Temperature chaos in a replica-symmetry-broken spin glass model — A hierarchical model with temperature chaos

M. Sasaki\textsuperscript{1} and O. C. Martin\textsuperscript{1,2}

\textsuperscript{1} Laboratoire de Physique Théorique et Modèles Statistiques, Bât. 100 Université Paris-Sud - F-91405 Orsay, France
\textsuperscript{2} Service de Physique de l’État Condensé, Orme des Merisiers-CEA Saclay 91191 Gif-sur-Yvette Cedex, France

(received 20 June 2002; accepted in final form 1 August 2002)

PACS. 75.10.Nr – Spin-glass and other random models.

Abstract. – Temperature chaos is an extreme sensitivity of the equilibrium state to a change of temperature. It arises in several disordered systems that are described by the so-called scaling theory of spin glasses, while it seems to be absent in mean-field models. We consider a model spin glass on a tree and show that although it has mean-field behavior with replica symmetry breaking, it manifestly has “strong” temperature chaos. We also show why chaos appears only very slowly with system size.

Introduction. – The fragility of the equilibrium state to an infinitesimal change of temperature is commonly referred to as “temperature chaos” [1]. Having such fragility away from a phase transition point probably requires the system to be frustrated, but whether temperature chaos actually arises in generic frustrated systems is still subject to controversy. In the context of spin glasses [2,3], temperature chaos is shown to be present for models on Migdal-Kadanoff lattices [4,5]. Furthermore, the standard scaling theories [1,6,7] suggest that this is a general property of glassy systems; in support of this, the Directed Polymer in a Random Medium [8] (DPRM), which is well described by the (spin glass) scaling theories, is known to have temperature chaos [9,10]. On the other hand, the Random Energy Model [11] has no temperature chaos [12], and what happens in the Sherrington-Kirkpatrick (SK) mean-field model of spin glasses is still unclear. A replica calculation for the SK model suggests the presence of temperature chaos [12], but the numerics indicate no chaos or only very weak chaos [13–15]. Furthermore, a more recent calculation by Rizzo [16] shows that temperature chaos is absent in perturbation theory about the critical temperature $T_c$ to the orders computed. To clarify this question of temperature chaos in mean-field spin glasses, in this paper we study a specific mean-field–like model. By determining the probability density of overlaps for two real replicas at two different temperatures, we show that this model has temperature chaos even though it has a mean-field behavior with replica symmetry breaking. Our quantitative study also gives a coherent picture of chaos and suggests why chaos is so weak in general.

The model based on a tree. – In this paper, we focus on the model introduced in ref. [17]. It is very similar to the model of a polymer on a disordered Cayley tree studied by Derrida and Spohn [18] (see also [19,20]); the differences are that values of both energy and entropy are assigned to each branch of the tree and each state thus has extensive entropy. It is also
close to the Random Entropy Random Energy model [21]; however, the energies and entropies are assigned hierarchically and the entropy is not introduced in an ad hoc way.

The model is constructed as follows. We consider a Cayley tree rooted at $O$. Each branch point $B$ (including $O$) creates $K$ branches which connect $B$ to its descendants. A tree with $L$ generations is obtained by repeating this procedure $L$ times. We regard the leaves (the bottom points) of the tree as the states of the system. A tree with $L$ generations has $K^L$ states. A random energy $\epsilon$ and a random entropy $\sigma$ are associated with every branch of the tree. The variables $\epsilon$ (respectively, $\sigma$) are drawn independently of the same distribution $\rho_E(\epsilon)$ ($\rho_S(\sigma)$).

To study temperature chaos in this model, consider a given realization of the quenched disorder (the random delta-function peaks, one at 0 and one at 1. Derivation of the overlap distribution with two different temperatures. – To study temperature chaos in this model, consider a given realization of the quenched disorder (the random energies and entropies); for that disorder, introduce two real replicas at equilibrium, one at temperature $T$, the other at temperature $T'$, both temperatures being below $T_c$. Of interest is the probability distribution of the overlap of these two replicas. We want to know how this distribution depends on $L$ and on the temperatures. We thus calculate the disorder-averaged “integrated probability” to find the two replicas at a distance less than or equal to $d$. This probability is explicitly defined as

$$ Y_{TT'}(L, d) \equiv \frac{1}{Z_T(L)Z_{T'}(L)} \sum_{ij/d_{ij} \leq d} e^{-X_T(i) - X_{T'}(j)}. \quad (1) $$

In this expression, $\overline{\cdots}$ represents the disorder average, $X_T(i) \equiv E(i)/T - S(i)$ is the free energy divided by $T$ of state $i$, and $Z_T(L)$ is the partition function at temperature $T$ for $L$ generations. Using an integral representation of $1/x$ for the two quantities $Z_T(L)$ and $Z_{T'}(L)$, we can rewrite eq. (1) as

$$ Y_{TT'}(L, d) = \int_{-\infty}^{\infty} dudv F_{TT'}(L, d; u, v), \quad (2) $$

$$ F_{TT'}(L, d; u, v) \equiv \exp \left[-e^{-u}Z_T(L) - e^{-v}Z_{T'}(L) - u - v \right] \sum_{ij/d_{ij} \leq d} e^{-X_T(i) - X_{T'}(j)}. \quad (3) $$

We can use $\sum_{ij/d_{ij} \leq d} \exp[-X_T(i) - X_{T'}(j)] = \sum_{B_d} \exp[-X_T(B_d) - X_{T'}(B_d)]z_T(B_d)z_{T'}(B_d)$, where $B_d$ is a general branch point in the $d$-th layer (counted from below) and $z_T(B)$ is the partition function at $T$ of the sub-tree rooted at a branch point $B$, in order to obtain

$$ F_{TT'}(L, d; u, v) \equiv \exp \left[-e^{-u}Z_T(L) - e^{-v}Z_{T'}(L) - u - v \right] \times \sum_{B_d} \exp \left[-X_T(B_d) - X_{T'}(B_d) \right]z_T(B_d)z_{T'}(B_d). \quad (4) $$
From this equation, we find

\[ F_{TT'}(d, d; u, v) = H_{TT'}(d; 1, 1; u, v), \quad (5) \]

\[ H_{TT'}(d; m, u; v) \equiv \left[ e^{-u_zT(B_d)} \right]^m \left[ e^{-v_zT'(B_d)} \right]^n \exp \left[ -e^{-u_zT(B_d)} - e^{-v_zT'(B_d)} \right]. \quad (6) \]

We can calculate \( H_{TT'}(d; m, n; u, v) \) (including \( H_{TT'}(d; 1, 1; u, v) \) which appears in eq. (5)) by the following recursion formulae. For \( m = n = 0 \), it is not so difficult to find

\[ H_{TT'}(0; 0; u, v) = \exp \left[ -e^{-u} - e^{-v} \right], \quad (7) \]

\[ H_{TT'}(d + 1; 0, 0; u, v) = \tilde{H}_{TT'}(d; 0, 0; u, v)^K, \quad (8) \]

where for a general two-variable function \( g(u, v) \) we have defined

\[ \tilde{g}(u, v) \equiv \int \text{d}\sigma \rho_E(\epsilon)\rho_S(\sigma)g(\epsilon + \sigma, \sigma + \epsilon/T - \sigma). \quad (9) \]

The recursion formula for general \( m \) and \( n \) is derived by applying the relation

\[ H_{TT'}(d; m, n; u, v) = \frac{\partial^m}{\partial u^m} \frac{\partial^n}{\partial v^n} H_{TT'}(d; 0, 0; u, v) \quad (10) \]

to eqs. (7) and (8). For example, the recursion formula for \( H_{TT'}(d; 1, 0; u, v) \) is

\[ H_{TT'}(d + 1; 1, 0; u, v) = \frac{\partial}{\partial u} \tilde{H}_{TT'}(d; 0, 0; u, v)^K \]
\[ = K \tilde{H}_{TT'}(d; 1, 0; u, v) \tilde{H}_{TT'}(d; 0, 0; u, v)^{K-1}. \quad (11) \]

Finally, a method similar to the one used in ref. [17] leads us to

\[ F_{TT'}(L + 1, d; u, v) = K \tilde{F}_{TT'}(L, d; u, v) \tilde{H}_{TT'}(L; 0, 0; u, v)^{K-1} \quad (L \geq d). \quad (12) \]

In summary, the disorder-averaged distribution of distances \( Y_{TT'}(L, d) \) can be computed by the following procedure: i) Calculate \( H_{TT'}(d; 1, 1; u, v) = F_{TT'}(d, d; u, v) \) by evaluating numerically the recursions which are derived by applying eq. (10) to eqs. (7) and (8). ii) Calculate \( F_{TT'}(L, d; u, v) \) by using the recursion equation (12). iii) Compute \( Y_{TT'}(L, d) \) by estimating numerically the integral in eq. (2).

Temperature chaos. – To show that this model has temperature chaos, let us first measure

\[ Y_{TT'}(L, d = 0) = \sum_i P_T^{eq}(i) P_{T'}^{eq}(i), \]

where \( P_T^{eq}(i) = \exp[-X_T(i)]/Z_T \). This is a generalization of \( \sum_i (P_T^{eq}(i))^2 \) which has been studied in many systems like the SK model [22] and the Random Energy Model [23]. The result is shown in fig. 1(A). We used \( K = 2, \rho_E(\epsilon) = 0.25\delta(\epsilon) + 0.5\delta(\epsilon - 1) + 0.25\delta(\epsilon - 2) \) and \( \rho_S(\sigma) = 0.5\delta(\sigma) + 0.5\delta(\sigma - 4) \) for those data. The critical temperature \( T_c \) is around 1.63 by the mapping to the Derrida-Spohn model and using the corresponding formula in [18]. We see that \( Y_{TT'}(L, d = 0) \) decays exponentially for \( T \neq T' \) while it converges to a non-zero value for \( T = T' \). (More precisely, a fit of the data at large \( L \) gives \( Y_{TT'}(L, d = 0) \approx A L^{-1/2} \exp[-BL] \).) These results tell us that the partition function below \( T_c \) is dominated by a few states, but these dominant states change with temperature, i.e., there is temperature chaos. We have also checked that temperature chaos is absent in the model without entropy (no \( \rho_S(\sigma) \); this is in agreement with ref. [12] which shows that the GREM does not have temperature chaos. Reference [12] has also shown that there is chaos.
The critical temperature $q_i$ for these data are $K$.

The origin of the strong chaos, let us focus on $Y_{TT'}(L, d = 0)$ of the model.

This means that the presence of $\delta f_T(B_d)$ only depend on $L - d$. These facts lead us to the scaling law eq. (13).

The validity of eq. (13) is confirmed in fig. 1(B) where $Y_{TT'}(L, (1 - q)L)$ for $q = 0.2, 0.4, 0.6, 0.8$ and 1.0 is plotted as a function of $qL$. Notice that $Y_{TT'}(L, (1 - q)L) = 0$ if $q = 1$, satisfy the scaling very well (note that $Y_{TT'}(L, 0)$ is calculated by eq. (14) with $\delta f_T = \delta f_{T'} = 0$). Furthermore, we see that the slopes for $Y_{TT'}(L, 0)$ and for the scaling function are the same. This means that the presence of $\delta f_T$ in eq. (14) does not change the slope because the variance of $\delta f_T$ is finite. Hereafter we regard the inverse of the exponent in this exponential decay as the chaos length $\ell(T, T')$ of the model.

This analysis shows that $\int_q^1 dq' P_{TT'}(q')$ decays as $\exp[-qL/\ell(T, T')]$ if $q \neq 0$, meaning that $P_{TT'}(q)$ also decays (up to power corrections) exponentially. This property corresponds to "strong" chaos in any reasonable classification of chaos. To obtain some insight into the origin of the strong chaos, let us focus on $Y_{TT'}(L, d = 0)$ which is the sum over all $K^L$ states of $\exp[-\{F_T(i) - F_{eq}(T)\}/T - \{F_{T'}(i) - F_{eq}(T')\}/T']$. (In this expression, $F_T(i)$ is the free energy of state $i$ at temperature $T$ and $F_{eq}(T)$ is the equilibrium free energy.) Now let us assume that among these $K^L$ states it is enough to consider just those that dominate the partition

**Fig. 1** – (A) $Y_{TT'}(L, d = 0)$ vs. $L$ for $(T, T') = (0.33, 0.2), (0.2, 0.2)$ and $(0.6, 0.33)$. The critical temperature $T_c$ is around 1.63. (B) $Y_{TT'}(L, (1 - q)L)$ for $(T, T') = (0.33, 0.2)$ vs. $qL$. The data are taken for $q = 0.2, 0.4, 0.6, 0.8$ and 1.0 with the same parameters as before.
function at some temperature \( T'' \). Since they are dominant states, the energy, the entropy and the free energy of these states are the same as the equilibrium ones at \( T'' \). Therefore, at any temperature \( T_m \) the free energies \( F_{T_m}(i) \) of these states are \( E_{eq}(T'') - T_m S_{eq}(T'') \) (= \( F_{eq}(T'') - S_{eq}(T'')(T_m - T'') \)). On the other hand, the Taylor expansion of \( F_{eq}(T_m) \) around \( T'' \) leads us to \( F_{eq}(T_m) = F_{eq}(T'') - S_{eq}(T'')(T_m - T'') - \frac{1}{2} \sigma(T'')(T_m - T'')^2 + \mathcal{O}((T_m - T'')^3) \), where \( \sigma \) is the heat capacity. By using this for \( T_m = T \) or \( T' \), we find that the contribution to \( Y_{TT'}(L, d = 0) \) for such a state is \( \exp[-\{ (T - T'')^2/T + (T - T'')^2/T' \} C(T'')/(2T'')] \). For \( \Delta T \equiv T - T' \ll 1 \), this is maximized at \( T'' = \frac{T + T'}{2} \) and we obtain

\[
Y_{TT'}(L, d = 0) \approx \exp \left[ - \frac{\Delta T^2 C(T)}{4T^2} \right].
\]  

(15)

In our model, \( C \) grows linearly with \( L \), leading to an exponential decay of \( Y_{TT'}(L, d = 0) \) with \( L \). On the contrary, the specific heat in the low-temperature phase is zero in the REM \([11]\) and in our model without entropy \([18]\) and thus there is no chaos in these systems.

Interestingly, this computation is only qualitatively correct and eq. (15) does not give the exact overlap length. The reason is that we have relied on typical contributions to \( Y_{TT'} \) while in fact it is dominated by rare events: a tiny fraction of the samples where the same state levelscancross, and these kinds of crossings generate temperature chaos in this model. Note that the reason why \( \sigma(T) \) grows linearly with \( L \) while \( \sigma(T') \) converges to a finite value. These results show that there are a few states which have almost the same lowest free energy, but whose entropies are very different from one another. Therefore, the relative order of these dominant states can change by a small change of the temperature, i.e., the free-energy levels can cross, and these kinds of crossings generate temperature chaos in this model. Note that this mechanism of temperature chaos was first proposed in the scaling theories \([1, 6, 7]\) and its validity is also confirmed in other systems \([10, 21]\). It is also worth noticing that \( \Delta S(i, T) \equiv S(i) - \langle S \rangle_T \) and \( \Delta E(i, T) \) are strongly correlated for the dominant states so that \( \Delta S(i, T) \approx \Delta E(i, T)/T \) because of the relation \( \Delta F(i, T) = \Delta E(i, T) - T \Delta S(i, T) \). This is the reason why \( \sigma_T^2(S) \) and \( \sigma_T^2(E) \) are almost the same in fig. 2.

The same results hold for state-to-state fluctuations defined as \( \hat{\sigma}_T^2(O) \equiv \langle O^2 \rangle_T - \langle O \rangle_T^2 \). First, \( \hat{\sigma}_T^2(F) \) stays \( O(1) \) since \( \hat{\sigma}_T^2(F) \leq \sigma_T^2(F) \). Second, \( \hat{\sigma}_T^2(E) \) grows linearly with \( L \) because \( \hat{\sigma}_T^2(E) \) is proportional to the heat capacity. From these two results, \( \sigma_T^2(S) \approx \sigma_T^2(E)/T \propto L \).

**Consequences for the overlap length.** Let us estimate \( Y_{TT'}(L, 0) \) to calculate \( \ell(T, T')^{-1} \) (recall that \( Y_{TT'}(L, 0) \approx \exp[-L/\ell(T, T')] \)). We denote the state with the lowest free energy at \( T \) by \( D_T \). If \( F_{TT'}(D_T') = E(D_T') - T'S(D_T') \) happens to be smaller than \( \langle F \rangle_T \), the dominant state at \( T' \) is still \( D_T \) (\( D_{T'} = D_T \)) so that \( Y_{TT'}(L, 0) \) for that sample is of order 1. Therefore,

\[
Y_{TT'}(L, 0) \approx \text{Prob}(F_{TT'}(D_T) \leq \langle F \rangle_{T'})
\]

\[
= \text{Prob}((T - T')\Delta E(D_T, T) \leq T[\langle F \rangle_{T'} - \langle F \rangle_T - (T - T')\langle S \rangle_T]),
\]  

(18)
where we have used $\Delta S(i,T) \approx \Delta E(i,T)/T$ to go from the first line to the second. Now assume that the distribution of $\Delta E(D_T,T)$ is Gaussian; this seems to be plausible since $\sigma_T(E)$ is linear in $L$, as if there were an underlying central-limit theorem process. Then we obtain

$$ Y_{TT'}(L,0) \sim \{L/\ell(T,T')\}^{-\frac{2}{3}} \exp \left[ -L/\ell(T,T') \right], \quad (19) $$

$$ \ell(T,T') = \frac{2\sigma_T^2(E)L(T-T')^2}{T^2[(F)_{T'} - (F)_T - (T-T')(S)_T]^2}. \quad (20) $$

The accuracy of eq. (20) was checked by comparing $\ell(T,T')$ estimated from $Y_{TT'}(L,0)$ and from eq. (20). The result was very satisfactory, i.e., the former is 131.3 and the latter 131.8 when the parameters are those used in fig. 1. We also found similarly good accuracy for the other sets of $(T,T')$ we tested. From eq. (20), we find

$$ \ell(T,T + \Delta T) \approx A(T) \left( \frac{\Delta T}{T} \right)^{-2} (\Delta T \ll 1), \quad (21) $$

$$ A(T) = 8\sigma_T^2(E)C(T)^{-2}T^{-2}L, \quad (22) $$

where again $C(T)$ is the heat capacity. It should be noted that the chaos exponent $\zeta$ defined via $\ell(T,T + \Delta T) \approx (\Delta T)^{-1/\zeta}$ is correctly given by the droplet theory [7,10] which predicts $\zeta = \frac{d-2\theta}{2}$ if $\sigma_T^2(S) \propto L^d$, and $\sigma_T^2(F) \propto L^{2\theta}$. (Indeed, fig. 2 shows $d_s = 1$ and $\theta = 0$ in this model). Figure 3 shows $A(T)$ of the model. We find that $A(T)$ has a minimum around $T \approx 0.2$ for which the value is about 33. This tells us that temperature chaos emerges only at large scales, e.g., when temperature is changed by 10% ($\Delta T/T = 0.1$), the chaos length is at least 3300. But note that eqs. (21) and (22) give us chaos volume if we consider the case $d \neq 1$ since $L$ is volume in this model. (Remember that energy and entropy are proportional to $L$.) Therefore, the minimum chaos length for $\Delta T/T = 0.1$ is not so large for $d = 3$, i.e., $3300^{1/3} \approx 15$.

(1) Rigorously speaking, eq. (22) is valid when $(F)_T/L = -k_B T \log Z(T)/L$. This relation is justifiable in the low-temperature phase where only a few states dominate the thermodynamics of the system, and we have checked this numerically.
Conclusions. – We have studied a GREM-like system with extensive entropy; it has strong temperature chaos, $P_{TT'}(q)$ decaying as $\exp[-q L/\ell(T, T')]$ if $T \neq T'$. Entropy fluctuations from valley to valley are the central ingredients for temperature chaos, as predicted by the scaling (droplet) theory [1, 6, 7]. Note that the overlap length $\ell(T, T')$ is proportional to $C(T)^{-1}(T - T')^{-2}$ (see eqs. (15) and (22)) and that $C(T)$ is typically small. If $C(T)$ also controls the decay of overlap probability in more general disordered systems, then it is no surprise that temperature chaos is difficult to detect in simulations. Finally, rejuvenation and memory effects observed in off-equilibrium dynamics [24, 25] are naturally interpreted by this model because it has both temperature chaos and a hierarchical structure. Consider, for example, the case where temperature is changed as $T \rightarrow T - \Delta T \rightarrow T$. A strong rejuvenated relaxation will be observed at $T - \Delta T$ due to temperature chaos, while memory will emerge when the temperature is returned to $T$ because of the hierarchical structure.

***

We thank J.-P. Bouchaud, F. Krzakala, H. Yoshino, and especially M. Mézard for helpful discussions. MS acknowledges a fellowship from the French Ministry of research. The LPTMS is an Unité de Recherche de l’Université Paris XI associée au CNRS.

REFERENCES

[1] Bray A. J. and Moore M. A., Phys. Rev. Lett., 58 (1987) 57.
[2] Mézard M., Parisi G. and Virasoro M. A., Spin-Glass Theory and Beyond, Lect. Notes Phys., Vol. 9 (World Scientific, Singapore) 1987.
[3] Young A. P. (Editor), Spin Glasses and Random Fields (World Scientific, Singapore) 1998.
[4] Banavar J. R. and Bray A. J., Phys. Rev. B, 35 (1987) 8888.
[5] Néy-Nifle M. and Hilhorst H., Phys. Rev. Lett., 18 (1992) 2992.
[6] Fisher D. S. and Huse D. A., Phys. Rev. Lett., 56 (1986) 1601.
[7] Fisher D. S. and Huse D. A., Phys. Rev. B, 38 (1988) 386.
[8] Halpin-Healy T. and Zhang Y., Phys. Rep., 254 (1995) 215.
[9] Fisher D. S. and Huse D. A., Phys. Rev. B, 43 (1991) 10728.
[10] Sales M. and Yoshino H., Phys. Rev. E, 65 (2002) 066131, cond-mat/0203371.
[11] Derrida B., Phys. Rev. Lett., 45 (1980) 79.
[12] Franz S. and Néy-Nifle M., J. Phys. A, 28 (1995) 2499.
[13] Billoire A. and Marinari E., J. Phys. A, 33 (2000) L265, cond-mat/9910352.
[14] Billoire A. and Marinari E., to be published in Europhys. Lett., cond-mat/0202473 (2002).
[15] Mulet R., Pagnani A. and Parisi G., Phys. Rev. B, 63 (2001) 184438.
[16] Rizzo T., J. Phys. A, 34 (2001) 5531.
[17] Sasaki M. and Martin O. C., cond-mat/0204413 (2002).
[18] Derrida B. and Spohn H., J. Stat. Phys., 51 (1988) 817.
[19] Majumdar S. N. and Krapivsky P. L., Phys. Rev. E, 62 (2000) 7735.
[20] Dean D. and Majumdar S., Phys. Rev. E, 64 (2001) 046121.
[21] Krzakala F. and Martin O. C., Eur. Phys. J. B, 28 (2002) 199, cond-mat/0203449.
[22] Mézard M. et al., J. Phys. (Paris), 45 (1984) 843.
[23] Derrida B. and Toulouse G., J. Phys. Lett., 46 (1985) L223.
[24] Jonason K. et al., Phys. Rev. Lett., 81 (1998) 3243.
[25] Nordblad P. and Svedlindh P., in Spin Glasses and Random Fields, edited by Young A. P. (World Scientific, Singapore) 1998.