Intermittent relaxation in hierarchical energy landscapes

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We numerically simulate a thermalization process in an energy landscape with hierarchically organized metastable states. The initial configuration is chosen to have a large energy excess relative to the thermal equilibrium value at the running temperature. We show that the initial energy surplus is dissipated in a series of intermittent bursts, or quakes, whose rate decreases as the inverse of the age of the system. In addition, one observes energy fluctuations with a zero-centered Gaussian distribution. These pertain to the pseudoequilibrium dynamics within a single metastable state and do not contribute to the energy dissipation. The derivative of the thermal energy with respect to the logarithm of time is asymptotically constant and comprises a temperature-independent part and a part with an Arrhenius temperature dependence. The findings closely mirror recent numerical simulation results obtained for microscopic glassy models. For these models, record-sized energy fluctuations have been claimed to trigger intermittent events during low-temperature thermalization. In the present model record-sized fluctuations are by construction needed to trigger changes from one metastable state to another. This property thus suffices to explain the statistical property of intermittent energy flow in complex metastable systems.

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I. INTRODUCTION

Many characteristics of low-temperature glassy dynamics are only weakly related to details of the microscopic interactions. Aging processes, for example, generically follow a change of an external parameter—e.g., a temperature quench. In experimental glassy systems a sequence of large, so-called intermittent, configurational rearrangements can be observed, which generate non-Gaussian tails in the probability density function (PDF) of configurational probes [1–6]. In microscopic model systems [7,8], the PDF of the energy fluctuations following a thermal quench also features a zero-centered Gaussian and an exponential tail which covers large negative changes. The former describes pseudoequilibrium fluctuations, and the latter is related to shifts between different metastable attractors. These and other features have been recently analyzed using an Edwards-Anderson spin-glass model [7] and an even simpler Ising model with four-spin plaquette interactions [9], which is known to possess central features of glassiness—e.g., a metastable supercooled phase and an aging phase [10,11]. For both models, the rate of intermittent energy flow out of the system was found to fall off with the reciprocal of the system age. For the plaquette model, the temperature dependence of the rate was also analyzed in detail.

The above aging properties can be understood using the idea that the attractors dynamically selected during the process are marginally stable [12,13]. The so-called *record dynamics* scenario [7,13] then links the intermittent events, or *quakes*, to record-sized energy fluctuations occurring within thermalized local domains. Record fluctuations are not associated with a definite scale. For this reason alone, they will not lead to observable effects, unless the energy landscape supporting the fluctuations is self-similar under a change of scale. Conversely, within a self-similar energy landscape, record-sized fluctuations are required to induce attractor changes.

Simple hierarchical models of configuration space are already known to explain many facets of complex relaxation [14–19]. In these mesoscopic descriptions, the configuration space of a physical system is coarse-grained into a graph whose nodes represent lumped sets of microscopic configurations with similar energies. Each node is thus simply characterized by its energy—i.e., the typical energy of its constituents—and by a degeneracy—i.e., the number of its constituents. Lumping is physically reasonable if the microscopic configurations lumped into the same node are able to reach a state of local thermal equilibrium on a time scale short compared to the time it takes to access configurations belonging to other nodes. Reference [18] provides an example where the lumping is explicitly carried out starting with a microscopic model. Connections between different nodes represent possible dynamical pathways. In tree models, the connectivity is at the lowest level possible for a connected configuration space. The unique path between two arbitrary nodes represents the dominant path in the original dynamical problem—i.e., typically for thermal dynamics, the path through the lowest possible energy barrier. In the tree graph shown in Fig. 1 the vertical axis represents the energy and a hierarchy of barriers of different sizes is present. By construction larger and larger barriers must be overcome starting from one of the bottom nodes in order to access larger sets of states. Correspondingly, any subtree contains a number of lesser subtrees characterized by smaller barriers.

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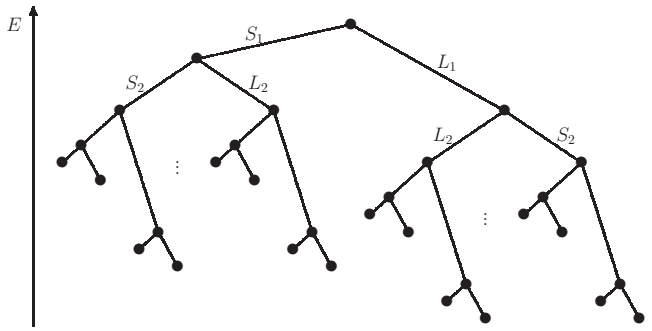

FIG. 1. The randomized *LS* tree used as model energy landscape in the simulations. Contrary to previous *LS* tree setups, the *L* and *S* branches are not of equal length for the whole tree, but level dependent. This extension leads to a diversification of the time scales present within the tree and thus breaks unphysical logarithmic oscillations in the energy decay.

Also note that the energy minima have different energies and represent physically different metastable configurations. This inequivalence was introduced in the context of the so-called *LS* tree model [19,20] of which Fig. 1 shows a generalization. The *LS* model's scale invariance is restricted to a discrete set of energy rescalings due to the presence of only two "elementary" energy scales—i.e., the energy differences *L* and *S* between neighboring nodes. To approach full rescaling symmetry, the present study considers a randomized version of the model. While exact analytical results are then no longer possible, the randomized model still offers a strikingly simple and general conceptualization of a highly complex relaxation behavior. In particular, only record-sized energy fluctuations can induce transitions out of a subtree into a larger subtree containing states of lower energy. Comparing the statistics of intermittent energy flow in a hierarchically structured energy landscape with the corresponding properties of microscopic models provides a direct check of whether record-sized energy fluctuations indeed are the main mechanism for thermal relaxation in complex systems.

In this article, energy traces are obtained from isothermal simulations of an ensemble of randomized *LS*-model aging after a thermal quench. The energy fluctuations are treated as time-resolved calorimetry data. Their PDF shows the fingerprints of intermittent heat flow. The form of the local density of states of the attractors is extracted from the Gaussian part of the fluctuations, and the rate of energy flow is extracted from the tail. The information is analyzed mathematically and related to the known geometrical properties of the model.

II. MODIFIED *LS*-TREE ENSEMBLES

In spatially extended systems with short-range interactions, one expects thermalization to occur independently within a number of slowly growing domains or clusters of neighboring degrees of freedom. The configuration space of the full systems correspondingly factorizes into a product of configuration spaces, each term belonging to a single domain. Domains are expected to have a hierarchical organization, which, in the present context, is rendered by the modified *LS* tree described below.

The randomized *LS* model used in the simulations can be pictured as an upward rooted tree with the vertical scale representing the energy as shown in Fig. 1. The *n*th level of the tree comprises all the nodes connected to the root by precisely *n* edges, with $n=0,\ldots,N$. With the exception of the "bottom" level with index $n=N$, each node is connected to two "daughters" of lower energy by a "longer" and a "shorter" edge. The modification of the original model [19,20] consists in choosing, independently for each level, new random values of *L* and *S*, as discussed further below. Accordingly, the energy differences along the "longer" and "shorter" edges are $\Delta E=L_n$ and $\Delta E=S_n$ for each level *n*. The above procedure removes the oscillation on a logarithmic time scale characteristic of a regular tree, concomitantly decreasing the energy scale corresponding to the smallest barrier in the system. Each node represents a lumped set of configurations and hence possesses a degeneracy. In the model, the degeneracy of a node equals the sum of the degeneracies if its L_n and S_n daughters, each multiplied by a factor κ_{L_n} and κ_{S_n}, respectively. Bottom nodes are not degenerate. With this prescription, the overall degeneracy of the model increases in a nearly exponential fashion, as the level index increases from the bottom. A list of values,

$$\mathcal{E}=\{2^{i/4-1}:\quad i=0,\ldots,19\}, \tag{1}$$

describes the possible energy differences. For each level of the tree, two values are drawn independently and with uniform probability from the list. They may be equal and are assigned to the respective *L* and *S* branches, ensuring that $L\geq S$.

Thermal relaxation is modeled as hopping between neighboring nodes, with up and down rates defined by

$$\Gamma_{\mathrm{up},j}=f_j\kappa_j e^{-\beta\,\Delta E_j},\quad \Gamma_{\mathrm{down},j}=f_j, \tag{2}$$

where the index $j\in\{L_n,S_n\}$ labels *L* and *S* edges at level *n*. The hopping rates obey the detailed balance condition $\Gamma(x,y)P_{\mathrm{eq}}(y)=\Gamma(y,x)P_{\mathrm{eq}}(x)$, where the equilibrium distribution is the Boltzmann distribution. So-called kinetic factors f_j are introduced to control the relaxation rate along each edge. Factors independent of *j* entail a trivial rescaling of the (arbitrary) time unit. In contrast, nonuniform factors considerably modify the dynamics on short time scales after a thermal quench [21]. For example, choosing $f_{S_n}\gg f_{L_n}$ favors downward transitions along the *S* edges, ensuring that an initial quench from the top node preferably ends near the shallowest metastable minimum. We achieve the same in a more *ad hoc* fashion by choosing the highest-lying and most shallow local energy minimum as the initial state for the aging dynamics.

III. DYNAMICS

The dynamical evolution of a single tree is studied using a rejectionless continuous-time Monte Carlo method [22], which operates with an intrinsic time variable *t*, initially set to zero. The following three steps are iterated: for the current

node, the possible transitions according to (2) are considered. In general, one upward and two downward transitions are available, except for the bottom states and the top state, which have, respectively, no downward and upward transitions. Among the neighbors to the current node, one is chosen with probability equal to the transition rate along the corresponding edge, divided by the sum of all rates out of the current node. A random waiting time is then drawn from an exponential distribution with average equal to the reciprocal of the transition rate. This waiting time is then added to the global time, and the position of the walker is finally updated.

Each tree in the ensemble is updated independently as described above. The result is an ensemble of time series, each describing the history of energy fluctuations of one member of the ensemble. The time series describing the total energy of the ensemble is then obtained by interweaving the time series pertaining to each tree into a single data stream ordered by increasing values of the time variable.

In the following, the symbol t stands for the system age—i.e., the time elapsed since the beginning of the simulation. The symbol t_w is the age of the system when data collection for the fluctuation PDF begins. Energy fluctuations are energy differences over a time interval $\delta t \ll t_w$.

IV. ENERGY TRANSFER STATISTICS

Our results are based on an ensemble of 2000 trees of height $N=12$, with 5000 independent runs on each tree. The model is set up with degeneracy growth parameters $\kappa_L=\kappa_S=2.20$ and kinetic factors $f_L=0.25$ and $f_S=1.00$. The latter of these values would generally carry units. However, the choice of the units does not affect the results, so they can be considered as being arbitrary here as well as in the figures showing the numerical results. The data pertain to systems initially quenched into the shallowest of the available minima—i.e., the minimum connected to the top node by a series of S links.

The PDF of the amount of energy exchanged within a time interval δt at system age $t_w+k\delta t$,

$$\Delta E = E(t_w + k\,\delta t) - E[t_w + (k-1)\,\delta t], \tag{3}$$

is collected over $k=1-100$ time intervals using $\delta t=1$ and starting at different values of t_w, in the range 10^3-10^5. The zero-centered Gaussian peak, flanked on the left by an exponential tail seen in Fig. 2, is the characteristic signature of intermittency. When k and δt are kept fixed, the relative weight of the intermittent tail decreases with increasing t_w. The width of the Gaussian fluctuations is independent of k and δt. We can then conclude that the fluctuations are (pseudo)equilibrium energy fluctuations within partially equilibrated subtrees. Clearly then, as the Gaussian fluctuations do not contribute to the net energy flow, the latter is carried exclusively by the tail of the distribution, which pertains to intermittent quakes.

The decay of the average energy is shown in Fig. 3.

After an initial transient stretching to approximately $t=200$, the energy decreases in time in a logarithmic fashion:

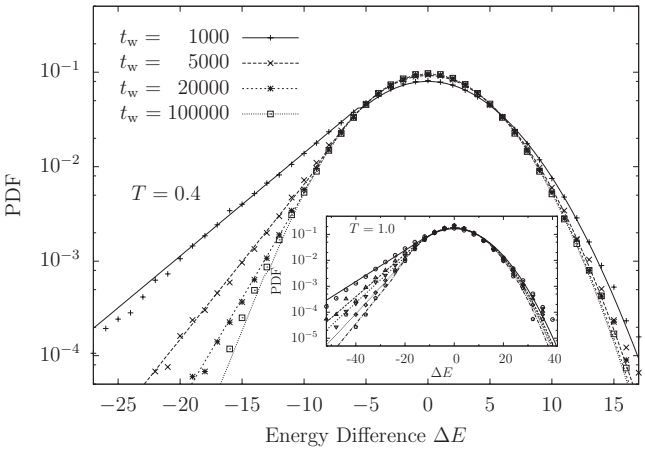

FIG. 2. The PDF of the amounts of energy exchanged between system and thermal bath within the time $\delta t=100$. Negative values represent an energy outflow, while positive values represent an energy inflow. The data are taken for four logarithmic equidistant times in the interval $t=[10^3-10^6]$. The inset (taken from [9]) shows an analogous figure obtained for simulation of a microscopic glassy model with plaquette interaction.

$$E(t,T) = -\,a(T)\ln(t) + \mathcal{C}. \tag{4}$$

In this model, a quake occurs when the lowest value of the energy seen in the simulation decreases. This event corresponds to a first visit to a new subtree containing states of lower energy and is—by construction—triggered by a record-sized (positive) energy fluctuation. The logarithmic rate of energy loss, $a(T)$, is thus the product of the logarithmic rate at which record-sized energy fluctuations occur with the average net amount of energy given off in a single quake. The logarithmic rate of record-sized energy fluctuation is independent of both temperature and time [13,23]. The average amount of energy given off in a single quake would also be temperature independent if the path leading to the new lowest-energy state were purely exothermal. However, since side branches in the tree can trap the walker on its way down, an activated contribution can be expected. Accordingly, we expect the thermal energy reached at a fixed time to

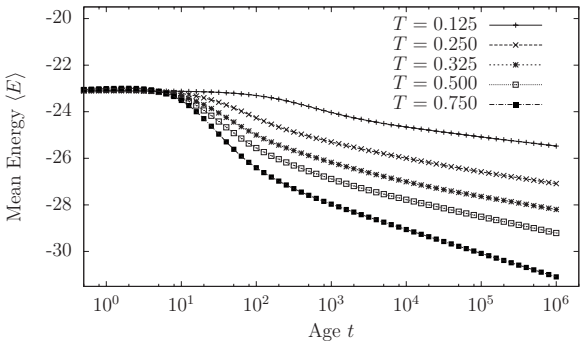

FIG. 3. The mean inner energy E of the tree ensemble plotted versus system age for different temperatures showing the progress of the relaxation process. Note that after some kind of startup phase lasting until $t\approx 200$ the energy shows a practically straight decrease at logarithmic time scale.

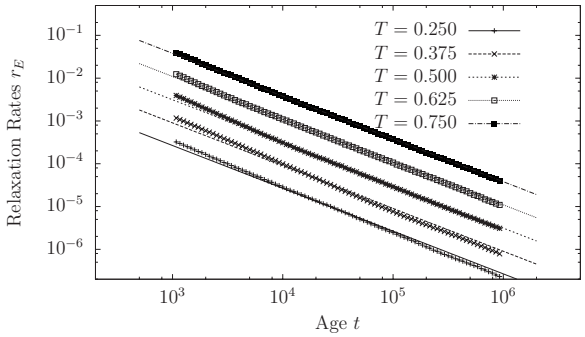

FIG. 4. The rate of energy loss r_E is plotted versus system age for different temperatures. The lines have the form $r_E=a(T)/t$ with the constant a as in Eqs. (4) and (5). To avoid clutter, the data set for each T is multiplied by 1,3,9,… in order of increasing T. A similar but much smaller shift of the curves in the same direction is present due to the temperature dependence of a.

be higher the lower the temperature, which is of course a hallmark of the nonequilibrium nature of the dynamics. The temperature-dependent offset $\mathcal{C}$ is related to the initial stage of the relaxation and has no importance for our treatment.

According to (4) the rate of energy loss $r_E=-dE/dt$ has the form

$$r_E(t,T) = -\frac{dE}{dt} = \frac{a(T)}{t}, \tag{5}$$

which fully agrees with the numerical results shown in Fig. 4 as well as with similar results for microscopic model simulations [7,9]. The figure depicts the rate of energy loss for selected temperatures (symbols) together with fits according to (5) (lines).

As just discussed, we expect the logarithmic rate of energy loss, $a(T)$, to have the form

$$a(T) = \overline{\delta_E} + c\,\exp(-b/T), \tag{6}$$

where $\overline{\delta_E}$ is the average contribution to the energy given off by paths not involving any energy barriers. The activated term involves a barrier which should be comparable in size to the smallest barrier present in the system. Figure 5 confirms Eq. (6) for the present model. The value $\overline{\delta_E}=0.195$ is

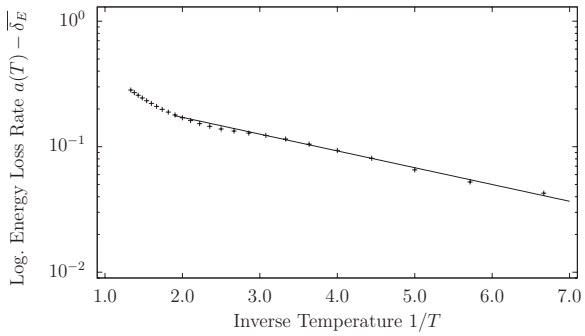

FIG. 5. The logarithmic rate of energy loss, $a(T)$ [see (5)], shifted by $\overline{\delta_E}$, is plotted vs the inverse temperature. The data are fitted to the expression $a(T)=\overline{\delta_E}+c\,\exp(-b/T)$, yielding $\overline{\delta_E}=0.195$, $b=0.307$, and $c=0.318$.

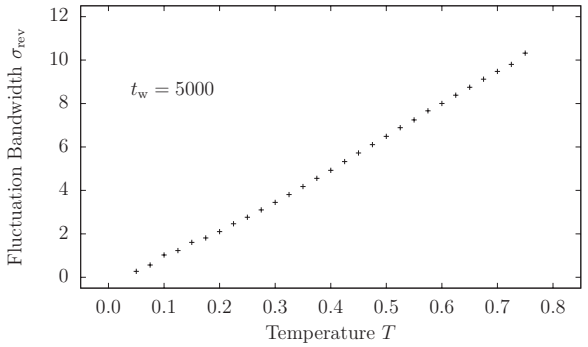

FIG. 6. The standard deviation $\sigma_{\rm rev}$ plotted vs temperature is obtained from the Gaussian part of the energy-exchange PDF.

the one judged to provide the best numerical agreement with the data. The parameters b and c were estimated by least-squares fitting. The value of the "barrier" parameter $b=0.307$ is close to the value of the smallest energy barrier present in the model, $b_{\rm min}=0.5$.

Figure 6 shows the bandwidth of the Gaussian fluctuation $\sigma_{\rm rev}$ versus the temperature. The curve is relatively featureless and increases with temperature as expected. For a classical system (with constant heat capacity) the fluctuation bandwidth would be proportional to T. The data shown have a slightly faster than linear increase with T.

The results presently obtained, with the possible exception of Fig. 6, very closely mirror the behavior of the Ising model with plaquette interactions recently investigated by one of the authors [9].

V. DISCUSSION AND CONCLUSION

Thermal hopping on a tree structure provides a simple framework to describe relaxation phenomena in complex systems [17,20,24–33]. The hierarchical model studied in this work is a modification of the even simpler *LS* model [20], whose two elementary energy scales are replaced with a wider spectrum of energy scales. This is physically more realistic and removes unphysical logarithmic oscillations [34] in the energy decay.

The intermittent energy relaxation of this model is strikingly similar to that observed at microscopic models [7,9]. For the model, the behavior can be understood as follows: At any given time, the probability distribution is, to a good approximation, supported within a finite subtree. A larger subtree must be entered in order to lower the hitherto lowest energy. Thus, record-sized energy fluctuations trigger, with a certain probability, quakes which then lead to the attainment of lower energies. Since the records occur at a rate proportional to $1/t$ [12,13,23], the rate of quakes is also proportional to $1/t$ and the quantity $r_E t=-a(T)$ is, modulo a constant proportionality factor, the energy given off in a single quake.

Further evidence for the crucial role of record-sized fluctuations was provided by an analysis of the Edwards-Anderson spin glass, which was done using two different dynamical update rules: thermal hopping [35] and extremal optimization [36]. In both cases, it was found that a record-

sized energy barrier needed to be overcome in order to lower the current lowest energy seen so far in the simulation. Since the update rules are completely different in the two cases and yet lead to the same result, the connection between record-sized energy barriers and low-energy states is likely to be a true geometrical property of complex energy landscapes.

In a thermalizing hierarchical model, record-sized energy fluctuations are needed to move from one metastable region of configuration space to a different region of lower energy. In this paper we have shown that this one property suffices to generate realistic spectra for the intermittent energy fluctuations.

[1] H. Bissig, S. Romer, L. Cipelletti, V. Trappe, and P. Schurtenberger, PhysChemComm **6**, 21 (2003).
[2] W. K. Kegel and A. van Blaaderen, Science **287**, 290 (2000).
[3] E. R. Weeks, J. C. Crocker, A. C. Levitt, A. Schofield, and D. A. Weitz, Science **287**, 627 (2000).
[4] L. Buisson, S. Ciliberto, and A. Garcimartín, Europhys. Lett. **63**, 603 (2003).
[5] L. Buisson, L. Bellon, and S. Ciliberto, J. Phys.: Condens. Matter **15**, S1163 (2003).
[6] L. Cipelletti, H. Bissig, V. Trappe, P. Ballesta, and S. Mazoyer, J. Phys.: Condens. Matter **15**, S257 (2003).
[7] P. Sibani and H. J. Jensen, Europhys. Lett. **69**, 563 (2005).
[8] P. Sibani, Europhys. Lett. **73**, 69 (2006).
[9] P. Sibani, Phys. Rev. E **74**, 031115 (2006).
[10] A. Lipowski and D. A. Johnston, Phys. Rev. E **61**, 6375 (2000).
[11] M. R. Swift, H. Bokil, R. D. M. Travasso, and A. J. Bray, Phys. Rev. B **62**, 11494 (2000).
[12] P. Sibani and P. B. Littlewood, Phys. Rev. Lett. **71**, 1482 (1993).
[13] P. Sibani and J. Dall, Europhys. Lett. **64**, 8 (2003).
[14] E. Vincent, J.-M. Hammann, and M. Ocio, in *Recent Progress in Random Magnets*, edited by D. H. Ryan (World Scientific, Singapore, 1992), pp. 207–236.
[15] J.-P. Bouchaud and D. S. Dean, J. Phys. I **5**, 265 (1995).
[16] J. Krawczyk and S. Kobe, Physica A **315**, 302 (2002).
[17] P. Sibani and K. H. Hoffmann, Phys. Rev. Lett. **63**, 2853 (1989).
[18] P. Sibani, J. C. Schön, P. Salamon, and J.-O. Andersson, Europhys. Lett. **22**, 479 (1993).
[19] K. H. Hoffmann, S. Schubert, and P. Sibani, Europhys. Lett. **38**, 613 (1997).
[20] P. Sibani and K. H. Hoffmann, Europhys. Lett. **16**, 423 (1991).
[21] C. Uhlig, K. H. Hoffmann, and P. Sibani, Z. Phys. B: Condens. Matter **96**, 409 (1995).
[22] J. Dall and P. Sibani, Comput. Phys. Commun. **141**, 260 (2001).
[23] J. Krug, J. Stat. Mech.: Theory Exp. (2007) P07001.
[24] K. H. Hoffmann, S. Grossmann, and F. J. Wegner, Z. Phys. B: Condens. Matter **60**, 401 (1985).
[25] K. H. Hoffmann and P. Sibani, Phys. Rev. A **38**, 4261 (1988).
[26] K. D. Ball, R. S. Berry, R. E. Kunz, F.-Y. Li, A. Proykova, and D. J. Wales, Science **271**, 963 (1996).
[27] U. Geppert, H. Rieger, and M. Schreckenberg, J. Phys. A **30**, L393 (1997).
[28] K. H. Hoffmann, Comput. Phys. Commun. **121–122**, 30 (1999).
[29] V. M. de Oliveira, J. F. Fontanari, and P. F. Stadler, J. Phys. A **32**, 8793 (1999).
[30] W. Hordijk, J. F. Fontanari, and P. F. Stadler, J. Phys. A **36**, 3671 (2003).
[31] D. J. Wales, *Energy Landscapes*, Cambridge Molecular Science (Cambridge University Press, Cambridge, UK, 2003).
[32] S. Schubert and K. H. Hoffmann, Europhys. Lett. **66**, 118 (2004).
[33] S. Schubert and K. H. Hoffmann, Comput. Phys. Commun. **174**, 191 (2006).
[34] M. Schreckenberg, Z. Phys. B: Condens. Matter **60**, 483 (1985).
[35] J. Dall and P. Sibani, Eur. Phys. J. B **36**, 233 (2003).
[36] S. Boettcher and P. Sibani, Eur. Phys. J. B **44**, 317 (2005).