Temperature chaos is a non-local effect

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Abstract. Temperature chaos plays a role in important effects, for example memory and rejuvenation, in spin glasses, colloids, polymers. We numerically investigate temperature chaos in spin glasses, exploiting its recent characterization as a rare-event driven phenomenon. The peculiarities of the transformation from periodic to anti-periodic boundary conditions in spin glasses allow us to conclude that temperature chaos is non-local: no bounded region of the system causes it. We precisely show the statistical relationship between temperature chaos and the free-energy changes upon varying boundary conditions.

Keywords: spin glasses
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1. Introduction

Temperature chaos [1–13], is one of the outstanding mysteries posed by spin glasses [14–20]. It consists of the complete reorganization of the equilibrium configurations by the slightest change in temperature. The topic is currently under intense theoretical scrutiny [21–24], not only because of its importance in analyzing spectacular experiments [25–32], but also as a crucial tool to assess the performance of quantum annealers [33, 34].

Here we exploit some of its very peculiar features to show that temperature chaos is a spatially non-local effect. For a disordered system, chaos should be studied on a sample by sample basis. In particular, for system sizes accessible to equilibrium computer simulations, chaos is a rare event, present only in a small fraction of the samples (as the system size increases, so does the fraction of chaotic samples [22]). We use this fact by thermalizing spin glasses down to a very low temperature (well below the critical temperature $T_c$). Then, for each simulated system, with periodic boundary conditions (PBC), we consider its image under a transformation where we make the boundary conditions anti-periodic (APBC) in one direction. As we discuss below, this transformation amounts to change in a tiny fraction of the coupling constants. Now, due to the gauge invariance in spin glasses, the couplings that have been changed by our transformation can be placed anywhere in the lattice. Interestingly enough, whether or not the PBC instance is chaotic carries essentially no information on the behaviour...
Temperature chaos is a non-local effect of its APBC transform. It follows that temperature chaos is not encoded in any localized region of the system.

We remark that our work relates as well to the long-standing controversy regarding the nature of the spin-glass phase. On the one hand, the replica symmetry breaking theory (stemming from the mean-field solution) envisages the spin-glass phase as composed of a multiplicity of states [16, 35]. Thus, from this point of view, the change of boundary conditions is a strong perturbation and there are no reasons to expect that temperature chaos effects will be significantly correlated for the PBC system and its APBC transform. On the other hand, the droplet picture [36–39] expects a single domain wall difference between the two types of boundary conditions, so there would be a strong correlation of the temperature chaos effects for the PBC/APBC systems. In this respect, our data favour replica symmetry breaking (because little correlation is observed). However, it has been pointed out many times that resolving this controversy requires studying much larger systems than are accessible to current simulations (or experiments [40]). This work is no exception. Furthermore, our analysis relies crucially on the fact that the system sizes are modest. Indeed, we rely that temperature chaos is a rare-event on small systems while, for larger systems, one expects that typical samples will display strong chaotic events.

The layout of the remaining part of this paper is as follows. In section 2 we recall the model definition and the crucial quantities we study. Some crucial features of temperature chaos are presented in section 3. Our main results are given in section 4. We briefly explore the relationships between the free-energy and temperature chaos in section 5. Our conclusions are given in section 6. Technical details are provided in two appendices.

2. The Edwards-Anderson model

Our \( S_u = \pm 1 \) spins occupy the nodes of a \( D = 3 \) lattice of size \( L^3 \) endowed with periodic boundary conditions. The Hamiltonian is

\[
\mathcal{H} = - \sum_{(u,v)} S_u J_{uv} S_v.
\]

The couplings \( J_{u,v} \) are \( \pm 1 \) with 50\% probability and only connect nearest neighbouring sites on the lattice. A particular realization of these couplings (quenched, i.e. fixed once and for all) is called a sample. Thermal averages for fixed \( \{ J_{u,v} \} \) are denoted by \( \langle \cdots \rangle_J \). This system has a second-order phase transition at temperature \( T_c = 1.102(3) \) [41].

For any original (periodic, PBC) instance its anti-periodic pair (APBC) is obtained by reversing the coupling \( J_{u,v} \) that joins sites \( (x = 0, y, z) \) and \( (1, y, z) \) for all values of \( y \) and \( z \) (only a \( 1/(3L) \) fraction of the bonds is changed\(^6\)). The APBC image could be a perfectly reasonable original instance, and, in fact, it is as probable as its PBC pair.

\(^6\) In [42] all the couplings undergo a tiny change, which produces a related, but different bond-chaos effect.
The system described by equation (1) has a gauge invariance [43]. The energy remains unchanged under the following transformation:

\[ J_{u,v} \rightarrow \epsilon_u \epsilon_v J_{u,v}, \quad S_u \rightarrow \epsilon_u S_u, \]  

where \( \epsilon_u = \pm 1 \) can be chosen arbitrarily for each site \( u \). Now consider the transformation where \( \epsilon_{(1,y,z)} = -1 \) and all other \( \epsilon_u = 1 \). This changes only the \( J_{u,v} \) that were reversed by the APBC transformation and those joining planes \( x = 1 \) and \( x = 2 \), moving, in this way, the transformed-couplings plane from \( x = 0 \) to \( x = 1 \). Using the same idea, we can place the transformed plane at any \( x \). Furthermore, one can deform the plane of inverted couplings locally in an essentially arbitrary way by considering a more complicated gauge transformation. In short, the PBC \( \leftrightarrow \) APBC transformation is non-local.

Another consequence of this gauge symmetry is the need to use real replicas of the system (i.e. copies that evolve independently, but share the same couplings) in order to form gauge-invariant observables (see, e.g. [40]).

We have simulated system sizes \( L = 8, 12 \) with parallel tempering [44, 45], carrying out several sets of runs for varying minimum temperatures: \( T_{\text{min}} = 0.15, 0.414, 0.479 \) for \( L = 8 \) and \( T_{\text{min}} = 0.414, 0.479 \) for \( L = 12 \). We have studied the same 4000 samples and their 4000 APBC counterparts for all \( T_{\text{min}} \). Since we want to study single-sample quantities and chaos, it has been very important to assess thermalization sample by sample by studying the temperature-mixing auto-correlation time of the parallel tempering [46]. In particular, we use the thermalization criteria of [40] (see also appendix A).

3. Some crucial facts about temperature chaos

Recently there has been much progress in the numerical characterization of temperature chaos [22, 23, 33]. A distinguishing feature of a chaotic sample is the very long auto-correlation time \( \tau \) for temperature-mixing along a parallel tempering simulation. Unfortunately, \( \tau \) is very difficult to measure with any precision, even for well equilibrated systems [40]. As shown in [22], see also appendix B, this difficulty can be skirted by choosing a different quantity, easier to measure but strongly correlated with \( \tau \).

In particular, we study the overlap between the spin configurations at temperatures \( T_1 \) and \( T_2 \),

\[ q_{T_1, T_2} = \frac{1}{L^3} \sum_u q_u^{T_1, T_2}, \quad \text{with} \quad q_u^{T_1, T_2} = S_u^{T_1} S_u^{T_2}, \]  

and use it to define a chaos parameter [47]:

\[ X_{T_1, T_2} = \left\langle \{q_{T_1, T_2}^2\} \right\rangle_j \left( \left\langle \{q_{T_1, T_2}^2\} \right\rangle_j \right)^{1/2}, \quad \]  

\[ I = \sum_{T_2} X_{T_1, T_2}. \]  

In these equations, \( \{S^{T_1}\} \) and \( \{S^{T_2}\} \) are extracted from different real replicas. \( X_{T_1, T_2} \) is small when the equilibrium configurations at \( T_1 \) and \( T_2 \) differ significantly. Instead, \( X_{T_1, T_2} \approx 1 \) in the absence of temperature chaos.
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We illustrate the ideas behind these parameters in figure 1—top, where we represent $X_{T_{\text{min}}}$ for two samples $A$ and $B$. The ratio of their respective temperature-mixing times is $\tau^A/\tau^B \approx 3000$. Consequently, for sample $A$ we can appreciate a very sudden drop in $X_{T_{\text{min}}}$ (which we name a chaotic event) for a low value of $T_2$, while sample $B$ has a smooth $X$. This behaviour can be summarized by saying that chaotic samples (such as $A$) have a low value of $I$ (essentially the integral of $X$), while non-chaotic samples have a high $I$. Figure 1—bottom shows that the probability of finding a chaotic event in a prefixed temperature interval increases for larger system size.

We note also from figure 1—top that the energy relates only in a very subtle way to temperature chaos. We shall further explore this relation below, since this quantity has been much emphasized in the literature [12, 13, 24, 49].

For fixed $\epsilon > 0$, $T_1$ and $T_2$ the probability of having $X_{T_1,T_2} > \epsilon$ drops exponentially in $L^3$ [21, 22].

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Finally, let us mention that we will base our analysis on \( I \). However, essentially identical results are obtained from the temperature-mixing time \( \tau \), as shown in appendix B.

4. Results

As figure 2 shows, the chaos integral \( I \) for a sample has very low correlation to the \( I \) value for its APBC transform. Yet, the \( I \)’s are not normally distributed (because the shape of the scatter plot is not elliptical). As a consequence, the characterization of correlations through the very small correlation parameter \( r = 0.074(16) \) is not complete. However, we can confirm the virtual absence of correlations is confirmed by a more refined analysis.

We start by considering the full probability distribution of \( I \) for our PBC samples, which spans a wide range of values and of course coincides with the \( p(I) \) for all the APBC samples. We then take the most typical samples, those contained in an interval of 20% probability around the median (the third quintile). All these samples, which span a very narrow \( I \) range, are non-chaotic. If we consider the APBC transforms of this median samples at a first glance one can observe that they span the whole \( I \) and therefore contain also chaotic instances. More precisely, one can construct the histogram of \( I \) values for the APBC images of the PBC median, which turns out to reproduce exactly the full probability distribution of \( I \) for this system. This is graphically shown in figure 3 but it can be proven using statistical methods. In particular, an Anderson–Darling non-parametric test [48] finds no difference between the full
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The free-energy change upon varying boundary conditions, $\Delta F = F_{\text{APBC}} - F_{\text{PBC}}$, has received much attention [12, 13, 24, 49]. However, to the best of our knowledge, the relation between $\Delta F$ and the spin correlations (e.g. the chaos parameter $X$ (4)), is yet
Temperature chaos is a non-local effect to be researched. We can investigate $\Delta F$ from our parallel tempering simulations by means of thermodynamic integration:

$$F = \frac{F(T_{\text{min}})}{T_{\text{min}}} - \frac{F(T_{\text{max}})}{T_{\text{max}}} = \int_{T_{\text{min}}}^{T_{\text{max}}} dT \frac{\langle H \rangle_{J, T}}{T^2}.$$  \hfill (6)

Here, $T_{\text{max}} = 1.6$ is the maximum temperature in our parallel tempering simulation. Note that, for large enough $T_{\text{max}}$, $\Delta F = \Delta F/T_{\text{min}}$. Indeed, for a temperature $T$ such that the high-temperature expansion converges $[50]$, $\Delta F(T)$ goes to zero exponentially in $L$.

Figure 1—top shows that chaotic events have an impact, albeit subtle, on the temperature evolution of $\langle H \rangle_{J, T}$. Hence, we expect some correlation between $X$ and the free energy. The question we address here is: how can we extract these correlations?

First, we note that $F$ is not a good chaos indicator by itself. This is clear already from figure 1, but can be seen more explicitly in figure 4—top, where we show that $F_{\text{PBC}}$ and $F_{\text{APBC}}$ are almost equal (their correlation parameter is about $r \approx 0.95$). However, on a closer inspection one realizes that chaotic events, even close to $T = 0$, result in minimal energy changes $[51]$. In other words, even in the most favourable case where only one member of the (PBC, APBC) pair has a chaotic event, the energy difference between the two samples is very small. Therefore, some sort of background subtraction is needed to enhance the chaotic signal:

$$F_{\text{sub}} = \int_{T_{\text{min}}}^{T_{\text{max}}} dT \frac{\langle H \rangle_{J, T} - \langle H \rangle_{J, T_{\text{min}}}}{T^2}.$$  \hfill (7)

Notice that, at very low temperature, (7) highlights the entropic contribution.

As we see in figure 4—centre, $F_{\text{sub}}$ is correlated with the chaos integral $I$. However, this correlation is only of $r = 0.546(12)$ and the scatter plot has a non-trivial structure, seemingly composed of two different populations. Therefore, $F_{\text{sub}}$, by itself, still does not seem a very good indicator of temperature chaos.

It is important to notice that the very strong correlation of $(F_{\text{PBC}}, F_{\text{APBC}})$, together with the (weaker) correlation of $(F_{\text{PBC}}, I_{\text{PBC}})$ is in no contradiction with our previous assertion that $(I_{\text{PBC}}, I_{\text{APBC}})$ are uncorrelated.

In order to see why, let us consider two stochastic variables, $A$ and $B$, that have the same variance $V$ and covariance $C$. Their covariance matrix has eigenvalues $\lambda_{\pm} = V \pm C$, and the corresponding normal coordinates are $N_{\pm} = (A \pm B)/\sqrt{2}$. It follows that the correlation coefficient is

$$r = \frac{C}{V} = \frac{1 - \frac{\lambda_{\pm}}{\lambda_{\pm}}}{1 + \frac{\lambda_{\pm}}{\lambda_{\pm}}}.$$  \hfill (8)

Clearly, $F_{\text{APBC}}$ and $F_{\text{PBC}}$, play the role of the stochastic variables $A$ and $B$ in the above reasoning. Now, as we shall explain next, there is a physical reason implying that $\lambda_+$ is orders of magnitude larger than $\lambda_-$. It follows that the correlation coefficient is $r \approx 1$ (as we find indeed). In other words, the only information in figure 4—top is $\lambda_+ \gg \lambda_-$. The physical reason underlying $\lambda_+ \gg \lambda_-$ is quite simple. On the one hand the sample to sample fluctuations of the free-energy are of order $L^{D/2}$. On the other hand, $\lambda_-$,
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\[ \text{Temperaure chaos} \]

which is the variance of \((\mathcal{F}_{\text{APBC}} - \mathcal{F}_{\text{PBC}})\sqrt{2}\) scales with the so called stiffness exponent \(\lambda_\perp \propto L^{2y}\) with \(y \approx 0.24\) in \(D = 3\) [52]. An elementary computation tells us that \(\lambda_- / \lambda_+ \propto L^{-x}\) with \(x = D - 2y \approx 2\).

A consequence of this analysis is that the free-energy difference \(\Delta \mathcal{F}_{\text{sub}} = (\mathcal{F}_{\text{sub,APBC}} - \mathcal{F}_{\text{sub,PBC}})\) is probably a much better chaos indicator than \(\mathcal{F}_{\text{sub}}\) by itself. This is confirmed by figure 4—bottom, which shows an enhanced correlation between \(\Delta \mathcal{F}_{\text{sub}}\) and \(\Delta I\), with a more Gaussian behaviour.

In conclusion, the free energy is related to temperature chaos as studied from the spatial correlation functions, but its sample-to-sample fluctuations are affected by several factors not related to chaos (see appendix D). Therefore, a refined analysis is needed to extract information about the chaos integrals from \(F\).

**Figure 4.** Temperature chaos and the free energy. We show several scatter plots for our \(L = 12\) and \(T_{\text{min}} = 0.414\) data. Top: for the free-energy (6) we plot \((\mathcal{F}_{\text{PBC}}, \mathcal{F}_{\text{APBC}})\) for each of our 4000 sample pairs. The green straight line is \(y = x\). Center: for the subtracted free-energy (7) we plot \((\mathcal{F}_{\text{sub,PBC}}, I_{\text{PBC}})\). Bottom: we plot \((\mathcal{F}_{\text{sub,PBC}} - \mathcal{F}_{\text{sub,APBC}}, I_{\text{PBC}} - I_{\text{APBC}})\).

\[ \text{Figure 4. Temperature chaos and the free energy.} \]

\[ r = 0.9606(13) \]

\[ r = 0.546(12) \]

\[ r = 0.648(9) \]
6. Conclusions

We have shown that temperature chaos, one of the most complex effects in glass physics, is a non-local phenomenon. Our approach has two fundamental ingredients: the recent rare-event characterization of chaos and the very special nature of periodic boundary conditions transformations in disordered systems. In fact, anti-periodic boundary conditions cannot be precisely located in a finite region of the system. So, changing a tiny $[O(1/L)]$ fraction of the coupling constants produces a dramatic effect in the physics of the considered sample (and the spatial location of the changed couplings has little importance).

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Appendix A. Simulation parameters

Our parallel tempering simulations closely follow [40]. Some details are provided in table A1 for the sake of completeness. There are two simulation phases. In the first phase, all the PBC instances (and their APBC images) are simulated for the same amount of time (which is referred to in table A1 as the minimum simulation time $N_{\text{HB}}^{\text{min}}$). At that point, we attempt a first estimate of the temperature-mixing time $\tau$ for each instance and check that the thermalization criteria were met [40]. We chose $N_{\text{HB}}^{\text{min}}$ in such a way that most instances (at least a 2/3 fraction) are well thermalized. For the remaining instances, the simulation length is increased and $\tau$ recomputed. The procedure continues until safe thermalization is achieved.

Some of the simulations for our PBC-samples were actually taken from [40], specifically the $(L = 8, T_{\text{min}} = 0.15)$ and $(L = 12, T_{\text{min}} = 0.414)$ simulations. We performed totally new simulations for the APBC image of this system. Additional simulations were performed in order to show the size-dependence in figure 1—bottom (the comparison of the chaos integral is easiest if we employ the same temperature grid in the parallel tempering for all system sizes).

Appendix B. Mixing time or chaos integral?

As we explained in section 3 the most appealing numerical characterization of temperature is the auto-correlation time $\tau$ for temperature-mixing along a parallel tempering
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Unfortunately, a high-accuracy computation of $\tau$ is not a light task, so we need an easier-to-compute alternative. A nice alternative is provided by the chaos integral $I$ defined in equation (5) [22]. Indeed, see figure B1—left, our estimations of $\tau$ and $I$ are very strongly correlated. Furthermore, our main theme (namely the very small correlation between the original PBC sample and its APBC-transform) is maintained when we work in terms of $\tau$, see figure B1—right.

**Table A1.** Parameters of our parallel-tempering simulations. In all cases we have simulated four independent real replicas for each of our 4000 samples. The $N_T$ temperatures are uniformly distributed between $T_{\text{min}}$ and $T_{\text{max}}$. In this table $N_{\text{mes}}$ is the number of heat-bath sweeps between measurements (we perform one parallel-tempering update every 10 heat-bath sweeps). The simulation length was adapted to the thermalization time of each sample (see [40]). The table shows the minimum, maximum and medium simulation times ($N_{\text{HB}}$) for each lattice, in heat-bath steps.

| $L$ | $T_{\text{min}}$ | $T_{\text{max}}$ | $N_T$ | $N_{\text{mes}}$ | $N_{\text{HB}}^{\text{min}}$ | $N_{\text{HB}}^{\text{max}}$ | $N_{\text{HB}}^{\text{med}}$ |
|-----|------------------|------------------|-------|-----------------|------------------|------------------|------------------|
| 8   | 0.150            | 1.575            | 10    | $10^3$          | $5 \times 10^6$  | $8.30 \times 10^6$ | $7.82 \times 10^6$ |
| 8   | 0.414            | 1.554            | 10    | $10^3$          | $10^7$           | $2.00 \times 10^7$ | $1.00 \times 10^7$ |
| 8   | 0.479            | 1.619            | 7     | $10^3$          | $10^7$           | $10^7$           | $10^7$           |
| 8   | 0.479            | 1.575            | 16    | $10^3$          | $10^7$           | $10^7$           | $10^7$           |
| 12  | 0.414            | 1.575            | 12    | $5 \times 10^3$ | $10^7$           | $1.53 \times 10^10$ | $4.60 \times 10^7$ |
| 12  | 0.479            | 1.640            | 12    | $2 \times 10^3$ | $8 \times 10^6$  | $7.49 \times 10^8$ | $1.08 \times 10^7$ |
| 12  | 0.479            | 1.575            | 16    | $2 \times 10^3$ | $8 \times 10^6$  | $2.56 \times 10^9$ | $1.94 \times 10^7$ |

**Figure B1.** The chaos integral and the temperature-mixing autocorrelation time carry similar information. We show here two scatter plots, obtained from our $L = 12$, $T_{\text{min}} = 0.414$ data. Left: we plot $(\log_2(PBC), I_{PBC})$ for each of our 4000 original PBC samples. Right: for the temperature-mixing time $\tau$, we plot $(\log_2(PBC), \log_2(\text{APBC}))$ for each of our 4000 sample pairs. All the $\tau$ are integrated autocorrelation times (see [40]) and are expressed in units of $N_{\text{mes}} = 5000$ heat-bath steps (see table 1).
Appendix C. Additional results

The purpose of this section is to show that neither the choice of temperature interval nor of studied system size is critical. This is evinced in figures C1–C3.

Appendix D. A geometric inequality on correlations

The assertion that the pair of stochastic variables \((I_{\text{APBC}}, I_{\text{PBC}})\) are essentially uncorrelated might be surprising in the view of the mild correlations for \((\mathcal{F}_{\text{PBC}}, I_{\text{PBC}})\) (or, equivalently, \((\mathcal{F}_{\text{APBC}}, I_{\text{APBC}})\)) and the very strong correlations depicted in figure 4 for

Figure C1. We show two scatter plots, as obtained from our \(L = 8\) and \(T_{\text{min}} = 0.15\) data. Left: the analogous of figure 5—left. Right: the analogous of figure 2.

Figure C2. The analogous of figure 3, as obtained from our \(L = 8\) and \(T_{\text{min}} = 0.15\) data.
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We shall first obtain an inequality, and then apply it to our problem. We start by considering a triplet of stochastic variables \( X_0, X_1, X_2 \). Let \( E(\cdots) \) denote the expectation value. For each \( X_i \), we define a related quantity \( x_i \):

\[
X_i = E(X_i) + \sigma_i^{1/2} x_i, \tag{D.1}
\]

where \( \sigma_i \) is the variance of \( X_i \). We note that the \( x_i \) are normalized, in the sense that \( E(x_i^2) = 1 \), that \( E(x_i) = 0 \) and that the correlation coefficient can be written as

\[
r_{ij} = E(x_i x_j). \tag{D.2}
\]

Now, we split the stochastic variable \( x_i \) for \( i = 1, 2 \) as

\[
x_i = r_0 i x_0 + \tilde{x}_i. \tag{D.3}
\]

Note that

\[
E(x_0 \tilde{x}_i) = 0, \quad E(\tilde{x}_i^2) = 1 - r_{0i}^2. \tag{D.4}
\]

It follows that

\[
r_{12} = E(x_1 x_2) = r_{01} r_{02} + E(\tilde{x}_1 \tilde{x}_2). \tag{D.5}
\]

Finally, we recall that the Cauchy–Schwarz–Bunyakovsky inequality unfortunately only implies \( |E(x_1 x_2)| \leq \sqrt{E(x_1^2) E(x_2^2)} \). Hence, the most we can tell about \( r_{12} \) judging from \( r_{01} \) and \( r_{02} \) is

\[
r_{01} r_{02} - \sqrt{1 - r_{01}^2} \sqrt{1 - r_{02}^2} \leq r_{12} \leq r_{01} r_{02} + \sqrt{1 - r_{01}^2} \sqrt{1 - r_{02}^2}. \tag{D.6}
\]

In our case, the variables of interest are \( X_1 = I_{\text{PBC}} \) and \( X_2 = I_{\text{APBC}} \). As for \( X_0 \) we can choose either \( F_{\text{PBC}} \) or \( F_{\text{APBC}} \) (these two quantities are so correlated that we can...
consider the most favourable case in which we identify them). Note that, in this approximation, $r_{01} = r_{02} = r$. Hence, only for $r > 1/\sqrt{2} \approx 0.71$ (much larger than the correlation we found), the inequality (D.6) guarantees some correlation, i.e. $r_{12} > 0$.

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