -\tilde{\beta}^{-1} \log \mathcal{Z}_{\mathrm{s}}$. For $T > \tilde{T}$ the fast variables would start acting as a heat bath for the slow ones, so thermodynamic stability requires $\tilde{m} \leqslant 1$. Note that $\tilde{m} < 1$ implies that the constraining entropy must be larger than that of the Boltzmann state (indeed, a large characteristic timescale does not imply low entropy).

The above argument can be generalized to an arbitrary hierarchy. The variables $\boldsymbol{\sigma}_\ell$ at each level ℓ are characterized by distinct timescales 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

$$\begin{aligned} \mathcal{Z}_\ell &= \mathrm{Tr}_{\boldsymbol{\sigma}_\ell}[\mathcal{Z}_{\ell+1}]^{\tilde{m}_{\ell+1}} \qquad (\ell < L) \\ \mathcal{Z}_L &= \mathrm{Tr}_{\boldsymbol{\sigma}_L}\; \mathrm{e}^{-\beta_L H(\{\boldsymbol{\sigma}\})} \end{aligned} \tag{5}$$

with $\tilde{m}_\ell = \beta_{\ell-1}/\beta_\ell \leqslant 1$, and $\beta_L = \beta$. The replica dimensions $\tilde{m}_\ell$ follow from the prescribed (stationary, but as yet unknown) values S_ℓ of the level-ℓ entropies, via $\beta_{\ell+1}\tilde{m}_{\ell+1}^2(\partial\mathcal{F}_\ell/\partial\tilde{m}_{\ell+1}) = S_\ell$, with $\mathcal{F}_\ell = -\beta_\ell^{-1} \log \mathcal{Z}_\ell$. Equivalently, using the specific nesting of the partition functions in (5) one shows that the $\{\tilde{m}_\ell\}$ are uniquely determined by the identities

$$\beta_{\ell+1}\tilde{m}_{\ell+1}^2 \frac{\partial}{\partial\tilde{m}_{\ell+1}}\mathcal{F}_0 = \Sigma_\ell \qquad \Sigma_\ell = \langle\langle\cdots\langle S_\ell\rangle_{\ell-1}\cdots\rangle_1\rangle_0 \tag{6}$$

in which $\langle\cdots\rangle_r$ denotes the average over the equilibrated level-r process. Due to the constrained minimizations underlying (5), the free energies $\mathcal{F}_\ell$ are generally not minimized; however, one can verify that $\mathcal{F}_0$ still serves as a generator of observables

$$H(\{\boldsymbol{\sigma}\}) \to H(\{\boldsymbol{\sigma}\}) + \lambda\psi(\{\boldsymbol{\sigma}\}): \qquad \lim_{\lambda\to 0}\frac{\partial}{\partial\lambda}\mathcal{F}_0 = \langle\psi(\{\boldsymbol{\sigma}\})\rangle. \tag{7}$$

This generalizes a formalism originally developed and applied for spin systems with slowly evolving bonds [8]. The construction reverts back to the conventional statistical mechanical picture if the constraining entropies S_ℓ are identical to those of the full Boltzmann state: then the constraining forces vanish and $\tilde{m}_\ell = 1$ for all ℓ.

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 $H(\boldsymbol{\sigma}) = -\sum_{i<j} J_{ij}\sigma_i\sigma_j$, but with suitably scaled independent random couplings J_{ij} (with average J_0/N and variance $J/\sqrt{N}$). In the remainder of this Letter we take $J_0 = 0$. We assume, following our previous arguments, that this system can be viewed as a hierarchy of $L+1$ levels of spins, each level ℓ with distinct disparate timescales and temperatures $\{\tau_\ell, T_\ell\}$

$$\{1,\ldots,N\} = \bigcup_{\ell=0}^{L} I_\ell \qquad \boldsymbol{\sigma} = (\boldsymbol{\sigma}_0,\ldots,\boldsymbol{\sigma}_L) \qquad \boldsymbol{\sigma}_\ell = \{\sigma_j | j \in I_\ell\} \tag{8}$$

with $|I_\ell| = \epsilon_\ell N$, and such that $\tau_\ell \ll \tau_{\ell-1}$ for all ℓ (thus larger values of ℓ correspond to faster spins). The selection of timescales for the spins is expected to depend on the realization 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. We calculate the disorder-averaged free energy $\mathcal{F}_0$ (the general multi-level generator of observables) with the replica trick

$$\overline{\mathcal{F}_0} = -\beta_0^{-1}\overline{\log \mathcal{Z}_0} = -\lim_{\tilde{n}\to 0}(\tilde{n}\beta_0)^{-1}\log \overline{\mathcal{Z}_0^{\tilde{n}}}. \tag{9}$$

Together with the relations (5), this leads us to a nested set of $\tilde{n}\prod_{\ell=1}^{L}\tilde{m}_\ell$ replicas. A spin at level ℓ 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 $\tilde{m}_\ell = \beta_{\ell-1}/\beta_\ell \leqslant 1$. Following standard manipulations, the asymptotic free energy per spin $f = \lim_{N\to\infty}\overline{\mathcal{F}_0}/N$ is then found to be

$$f = \lim_{\tilde{n}\to 0}\frac{1}{\tilde{n}\beta_0}\,\mathrm{extr}\left[\frac{J^2\beta^2}{4}\sum_{\{a\}_L,\{b\}_L} q_{\{b\}_L}^{\{a\}_L\,2} - \sum_{\ell=0}^{L}\epsilon_\ell \log \mathcal{K}_\ell\right] \tag{10}$$

$$\mathcal{K}_\ell = \mathrm{Tr}_{\{\sigma^{\{c\}_\ell}\}}\exp\left[\frac{J^2\beta^2}{2}\sum_{\{a\}_L,\{b\}_L} q_{\{b\}_L}^{\{a\}_L}\sigma^{\{a\}_\ell}\sigma^{\{b\}_\ell}\right]. \tag{11}$$

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

$$q_{\{b\}_L}^{\{a\}_L} = \lim_{N\to\infty}\frac{1}{N}\sum_{\ell=0}^{L}\sum_{j\in I_\ell}\langle\sigma_j^{\{a\}_\ell}\sigma_j^{\{b\}_\ell}\rangle. \tag{12}$$

With the new definitions $m_\ell = \prod_{k=\ell}^{L}\tilde{m}_k = \beta_{\ell-1}/\beta$, $\beta_0\tilde{n} = \beta n$, the connection with the original Parisi solution becomes clear. What remains is to assume full ergodicity within each level in the hierarchy of timescales

$$q_{\{b\}_L}^{\{a\}_L} = q_{\ell[\{a\}_L,\{b\}_L]} \tag{13}$$

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

$$f = \frac{\beta J^2}{2}\sum_{\ell=0}^{L}\left[\frac{1}{2}m_{\ell+1}(q_{\ell+1}^2 - q_\ell^2) - \epsilon_\ell\sum_{r=\ell}^{L}m_{r+1}(q_{r+1}-q_r)\right] - \frac{1}{m_1\beta}\sum_{\ell=0}^{L}\epsilon_\ell\int \mathrm{D}z_0\,\log[\mathcal{N}_\ell^1] \tag{14}$$

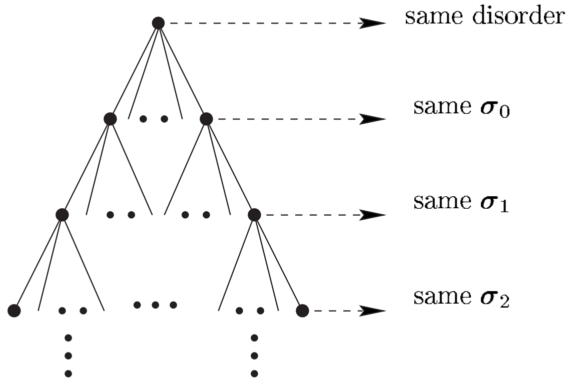

Figure 1. The ultra-metric tree, which here is a direct consequence of the hierarchy of spin clusters, evolving at disparate timescales.

where $q_{L+1} = m_{L+1} = 1$, $\mathrm{D}z = (2\pi)^{-1/2} \exp(-z^2/2)\,\mathrm{d}z$, and

$$\mathcal{N}_\ell^r = \begin{cases} \int \mathrm{D}z_r [\mathcal{N}_\ell^{r+1}]^{\frac{m_r}{m_{r+1}}} & \text{for} \quad r \leqslant \ell \\ 2\cosh\left(J\beta m_{\ell+1} \sum_{s=0}^{\ell} z_s \sqrt{q_s - q_{s-1}}\right) & \text{for} \quad r = \ell + 1. \end{cases} \tag{15}$$

The physical meaning of q_ℓ is

$$q_\ell = \lim_{N\to\infty} \frac{1}{N} \sum_j \overline{\langle \cdots \langle \langle \langle \cdots \langle \sigma_j \rangle_L \cdots \rangle_{\ell+1} \rangle_\ell^2 \rangle_{\ell-1} \ldots \rangle_0} \tag{16}$$

in which $\overline{\cdots}$ denotes the disorder average. The physical saddle-point is the analytic continuation of the one which minimizes f for positive integer values of $\{\tilde{n}, \tilde{m}_\ell\}$. For such values, the minimum with respect to the ϵ_ℓ (with $\sum_{\ell=0}^{L} \epsilon_\ell = 1$), in turn, is found to occur for $\{\epsilon_L^* = 1, \epsilon_\ell^* = 0\,\forall \ell < L\}$, i.e. in the thermodynamic limit the slow spins form a vanishing fraction of the system as a whole. Note, however, that the *number* of slow spins can still (and is expected to) diverge as $N \to \infty$. We have now exactly recovered the Lth-order Parisi solution. The values of m_ℓ follow from (6), which translates into

$$\beta m_{\ell+1}^2 \frac{\partial}{\partial m_{\ell+1}} f = \overline{\Sigma}_\ell / N. \tag{17}$$

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

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 timescales 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_ℓ at level ℓ of the Parisi matrix is found to be the ratio of the effective temperature T_ℓ of that level and the ambient temperature T. Extremization of the free energy per spin with respect to m_ℓ 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 $m_\ell \leqslant 1$ for all ℓ. Ultra-metricity (see figure 1) is a direct consequence of the existence of a

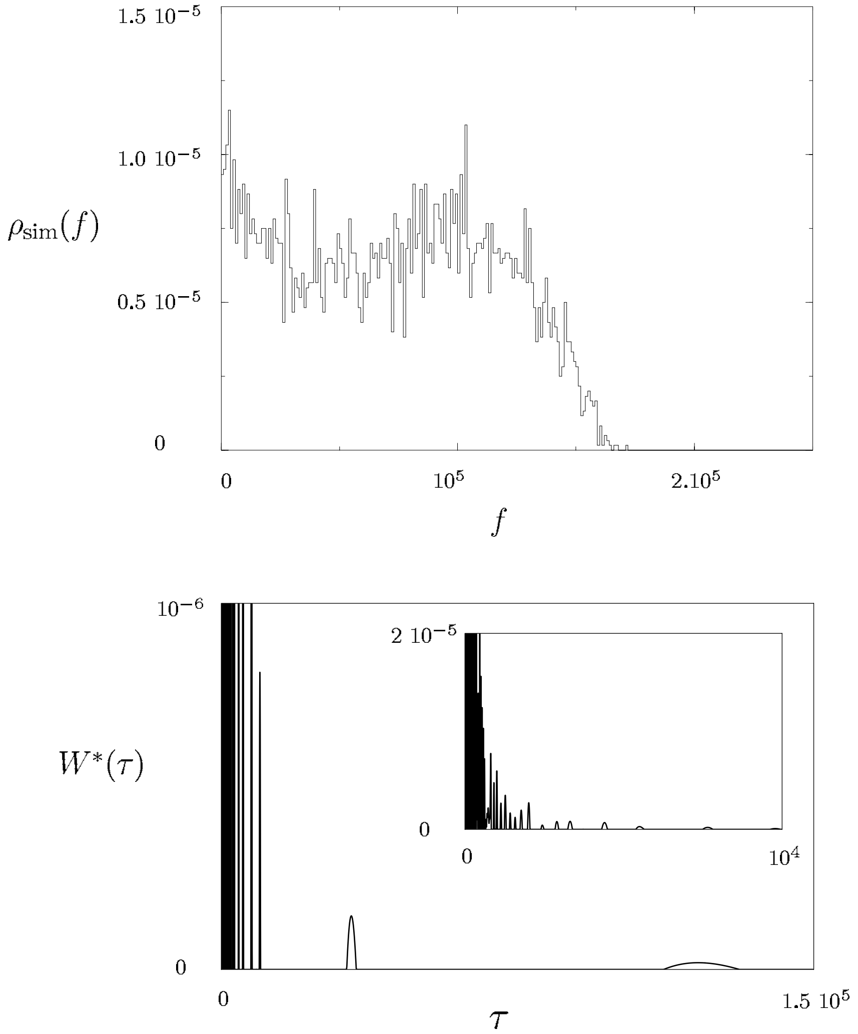

Figure 2. Upper graph: distribution of the number of flips f per spin for a simulation of the SK model with $N = 6000$, during $t = 10^6$ Monte Carlo updates per spin, after a waiting time of $t_w = 6 \times 10^5$, at $T = 0.25$. Lower graph: corresponding estimate of the most probable distribution $W^{\star}(\tau)$ of timescales τ. Inset: the small τ area enlarged.

hierarchy of timescales. At each level ℓ, the different descendants of a node represent different configurations of the $\boldsymbol{\sigma}_{\ell+1}$, which share the same realization of the disorder and of the slower spins.

Since our proposal relies fundamentally on the existence of clusters with widely separated characteristic timescales, we sought to provide independent evidence for this assumption by measuring the distribution $\rho_{\mathrm{sim}}(f, t)$ of the number of flips f per spin at time t in numerical simulations of the SK model, see figure 2. Upon assuming an independent characteristic timescale τ_j for each spin σ_j, and a distribution $W(\tau)$ for these timescales, one obtains a

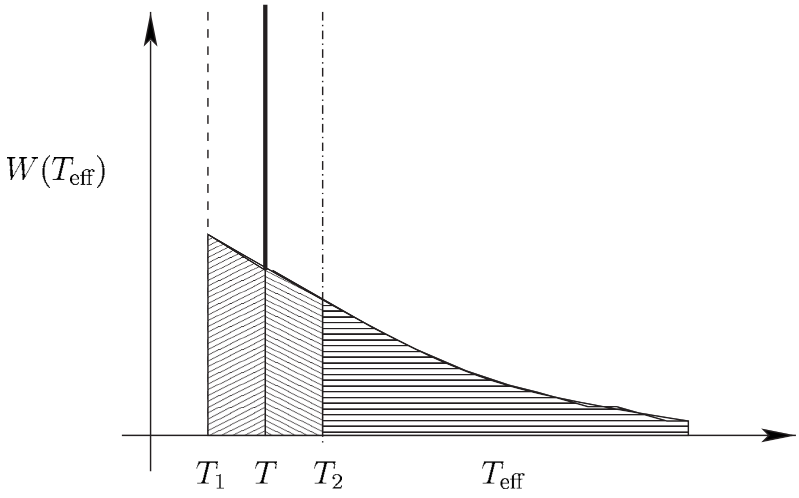

Figure 3. Qualitative sketch of the distribution $W(T_{\text{eff}})$ of (effective) temperatures (note: timescales increase with T_{eff}) at ambient temperature T (resp. T_1, T_2) in the spin-glass phase.

simple theoretical prediction for this distribution

$$\rho_{\text{th}}(f, t|W) \simeq \int_0^\infty \mathrm{d}\tau\; W(\tau) \begin{pmatrix} t \\ f \end{pmatrix} \frac{1}{\tau^f} \left(1 - \frac{1}{\tau}\right)^{t-f}. \tag{18}$$

Minimizing the deviation $\sum_{f=0}^{\infty}[\rho_{\text{sim}}(f,t) - \rho_{\text{th}}(f,t|W)]^2$ with respect to $W(\tau)$ yields an estimate of the most probable distribution of the timescales $W^*(\tau)$, see figure 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 timescales) are found to grow with increasing system size and/or time, whereas the fraction (but not the number) of 'slow' spins appears to decrease with increasing system size. Although our simulations reach timescales of the order of N^2 updates per spin, it should be emphasized that full equilibration has not yet been obtained, since this would have required simulation times of order $\exp(aN^{\frac{1}{2}})$ [10]. The equilibration problem is made worse by the conflicting additional requirement of choosing N sufficiently large to rule out finite size effects.

In figure 3 we sketch the qualitative picture emerging from our interpretation of the Parisi scheme. Most spins evolve at the fastest (microscopic) timescale, at ambient temperature T; a small fraction evolves at (infinitely) slower timescales, 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 $T \leqslant T_{\text{eff}} \leqslant T_2$ will be erased, which may explain thermocycling experiments (for a recent review see e.g. [9]). We expect the qualitative features of our picture to survive in short-range systems, where the timescales need not be infinitely disparate due to activated processes. The origin of the slow timescales 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 localized spin clusters. The fact that the characteristic timescale 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), both for full- and 1-RSB models. This may allow us to calculate the complexity in such systems. An important question is whether, for mean-field models in equilibrium, cluster membership of spins is a dynamic or static attribute. If spins can change mobility on sufficiently large timescales (infinitely larger than that of the slowest cluster), this would explain why our present simple treatment leads to the correct solution. Furthermore, it needs to be investigated whether slow clusters survive above the thermodynamic spin-glass temperature T_{sg}. Our results 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 [13–15].

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