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Competition between Energy- and Entropy-Driven Activation in Glasses

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In simplified models of glasses we clarify the existence of two different kinds of coexisting activated dynamics, with one of the two dominating over the other. One is the energy barrier hopping that is typically used to understand activation, and the other, which we call entropic activation, is driven by the scarcity of convenient directions in phase space. When entropic activation dominates, the height of the energy barriers is no longer the primary factor governing the system's slowdown. In our analysis, dominance of one mechanism over the other depends on temperature and the shape of the density of states. We also find that at low temperatures a phase transition between the two kinds of activation can occur. Our observations are used to provide a scenario that can harmonize the facilitation and thermodynamic pictures of the slowdown of glasses into a single description.

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I. INTRODUCTION

Glasses are inherently slow systems. Their slowness ⁵⁴ 16 can be captured by mean-field (MF) theory, which re- 55 17 cently motivated a series of breakthroughs that allowed ⁵⁶ 18 for a deeper understanding their sluggish behavior [1-3]. ⁵⁷ 19 However, MF theory predicts divergences of the relax-58 20 ation time that do not occur in real systems, because it ⁵⁹ 21 does not capture relaxation mechanisms that appear in $_{60}$ 22 low-dimensions. These are generically called *activation*, 61 23 and they are most often pictured as the hopping of energy 62 24 barriers [4, 5]: since in MF the barriers diverge with the $_{63}$ 25 system size N, a simple argument is that activation in $_{64}$ 26 MF cannot occur because barriers cannot be hopped [6]. 65 27 However, activation can be studied in MF models by $_{66}$ 28 restricting to finite-N and long times [7, 8]. Several works ₆₇ 29 focused on comparing the dynamics of simple MF mod-68 30 els, such as the Random-Energy Model (REM) [9], to 69 31 the Trap Model (TM) [10-12], to establish whether the ₇₀ 32 barrier hopping dynamics can be assimilated to jump-71 33 ing between traps with a fixed threshold energy [13-21]. 72 34 Other works studied the saddles connecting minima $[22-_{73}]$ 35 25], extensions of the Franz-Parisi potential [26], or path-74 36 integral approaches to study the dynamics between dif-75 37 ferent minima [27]. 38

Comparisons with the TM were also performed in mod-39 els with a trivial landscape, such as the Step [28] or Fun-40 nel models [29], where it was shown that entropic effects 41 can lead to Trap-like activation, if instead of considering ⁷⁶ 42 basins in phase space we construct them dynamically. 43 Indications of entropic effects in long-time dynamics was 77 44 also found in less idealized systems, such as the *p*-spin $\frac{1}{78}$ 45 model [30, 31], finite-connectivity Step models [32], or 79 46 even 3D Lennard-Jones mixtures between the dynami-47 cal temperature $T_{\rm d}$ and the onset temperature $T_{\rm o}$ [33] 48 and experimental metallic glasses [34]. In these works, $\frac{1}{82}$ 49 however, the underlying framework is either that acti-50 vation only exists as barrier hopping [4, 11]; either that 51

it is an entropic effect that can be assimilated to barrier hopping [28, 29]; or it is a transient behavior which eventually turns into hopping [7, 32, 35]. This is hard to reconcile with other pictures of the dynamical arrest of glasses, such as facilitation [36, 37], that argue that the landscape (energy barriers) is not crucial to explain the slowness of glasses, which should instead be attributed to kinetic constraints.

Here, we clarify the nature of these entropic effects, showing how under the right lens they can be used to unify the landscape with the facilitation pictures. We take a paradigmatic model of glasses, the REM [9], and show that both energy- and entropy-driven activation mechanisms coexist. When energy-driven activation dominates, the system's slowness is driven by the energy barrier separating basins, while when entropic activation dominates, the height of the barrier becomes unimportant, and the slowness is instead driven by the scarcity of convenient directions. In our analysis, the dominance of one mechanism or the other depends on the density of states $\rho(E)$, and on the temperature $k_{\rm B}T \equiv \beta^{-1}$, which is the control parameter of a non-equilibrium phase transition between the two different activated regimes (we set $k_{\rm B} = 1$ in this work).

II. MODELS

In the REM, we have a system with N spins, $s_i = \pm 1$. The dynamics takes place by flipping a single spin at a time: from any configuration one can reach N neighboring states. The energy of a configuration is independent of the configuration itself, and is drawn from a probability distribution $\rho(E)$. Two choices of $\rho(E)$ are used in literature. The initial formulation of the REM used a Gaussian energy distribution [9],

$$\rho_g(E) = \frac{1}{\sqrt{2\pi N}} e^{-\frac{E^2}{2N}},$$
 (1)

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while more recent efforts also considered the Exponential¹⁰⁵
 REM (EREM) [20], which has

$$\rho_e(E) = \beta_c e^{\beta_c E} \Theta(-E) , \qquad (2)_{100}^{10}$$

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where we set $\beta_{\rm c} = 1$. These models have a transition¹⁰⁹ from a paramagnetic to a glassy phase at $\beta_{\rm g} = \sqrt{2 \ln 2_{111}}$ and $\beta_{\rm e} = \beta_{\rm c}$, respectively.

90 III. CHARACTERISTIC ENERGIES

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A. Threshold Energy

In both models, we can define a threshold energy, $E_{\rm th}$,¹¹⁵ analogous to that of the *p*-spin model [38], above which¹¹⁶ no barriers are typically found. We calculate it as the¹¹⁷ energy for which the probability that a neighboring con-¹¹⁸ figuration has a lower energy is 1/N [20, 39], ¹¹⁹

$$\frac{1}{N} = \int_{-\infty}^{E_{\rm th}} \rho(E) dE \,. \tag{3}_{122}^{121}$$

From Eq. (3) one obtains that, to leading order, the¹²⁴ threshold energies of REM and EREM are 125

$$E_{\rm th}^g = -\sqrt{2N\ln N}\,,\tag{4}$$

$$E_{\rm th}^e = -\frac{1}{\beta_c} \ln N \,. \tag{5}_{126}$$

This definition ensures that there are asymptotically no₁₂₈ barriers above $E_{\rm th}$, and descends from the mutual inde-129

pendence of neighboring configurations in the (E)REM. ¹³⁰
After long times, the system typically finds itself in a¹³¹
configuration with an extensively deep energy [20, 39],¹³²
which we call trap (or basin). To transition from one¹³³
trap/basin to another, the system needs to climb to the¹³⁴
threshold. Energetic activated dynamics is mainly driven¹³⁵

by the jumps on these energy barriers, in a manner that is analogous to what happens in the Trap Model, in which the time spent in a trap of energy E follows and Arrhenius law, $\tau \sim \exp[\beta(E_{\rm th} - E)]$. This was indeed found to be the case, by looking at the limiting values of the aging functions and comparing them with the predictions of the TM [18, 20].

B. Attractor Energy

We can also define another characteristic energy, which stems from toy models which represent a purely entropic kind of activation [28, 29, 40]. This quantity was called threshold energy in Refs. 28 and 29. As we will show, it is quantitatively and qualitatively different from the threshold energy, so we henceforth refer to it as the *at*tractor energy, $E_{\rm a}$. This quantity was first defined in Ref. 41, as the energy such that the energy of the next step is, on average, neither higher nor lower. However, we find it more intuitive to work with the definition given in Ref. 28, according to which $E_{\rm a}$ is the energy at which the probability $P_{\uparrow}(E)$ of increasing the energy at the next step is equal to the probability $P_{\downarrow}(E)$ of decreasing it:

$$P_{\uparrow}(E_{\rm a}) \equiv P_{\downarrow}(E_{\rm a}) \,. \tag{6}$$

 $P_{\uparrow}(E)$ (or $P_{\downarrow}(E)$) is calculated by considering the probability of finding neighbors with a higher (or lower) energy E', and the transition rate $w(E \to E')$ telling whether a move towards such an energy is accepted. We consider Monte Carlo Metropolis dynamics, $w(E \to E') =$ $\min(1, \exp(-\beta(E' - E)))$. As for the distribution of neighboring energies, it is particularly easy to calculate in the (E)REM, because the energy distribution of the neighbors is the same as that of the whole system. Therefore. one has

$$P_{\downarrow}(E) = \int_{-\infty}^{E} dE' \rho(E') w(E \to E') = \int_{-\infty}^{E} dE' \rho(E') , \qquad (7)$$

$$P_{\uparrow}(E,\beta) = \int_{E}^{\infty} dE' \rho(E') w(E \to E') = \int_{E}^{\infty} dE' \rho(E') e^{-\beta(E'-E)}, \qquad (8)$$

where we made it explicit that P_{\uparrow} depends on β . We note₁₄₃

¹³⁷ that, since the configurations in the (E)REM are i.i.d.,

¹³⁸ $P_{\downarrow}(E)$ is the cumulative distribution of $\rho(E)$, so we can ¹³⁹ write $P_{\downarrow}(E_{\rm th}) = \frac{1}{N}$.

Since $P_{\uparrow}(E,\beta)$ varies with β while $P_{\downarrow}(E)$ does not, also E_{a} must vary with temperature. For the Gaussian REM, we find that the attractor energy is

$$E_{\rm a}^g = -\frac{N\beta}{2} \,, \qquad \qquad (9)_{\rm _{145}}^{\rm ^{144}}$$

whereas for the EREM it is

$$E_{\rm a}^e = \begin{cases} \frac{1}{\beta - \beta_{\rm c}} \ln\left(\frac{2\beta_{\rm c} - \beta}{\beta_{\rm c}}\right) ; & \text{if } 0 < \beta < 2\beta_{\rm c} , \\ -\infty ; & \text{if } \beta > 2\beta_{\rm c} . \end{cases}$$
(10)

The attractor energy for the EREM is the same that is found in Ref. 28 in a model which corresponds to a global



FIG. 1. Left: Phase diagram of the EREM, with the as-180 sociated characteristic energies and dynamical regimes. For₁₈₁ $\beta < \beta_{\rm c}$ we have the equilibrium phase. The solid line is₁₈₂ the equilibrium energy $\langle E \rangle$. At $\beta = 2\beta_{\rm c}$ we have the transition from the entropically to the energetically activated regime. The dashed line is the attractor energy. The horizontal dashed-dotted line represents $E_{\rm th}(N = 10)$. $E_{\rm th}$ exists $\forall \beta$ but is only relevant for $\beta > 2\beta_{\rm c}$. **Right**: two diagrams¹⁸⁶ showing how activated dynamics qualitatively takes place in¹⁸⁷ each of the regimes.

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¹⁴⁶ dynamics in the EREM. ¹ This is due to the fact that¹⁹¹ ¹⁴⁷ in the EREM the distribution of neighboring energies ¹⁴⁸ (local) is equal to $\rho_e(E)$ (global).

Note that $E_{\rm a}$ is not directly related to the equilibrium¹⁹² 149 energy $\langle E \rangle$. For example, in the EREM, there is no equi-150 librium energy from $\beta \geq \beta_{\rm c}$ (the equilibrium energy di-193 151 verges to $-\infty$ at $\beta = \beta_c$, ² but E_a^e still is finite for₁₉₄ 152 $\beta_{\rm c} \leq \beta < 2\beta_{\rm c}$. We depict this in Fig. 1. In other words, 195 153 the system still is *attracted* towards finite energies even₁₉₆ 155 though the equilibrium energy is divergingly negative. In₁₉₇ 156 fact, it is straightforward to check that when $E < E_{\rm a}$ (or₁₉₈ 157 $E > E_{\rm a}$) the next configuration during the dynamics is₁₉₉ 158 more likely to have a higher (or lower) energy. Intuitively,200 159 what happens is that even when neighbors with lower en-201 160 ergy exist, they are to hard to find, and the system will₂₀₂ 161 find it more convenient to just increase the energy. How-203 162 ever, the system will immediately abandon high-energy₂₀₄ 163 configurations, while it will stay a very long time in the₂₀₅ 164 low-energy ones. 165 206

IV. ENERGY- AND ENTROPY-DRIVEN ACTIVATION

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A. Energy-driven

We call *energy-driven* the typical thermally activated²¹⁴ dynamics consisting of hopping barriers with an Arrhenius rate. Since in the (E)REM the overwhelming major-

²In the EREM we have
$$\langle E \rangle = \frac{\int_{-\infty}^{0} e^{(\beta_{\rm C} - \beta)} E dE}{\int_{-\infty}^{0} e^{(\beta_{\rm C} - \beta)} dE} = -\frac{\beta_{\rm c}}{\beta_{\rm c} - \beta}.$$

ity of the barriers are at $E = E_{\rm th}$ (see *e.g.* Ref. 21), this kind of activation resembles the dynamics of the Trap Model [10, 11, 18, 20].

B. Entropy-driven

Contrary to $E_{\rm th}$, $E_{\rm a}$ can also exist in systems with a single energy basin, such as the Step [28] or the Funnel model [29]. In these systems, despite the absence of energy-driven activation, the dynamics is a renewal process, provided that one identifies the traps dynamically, as all the configurations visited while $E < E_a$ [28]. With this construction, the relationship between aging functions and trapping time distributions is the one predicted by the TM [28], and the typical time scales grow exponentially in N [29]. In other words, $E_{\rm a}$ identifies an activated dynamics which is *not* driven by the height of the energy barriers (as there are none), but which shares many signatures of energy-driven activation. This kind of activated dynamics is instead driven by the scarcity of convenient directions, and was therefore called entropydriven [28].

C. Interplay between the two mechanisms

In the (E)REM, we can study the interplay between these two mechanisms. Since $E_{\rm th}$ is the minimal height at which the system must go in order to leave a trap, the entropic mechanism is not expected to play a role when $E_{\rm a} < E_{\rm th}$. We see that, for sufficiently large sizes, in the REM $E_{\rm a}^g(\beta) < E_{\rm th}^g \forall \beta$. Therefore, we expect that activation in the REM is purely energy-driven.

In contrast, in the EREM we have different behaviors depending on β . When $\beta > 2\beta_c$, we have $E_a < E_{th}$, so the slow dynamics should be energy-driven. When instead $\beta_c < \beta < 2\beta_c$ (excluding a range of β close to $2\beta_c$ which shrinks with increasing N), we have $E_a > E_{th}$. This indicates that even when the system manages escaping a trap, reaching E_{th} , it will likely keep going up in energy, attracted towards E_a . Thus, the height of the barrier, $(E_{th} - E)$, is not that important. The reason for this is that even though in this regime there are directions in phase space which would decrease the energy, they are too rare, and the system would rather keep increasing its energy than "invest time" looking for a descending direction. In Fig. 1 we show a diagram of how activation takes place in each of the two out-of-equilibrium phases.

Since activated dynamics is relevant in the limit of large but finite N, we can work out the transition inverse temperatures β_* by setting $E_{\rm a}(\beta_*, N) = E_{\rm th}(N)$. This gives us the N-dependent transitions

$$\beta_*^g = 2\sqrt{\frac{2\ln N}{N}} \stackrel{N \to \infty}{\longrightarrow} 0, \qquad (11)$$

$$\beta_*^e = \beta_c \frac{2\ln N + W(-\frac{\ln N}{N})}{\ln N} \xrightarrow{N \to \infty} 2\beta_c , \qquad (12)$$

¹By global dynamics we mean that any number of spins is flipped at each time step, in contrast with the single-flip dynamics considered in this paper. With global dynamics local minima disappear.



FIG. 2. Median $E_{\text{ridge}}(\beta; N)$ in the EREM (a) and REM (b). Different lines stand for different system sizes. Here and in Fig. 3, results from memory-1 dynamics are shown in solid lines, and results from full-memory dynamics (N < 30) are shown as markers.

where W(z) is the Lambert function. In the Gaussian 215 REM the entropic phase disappears for increasing N. In 216 the EREM, instead, the transition stays at a finite tem-217 perature, and we have entropy-driven activation at low 218 β , and energy-driven activation at high β . 219

v. **RIDGE ENERGY AND PHASE** 220 TRANSITION 221

We run Monte Carlo simulations (details in App. A) 222 to verify this transition from an energy-driven phase at 223 high β , to an entropy-driven phase at lower β . Since 224 REM and EREM do not allow for exact simulations at 225 large system sizes, for sizes $N \geq 30$ we rely on modi-226 fied dynamics, where every time that a new configuration 227 is visited, all its neighbors' energies, except that of the 228 last-visited configuration, are drawn anew. We call this 229 *memory-1 dynamics*, and elaborate more on it in App. B. 230

Our intent is now to relate this transition to physi-250 231 cal observables. We measure the ridge energy, $E_{\rm ridge}$,²⁵¹ 232 defined as the highest-reached energy during each basin²⁵² 233 transition, *i.e.* in each of the time intervals during which²⁵³ 234 $E(t) > E_{\rm th}$. With energy-driven activation, we expect²⁵⁴ 235 that $E_{\rm ridge}(\beta; N)$ will stay close to $E_{\rm th}(N)$, while for²⁵⁵ 236 entropy-driven activation it will overshoot to higher val-256 237 ues. In Fig. 2 we plot the median $E_{\rm ridge}$ as a function²⁵⁷ 239 of β , for EREM and REM. While in the REM the ridge²⁵⁸ 240 energies decrease steadily $\forall \beta$, in the EREM we see two²⁵⁹ 241 distinct entropy-driven (low β) and energy-driven (high²⁶⁰ 242 β) phases. 261 243

As we show in Fig. 3, the ridge energy scales with $N \text{ in}^{262}$ 244 the way we expect. In the EREM at low β we are in the₂₆₃ 245 entropic phase, and $E_{\rm ridge} \sim -1 \sim E_{\rm a}$. In the energy-264 246 driven phase, instead, $E_{\rm ridge} \sim -\ln(N) \sim E_{\rm th}$. In the₂₆₅ 247 REM, where we only have energy-driven activation, the₂₆₆ 248 ridge energy follows $E_{\rm th}$ at every β . 249 269



FIG. 3. Median E_{ridge} as a function of N in the EREM and REM (inset). Different lines correspond to different values of β . The black dashed line represents $E_{\rm th}(N)$ for each model, according to Eqs. (4) and (5).



FIG. 4. The density of ridge energies in the EREM model, using memory-1 dynamics, for N = 10000.

Through the lens of the median $E_{\rm ridge}$, the transition appears at β slightly smaller than 2, which we understand through two observations. First, β^e_* [Eq. (12)] indicates when $P_{\uparrow} > P_{\downarrow}$. However, in order to reach $E_{\rm a}$ from $E_{\rm th}$, the system needs to go through a large number of steps (*i.e.* growing with N) with ascending energy. If P_{\uparrow} is only slightly larger than P_{\downarrow} (which is what happens at β slightly lower than 2), this is not enough to accept a sufficiently large number of steps to go all the way up to energies of order 1. Second, this transition from energyto entropy-driven activation has features of a first-order phase transition. We see this from Fig. 4, where we plot the distribution $P(\frac{E_{\text{ridge}}}{|E_{\text{th}}|})$ at three different temperatures. At low β it is peaked around 0, while at high β it is peaked around -1, as expected. Around the transition, instead, we see the characteristic two-peak structure of first-order phase transitions.

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VI. CONCLUSIONS

A. Summary

We showed that the "threshold energy" calculated dy-³²⁴ 272 namically in models with a trivial landscape $[28, 29]^{325}$ 273 does not correspond to the typical landscape-based def-³²⁶ 274 inition of threshold energy, and decided to rename it as³²⁷ 275 attractor energy. Threshold and attractor energies de-³²⁸ 276 fine two different kinds of activated dynamics, entropy-³²⁹ 277 and energy-driven, which can coexist, though typically³³⁰ 278 one dominates over the other. Energy-driven activa-³³¹ 279 tion corresponds to the typical picture of Arrhenius-like³³² 280 basin hopping, whereas entropy-driven activation is not³³³ 281 driven by barrier heights, but rather by the scarcity of $^{\scriptscriptstyle 334}$ 282 convenient directions. While at sufficiently low temper-³³⁵ 283 atures energetic activation always exists in landscapes³³⁶ 284 with multiple minima, the existence of a higher-T phase³³⁷ 285 where entropy-driven activation dominates depends on 286 the shape of $\rho(E)$. In this entropic activation phase, the 287 attractor energy $E_{\rm a}$, towards which the system is reg-³³⁸ 288 ularly driven, is higher than the threshold energy $E_{\rm th}$,³³⁹ 289 the height of the barriers loses relevance and we have a 290 breakdown of the Arrhenius behavior. 340 291

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В.

Reconsidering the importance of saddles

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One consequence is that the study of the transition³⁴⁵ paths of glasses by searching the lowest saddles, a techni-³⁴⁶ cally daunting task [22–25], is potentially not informative³⁴⁷ for the dynamics at temperatures around the glass tran-³⁴⁸ sition. Calculating the attractor energy, with its compar-³⁴⁹ ison to the threshold, is simpler and has the potential of³⁵⁰ unlocking the true activated nature of the dynamics. ³⁵¹

300 C. Rationalizing observations in other systems 354

Additionally, entropic activation can elegantly ex-301 plain an apparently puzzling result recently found by T. 302 Rizzo [27], who calculated, in the spherical *p*-spin model,³⁵⁶ 303 the path from one equilibrium low-temperature configu-304 ration to another. He found that the maximum energy₃₅₇ 305 reached during this transition is considerably higher than 358 306 $E_{\rm th}$ even though the largest barriers should not exceed³⁵⁹ 307 $E_{\rm th}$. We see that the same phenomenon occurs in the₃₆₀ 308 EREM, in a similar setting (we followed the system from₃₆₁ 309 one trap at $E < E_{\rm th}$ to another one), where we showed₃₆₂ 310 that the system is pushed towards a higher energy $E_{\rm a}$ by $_{363}$ 311 the scarcity of paths with energy close to $E_{\rm th}$. We can₃₆₄ 312 thus attribute this behavior to the same entropic effects, 365 313 and conjecture that at lower temperatures the paths will₃₆₆ 314 be close to $E_{\rm th}$ (as per the transition that we found in₃₆₇ 315 the EREM). 368 316

This is also consistent with recent numerical obser-369 vations by Stariolo and Cugliandolo in the discrete *p*-370 spin model, that the trapping time distributions seem to 371 follow the Step-model predictions better than those of the Trap Model [30, 31]. In particular, they define the traps dynamically by taking, instead of the position of the saddle, the highest point reached during the dynamics. Therefore, they are calculating the traps through the attractor instead of the threshold energy, which explains the observed Step-like behavior. Furthermore, they find that the energy of the ridge is larger than $E_{\rm th}$, which is an indication that the lowest-energy path is not used, just as we find here.

Also in 3D systems, such a Lennard-Jones mixtures, although activated dynamics takes place between $T_{\rm o}$ and $T_{\rm d}$ [4, 5, 42], it was recently shown that it is not dominantly of an energy-driven kind, since, for example, the system is moving at energies significantly higher than the ridges separating metabasins [33]: the height of the barriers separating basins does not play a crucial role in this regime.

D. The nature of activation in different kinds of models

A typical intuition of why MF results do not apply in low dimensions is that the energy barriers diverge with the system size. However, in systems like hard spheres there are no energy barriers, so it seems like beyond-MF effects are not attributed to the right mechanism. It was suggested in several occasions that the low-D correspondent of a MF model can be non-trivial [43–45]. Our analvsis suggests that we should often think of activation less as the hopping of energy barriers, and more as a search for convenient directions, which require a collective cooperative behavior that is hard to obtain by randomly moving particles. We should therefore regard activation as a process beyond MF, not because the barriers are diverging, but rather because it involves processes (energetic and entropic) which take place on time scales $t \gg N$ (usually $t \sim e^N$).

E. Connection to Facilitation Theory

The dynamical facilitation picture shows that a strong glass-like slowdown can appear in a trivial landscape (without barriers), with the dynamics being slowed down by dynamical constraints [36, 46]. These dynamical constraints are localized in space, so we do not aim at a 1:1 correspondence with a mean-field model (as the (E)REM), but we do note that the entropic barriers that lead to the entropic phase in the EREM are (soft) kinetic constraints. In fact, they mark directions in phase space along which motion is suppressed (with high probability a spin cannot be flipped), and they also appear in the absence of potential energy barriers [28, 29, 41, 47, 48]. As an extra, here, kinetic constraints are not the only slow dynamics mechanism, but they act concurrently with energetic activation; in addition to the fast mechanism of ³⁷³ nomenological ingredients of facilitation are present, to-425

gether with additional mechanisms that should appear in426
 the description of a glass.

Since the dynamical constraints, as well as activation, 428 376 appear at T_{0} [4, 36], we suppose a correspondence with⁴²⁹ 377 the thermodynamic transition in the EREM (at $\beta = \beta_c$).⁴³⁰ 378 Cooling further, one observes entropy-driven activated⁴³¹ 379 dynamics between $T_{\rm o}$ and $T_{\rm d}$ [33], and at $T_{\rm d}$ the dy-432 380 namics is deemed to become energy-driven [49]. Also in₄₃₃ 381 the EREM, entropic activation stays dominant until the434 382 transition to the energetic phase at $\beta = 2\beta_{\rm c}$, suggesting₄₃₅ 383 a correspondence between T_d and the entropic-energetic 384 transition we observed in the EREM. However, in order 385

to confirm these speculations we need to be able to ob-436 serve entropic activation in more complex models.

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F. Verifying entropic activation in more complex 436 models

In simple models such as the EREM or the $Funnel_{441}$ 390 model, the entropic phase is present both for local and_{442} 391 global phase space dynamics [29]. However, this is not_{443} 392 necessarily true for more complex models such as the_444 393 *p*-spin. A starting point which would allow to study cor_{445} 394 related energy levels without changing the overall $\rho(E)_{446}$ 395 would be the Correlated REM [21] and the Number Par-447 396 titioning Problem (NPP) [50]. These two models have₄₄₈ 397 different kinds of correlations since, in the first, the₄₄₉ 398 basins are smooth, while in the NPP the traps are anti- $_{450}$ 399 correlated with their neighbors. In particular, in the NPP_{451} 400 it was observed that, at $\beta = 2\beta_c$, there is a transition₄₅₂ 401 within the glass phase, associated with a violation of the $_{453}$ 402 fluctuation-dissipation theorem, with relevant differences₄₅₄ 403 between local and global dynamics. The relationships₄₅₅ 404 between our findings and those of Ref. 50 could be stud- $_{456}$ 405 ied analytically within the framework of Ref. 51, which $_{457}$ 406 studies the Step model in the limit of slowly decorrelating₄₅₈ 407 408 variables. 459

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Appendix A: Numerical details

1. Monte Carlo Simulations

Our simulations are performed with the Metropolis Monte Carlo algorithm [52]. Depending on the value of β , we use two equivalent implementations, which we call "standard" and "Gillespie". The standard dynamics is a textbook Monte Carlo simulation with Metropolis acceptance criteria (see e.g. Ref. 53 for a detailed description). The run time of the standard procedure is tightly bound, with t_{max} time steps. However, at large β , the rejection rate of standard dynamics is high and it may take many steps for a new configuration to be accepted. We therefore use the Gillespie procedure (which is formally equivalent) is much more efficient. The Gillespie algorithm is a rejectionless method, that computes the time that the system spends in a given configuration, and transitions without rejection to one of the neighbors, according to how probable it is to transition to each neighbor. For a more detailed and didactic explanation of the Gillespie algorithm we refer the reader to Ref. 54. While the Gillespie method this is efficient at large β , it is extremely inefficient at small β . Thus, we set a cutoff of $\beta/\beta_c = 2.3$, such that when $\beta/\beta_c < 2.3$, dynamics are run using the standard procedure, and Gillespie otherwise. We also use $t_{\rm max} = 10^7$ for all calculations.

Note that the standard and Gillespie procedures are formally equivalent [54]. To demonstrate this empirically, we show the mean energy E(t) for various choices of Nand β (with $\beta_c = 1$) in the EREM, in Fig. 5.

2. Inherent Structures

To ensure that we only measure transitions between different traps, with memory dynamics we measure the inherent structure (IS) before and after the transition, and keep the transition only if they are different. To measure the IS we take the steepest descent path towards the nearest minimum. Since the system is discrete, we define steepest descent as a trajectory which at each step goes to its lowest-energy neighbor, until a minimum is reached.



FIG. 5. Energy as a function of time, in simulations with₅₀₁ Gillespie (red) and regular Monte Carlo (blue) dynamics.₅₀₂ Each row is a different inverse temperature. On the first column we have the full memory dynamics, while on the second ⁵⁰³ we have the memory-1 dynamics (App. B). ⁵⁰⁴

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Threshold Energy

3.

As already pointed out in Ref. 20, the subleading cor_{509} rections in the threshold energy of the REM are $large_{510}$ (around 13% in the largest sizes). Therefore, in our REM₅₁₁ simulations we calculated the threshold energy numeri-₅₁₂ cally. For the EREM simulations, we used Eq. (4).

481 Appendix B: Memory and Memory-1 dynamics 516

In REM and EREM, the energy of each configuration⁵¹⁸ is a fixed random variable. This means that, for N spins,⁵¹⁹ there are 2^N energies sampled from $\rho(E)$, each of which⁵²⁰ is permanently paired to some configuration. Therefore, in order to perform a long simulation in these models, we need to store the energy of all the 2^N states, to ensure that if a configuration is visited twice its energy has not changed. Storing 2^N double precision floating point numbers is expensive in terms of memory, and limits the largest system sizes that we can simulate. This is why, in order to simulate $N \geq 30$, instead of storing the all the 2^N energies, we only stored the last visited one, and sampled anew the remaining N - 1 neighbors. We call this dynamics *memory-1*, in contrast with the *memory* dynamics which stores all the energies throughout the whole simulation.

This simplification neglects loops in the dynamics, which for large N are arguably rare, and does not allow the system to directly return to configurations visited more than one step earlier. The latter can be seen as an advantage, since we want to wash back and forth motion out of the dynamics we are measuring [4, 20]. Since the REM and EREM dynamics is a renewal process [20], we can expect that anyhow after some time the previously visited phase space should be forgotten.

An additional difference between memory and memory-1 dynamics is that the latter does not suffer from finite size effects descending from the phase space being of limited size: with memory dynamics there exists a lowest-reachable energy, while with memory-1 it is always possible to reach a lower energy. In other words, memory-1 dynamics suffer less from finite-size effects than the exact dynamics, and in any case this kind of effects does not affect the calculation of $E_{\rm ridge}$. In Fig. 6 we show the comparison between the two dynamics for varying β and N. At all temperatures, the difference between the two dynamics present finite-size effects, which decrease as the system becomes larger.

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FIG. 6. Energy as a function of time for memory and memory-1 dynamics. The dashed curve is the slope $-T \ln(t)$ that one would expect in the infinite-size limit.

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