Diffusion in hierarchies

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In this paper we show that diffusion processes in a "complex" phase space with many local minima can be mapped into a random-walk problem on a tree structure. We then rigorously solve the latter problem for regular trees, under quite general assumptions about the rates. Finally, we extend our results to the case of inhomogeneous trees.

I. INTRODUCTION

Hierarchies and hierarchical models are now popular modeling tools in theoretical physics, for at least one reason: their mathematics is tractable, and yet nontrivial results can be obtained, such as, for example, algebraic and stretched exponential decays with temperature-dependent exponents.[1-12]

Recently, this type of model has been used to calculate an experimental quantity, the ac susceptibility of a spin glass.[13] The good agreement obtained suggests that hierarchies are more than just toy models. Since, however, the extent of their applicability to a real physical system has not yet been discussed in general terms, we try in this paper to establish some links to a widely used dynamical description, which is thermally activated diffusion in a mountain landscape given by the energy surface.

We first develop an intuitive picture of the process, leading quickly to the temperature-dependent exponents which have been found, for the hierarchical models, by several different mathematical methods. We then show that the diffusion problem can be mapped (under certain restrictions) into a random-walk problem on a suitably defined tree structure. Finally, we treat the latter problem in a complete and a more general way than hitherto attempted. We believe that the ideas developed in this paper are relevant for a number of fields, such as the study of chemical reactions, the relaxation in amorphous materials, and the theory of annealing processes.

II. HEURISTICS OF DIFFUSION IN A MOUNTAIN LANDSCAPE

We start our discussion by rederiving the temperature dependence of the exponents of models found in the literature in a way which emphasizes the difference in the physical interpretation of the models. Our system is a particle diffusing in R^d. Its energy $E(x)$ is given as a function of the state $x \in R^d$. Without loss of generality we assume that $E(x) > 0$ for all x. One can visualize $E(x)$ as a mountain landscape over R^d. The time evolution of the system is described by the distribution $P(x,t)$, which gives the probability to find the particle at state x at time t. We now consider a sequence of real numbers V_n (the heights of the passes) and of subsets A_n of R^d (the valleys), which are iteratively defined in the following way. Initially the particle is confined to a certain valley A_0, i.e., A_0 is the support of the initial distribution. At time t_1 the lowest available pass, of height V_1, is crossed, and the distribution relaxes into a new larger valley $A_1 \supset A_0$. In general, we assume that being in A_{n-1}, the system diffuses through the lowest available pass, of height V_n, at time t_n, after it started in A_0, into the set $A_n \supset A_{n-1}$. Note that since the nth valley includes all the smaller ones, by construction, there is no difference between the waiting time in the nth valley and the total time elapsed since the start of the diffusion process.

At each t_n, the diffusion profile P_n is (approximately) supported in A_n. Hence, letting the symbol A_n denote the area (Lebesgue measure) of the valley as well, we set $P_n \sim 1/A_n$. The time dependence of P_n is thus given by specifying the area of the nth valley and the time the system spends in it. The first quantity depends on the geometry of the phase space only, while the second involves the dynamics of the process under consideration.

Suppose that the nth valley is a rescaled version of the $(n-1)$th. Then

$$A_n = z A_{n-1} = z^n A_0 \ . \tag{1}$$

Assuming that the linear size of the region *available* to diffusion (which might not be the whole valley, due to the presence of high massifs) increases by a factor of m, each time a pass is crossed, we get

$$A_n = (m^{d_f})^n = z^n A_0 \ , \tag{2}$$

hence the fractal dimension of the landscape is found to be

$$d_f = \ln(z)/\ln(m) \ . \tag{3}$$

We have thus related the parameter z to the fractal dimension d_f. It is noteworthy that $d_f \to 0$ when $z \to 1$, which means that in the limit $z \to 1$ the landscape is made up of very high massifs and threadlike canyons, in which the diffusion takes place.

We now show how different choices of V_n and t_n easily lead to the exponents. There are two different types of

thermally activated dynamics, one with long-range hops and one with nearest-neighbor hops. Both terms are understood in the sense of the usual Euclidean metric on R^d.

The case of long-range hops is not compatible with the present picture in which the underlying dynamics is just diffusion, which is intrinsically local. We consider it anyway for the sake of completeness and take the usual choice of waiting times, i.e., $t_n = \exp(V_n/T)$, the Arrhenius law. The second case is more involved, since in general the waiting time t_n will partly be spent in trying to find the pass, and partly in trying to overcome the barrier. If we assume that the first subtask is completed in a time proportional to the area of the valley A_n, the second depends on the barrier energy in the usual Arrhenius way, and they are independent of each other, we get immediately

$$t_n = (z/k)^n \exp(V_n/T) , \tag{4}$$

where k is a free parameter, which accounts for entropic effects. However, at this level of description we are unable to justify the introduction of the parameter k further and we refer the reader to Sec. IV for a more complete discussion.

The first choice of dynamics (long-range hops) yields, for $V_n = n$,

$$n(t) = T \ln t , \tag{5}$$

$$P(t) = t^{-T \ln z} , \tag{6}$$

while for $V_n = \ln(n)$ we find

$$n(t) = t^T , \tag{7}$$

$$P(t) = \exp[-(\ln z) t^T] , \tag{8}$$

which are the results of Ogielski and Stein.[5] The second choice again, for $V_n = n$, gives

$$P(t) = t^{-T \ln z/[1 - T \ln(k/z)]} , \tag{9}$$

which was found by Grossmann, Wegner, and Hoffmann[2,3] and others.

Other types of relaxations can be found for various dependences of V on n. We shall not, however, pursue this issue further before Sec. IV. In Sec. III we try to develop another formalism for the diffusion problem, which clearly shows how the tree structures enter the mathematical description of the problem.

III. FROM DIFFUSION IN R^d TO RANDOM WALKS ON A TREE

The rough qualitative picture of diffusion in a mountain range developed in Sec. II has a couple of shortcomings: it contains approximations which are hard to quantify, and it conveys the idea of a strict linkage between the concept of hierarchy of valleys and the dynamical hypothesis that the lowest pass is always chosen by the diffusing system.

We show below that a tree structure can be introduced by geometrical arguments only. There are indeed several possible ways of obtaining a tree structure from a given energy surface, which differ in some details. In a second step, involving a coarse graining, we then map the original dynamics into a stochastic process on the tree. Below we give two instances of the tree construction.

Construction 1. We recall that the energy function E, defining the shape of the landscape, is non-negative. Let $S(h)$ be the subset of R^d below height h, i.e., $S(h) = E^{-1}((0,h))$. Pictorially, if the landscape is flooded up to height h, $S(h)$ is the "sea" and $R^d \setminus S(h)$ the land.

Let us assume that $S_L(h)$ is a connected subset of $S(h)$, which contains no islands. This assumption can usually be made without a loss of generality for that part of state space, which is interesting for the low-temperature regime. For more details see Appendix A. $L = L_0, L_1$ is a label, which consists of a sequence of digits, with L_1 being the last digit and L_0 being the sequence up to the penultimate digit. We now want to follow the connectivity properties of $S(h)$ as the water level h decreases. On lowering h two things can happen: either $S_L(h)$ divides at $h = h_L$ into two or more connected subsets $S_{L,1} S_{L,2}, \ldots$, with $S_L(h_L) = S_{L,1}(h_L) \cup S_{L,2}(h_L) \cup \ldots$ (the generic situation, however, is having two subsets); or the set $S_L(h)$ becomes empty without bifurcating. The sets $S_{L,i}$ might well contain islands, which are local energy maxima. This is not important for our construction; see Appendix A. For each newly created connected subset $S_{L,i}(h)$ the previously described procedure is repeated.

Now we can define the nodes of the tree: for every label L the node N_L is a subset of R^d given by

$$N_L = S_L(h_{L_0}) \setminus S_L(h_L) = S_L(h_{L_0}) \setminus \bigcup_i S_{L,i}(h_L) . \tag{10}$$

Since for every $x \in N_L$ we have $h_L \le E(x) \le h_{L_0}$, we assign to each node N_L the coarse-grained energy $\tilde{h}_L = (h_{L_0} + h_L)/2$. The reader should be aware that at the level of description we are aiming for, any other height between h_{L_0} and h_L could have been chosen.

By construction all the sets N_L are disjoint. Now note that for each node N_L there is a unique "parent" node N_{L_0}, which surrounds N_L, and a node N_L may itself have a number of "daughter" nodes $N_{L,i}$, which are in turn surrounded by N_L. The tree is then generated by connecting a pair of nodes if they have a parent-daughter relation. In Fig. 1 the preceding construction is graphically depicted showing a one-dimensional cut through a state space. The reader should note that due to the projection used connected sets may appear to be unconnected. Another way of obtaining the tree structure is the following.

Construction 2. We introduce equidistant energy levels

$$E(l) = \Delta l \tag{11}$$

and take $S(h) = E^{-1}((0,h))$ as previously. The set $N(\Delta l) = S(\Delta l) \setminus S(\Delta(l-1))$ can be written as a union of connected subsets $N_{l,k}$,

$$N(\Delta l) = \bigcup_k N_{l,k} . \tag{12}$$

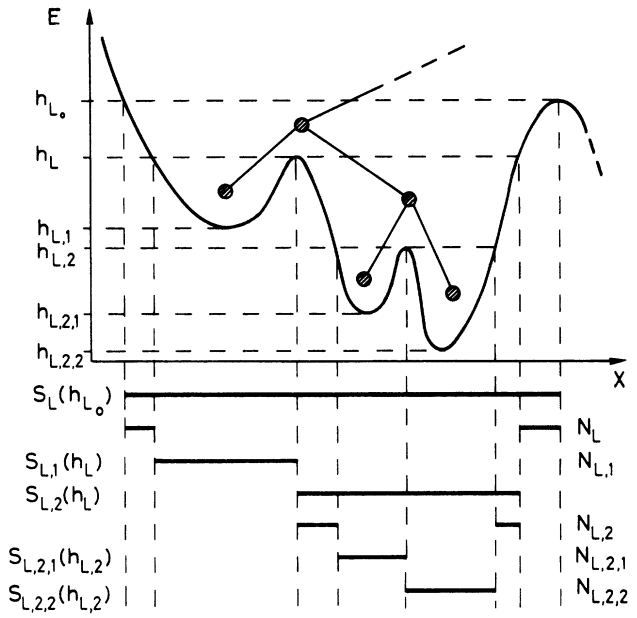

FIG. 1. Tree construction 1 is graphically depicted. The energy is shown as a function of the state for a one-dimensional cut through the high-dimensional state space. The heights at which connected subsets become unconnected or empty are marked at the left. At the bottom the projections of the connected subset S_L and its descendants and the projection of the node N_L and its descendants are shown. One should note that the connected sets N_L appear to be unconnected due to the projection.

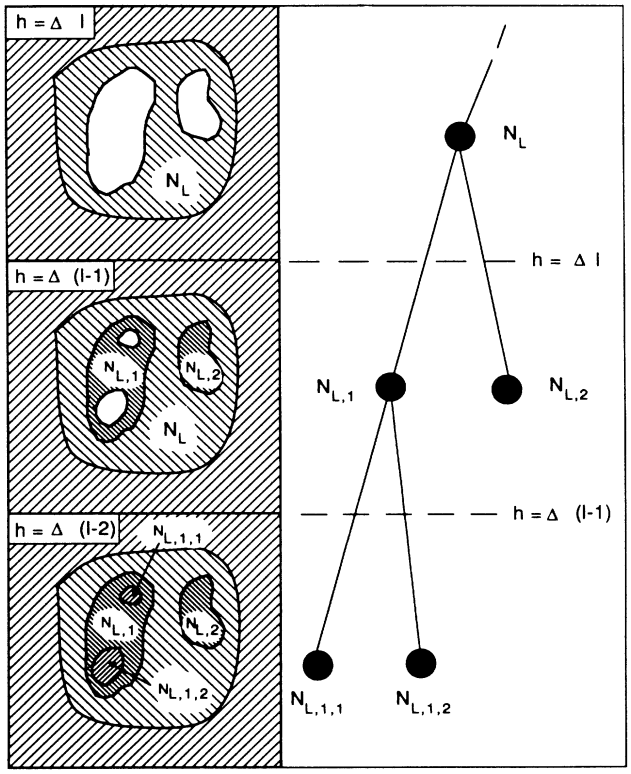

FIG. 2. Tree construction 2 is graphically depicted. The three pictures on the left show a two-dimensional energy surface from a bird's eye view, the lines represent points of equal heights. The white area is the "sea." From the top to the bottom the sea level is lowered in equidistant steps Δ, the respective height is given in the upper left corner. As the sea level sinks, the nodes are created. On the right side the emerging tree structure is shown.

We call $N_{l,k}$ a node of the tree. In this notation the first index indicates the level, while the second gives an arbitrary numbering of the nodes within a level. In order to emphasize the hierarchical ordering of the nodes, it is more convenient to use the same notation as in construction one: Let N_L be a connected subset at level l. Then all the connected subsets of level $l-1$ which lie in the interior of N_L become the daughter nodes of N_L and they are labeled as $N_{L,1}, \ldots, N_{L,z}$. The branching ratio z will vary now from node to node but the energy is by definition a linear function of the level. This procedure is then repeated down to lower levels until a node has no descendants; such a node contains a local energy minimum. Note that local maxima will appear as holes in N_L, which are not "filled" with descendants. Again such an event is most unlikely, for details see Appendix A. The tree represents again the topological situation which a random walker in the state space encounters: To go from node $N_{L,1}$ to $N_{L,2}$ it has to go through N_L. Figure 2 depicts this construction graphically.

The tree in this construction differs from the one of the first construction in having the cuts not defined locally by the height at which sets get disconnected or empty but globally by equidistant energies. This offers some advantages from a technical point of view. When $\Delta \to 0$, the multifurcations in the second construction no longer occur, and the tree appears as occasionally branching long chains of nodes. All the states lying on each linear piece of the tree can then be lumped together, at the price of changing the hopping rates, and the result is equivalent to what is obtained in the first construction.

Consider the random motion of a point in the landscape. Rather than calculating the full time-dependence of the probability density in R^d, we can choose to monitor the presence or absence of the point from each of the sets represented by a node. Since these can only be exited by going "uphill" to the parent set or "downhill' to one of the daughter sets, we have hereby defined a stochastic process on the tree which, however, will not in general be a random walk, because successive steps are correlated.

In order to see how the correlations arise, consider a landscape where $\nabla E/k_bT$ is small everywhere: T is the temperature and $\nabla E/k_bT$ controls the magnitude of the drift term in the Brownian motion which, by assumption, is small. A diffusing particle will then cross many times any boundary line arbitrarily drawn in the landscape. Hence there will be a positive correlation between a jump from one set to another and the reverse jump at the next move, and, at the coarse grained level of description we have chosen, the system will bounce several times back and forth between two neighbor nodes in the tree.

However, this situation does not arise under two conditions: (1) roughness of the energy surface and (2) low

temperature. By a rough surface we mean a surface with a slope which is weakly correlated over distances small compared to a typical distance across a node. With low tempeature we mean that $k_B T$ is small compared to a typical height of the bumps of the surface. This together with the roughness ensures that the system has lost the memory of where it entered the node by the time it leaves the node.

Let us now assume that the temperature is sufficiently low, and the landscape sufficiently rough. The original diffusion problem can thus be mapped into a random walk on a tree structure. Instead of deriving the parameters for the random walk from a given energy surface, we rather take the viewpoint that the parameters are arbitrarily given functions and we then proceed to classify the possible solution to the diffusion problem on the tree.

IV. HOMOGENEOUS TREES

The preceding discussion has lead to a reformulation of the diffusion problem in R^d into the problem of a random walk on an inhomogeneous tree structure. As shown in Fig. 2, the tree contains dead ends, which are local (metastable) states. At this level of generality, the problem is hard to solve rigorously, for reasons which will become clear later. The simpler case of diffusion on an ultrametric space (the baseline of the tree) has recently been solved by Bachas and Huberman[9] and Kumar and Shenoy,[8] but has no direct bearing on the problem of diffusion in a mountain landscape, which, as we have argued, leads to a *nearest*-neighbor hopping model in a tree.

We therefore first restrict our treatment to the case in which the tree bifurcates uniformly, allowing the branching ratio and the hopping rates to depend in an arbitrary manner on the level height. In Sec. V we then argue that the results obtained can be extended to a random tree structure satisfying some regularity conditions.

A. Propagator formula

Let k_j^u and k_j^d be the hopping rate from a level j node to its parent node and to one of the daughter nodes respectively. Since all the nodes at a given level are mathematically equivalent, any quantity will depend on the level index only. The total rate downwards is zk_j^d, where z, the branching ratio, is assumed to be level independent for notational convenience, and the total rate upwards is k_j^u.

Let $\tilde{G}(f,s \mid i)$ be the Laplace transform of the probability of being at a level-f node, with start point at a level-i node. As shown by Hoffmann, Grossmann, and Wegner[2] the basic relation

$$\tilde{G}(f,s \mid i)=\sum_{l=k_0}^{\infty}[Q^l(f,s \mid i)-Q^{l-1}(f,s \mid i)]z^{f-l} \tag{13}$$

holds true. In the preceding formula, the Q^l's are analog quantities to $\tilde{G}$, except that they refer to the random walk on the levels obtained by projecting the original motion on the vertical axis. The arguments f and i of Q^l must thus be interpreted as the heights of the initial and final level. Finally, the superscript l indicates that we impose an absorbing boundary condition at level $(l+1)$, and k_0 is the level of the closest common ancestor of f and i. The equation can be understood by observing that $Q^l(f,s \mid i)-Q^{l-1}(f,s \mid i)$ is the Laplace transform of the probability of being somewhere in the tree at level f, starting at level-i node, and having reached but not exceeded level l. Sine all the nodes with the same level index are equivalent, the probability of being at one particular level-f node is obtained by dividing $Q^l(f,s \mid i)-Q^{l-1}(f,s \mid i)$ by z^{l-f}, which is the number of level f descendants of a level-l node. In summary, each term in the sum of Eq. (13) counts the contribution to G from the walks which reach but do not exceed level l.

Each Q is the solution of a random-walk problem on a finite set of nodes, having a discrete set of eigenvalues, λ_i^l, $i=0,1,2,\ldots,l$, in order of increasing magnitude. The small-s and large-time asymptotics are determined by the behavior of the lowest eigenvalue λ_0^l (which appears as a pole in Q^l). In order to discuss its dependence on l, it is expedient to introduce a (free) energy function by the formula

$$F(j)-F(j+1)=T\ln(k_j^u/zk_{j+1}^d)\ , \tag{14}$$

which is just detailed balance "the other way around." Given $F(0)$ and the rates, any $F(j)$ can be calculated by iteration. F acts as an "effective" potential well, in which the motion up and down the *levels* takes place.

As previously mentioned, it is convenient to introduce a parameter k in the model definition, which accounts for the inner structure of the nodes by enhancing the upwards hopping rate relative to what would be obtained by energy considerations alone. As in Ref. 14 we therefore take

$$k_j^u=k\exp(-\Delta_j/T)\ , \tag{15}$$

$$k_j^d=1\ , \tag{16}$$

where $\Delta_j=E(\tilde{h}_{j+1})-E(\tilde{h}_j)$ is the energy difference between adjacent nodes. The factor k is introduced here to take care of entropic effects: the nodes of the tree represent a large number of the original states. This coarse graining of the state space will modify the simple Arrhenius law which applies for transitions between single states, as can be seen from the fact that at equilibrium the probability of being in one node is proportional to the appropriate Boltzmann factor and to the node degeneracy, i.e., the number of states contained in the node.

The effective potential of Eq. (14) is then

$$F(j)=E(j)-T\ln(k/z)j\ , \tag{17}$$

a formula which clearly suggests that F be interpreted as a free energy.

Since we are interested in the long-time and small-s asymptotics of $Q^l(f,s \mid i)$, and the discrete hopping model is equivalent to continuous diffusion in this limit, we choose the latter description which is mathematically easier to handle. The rest of the section is therefore concerned with solving the Fokker-Planck equation

$$\frac{\partial}{\partial t}Q^l(x,t\mid x_i)=\frac{\partial}{\partial x}\left[\frac{\partial Q^l}{\partial x}+\frac{1}{T}\frac{\partial F}{\partial x}Q^l\right] \tag{18}$$

in the interval $(0,l)$ with reflecting and absorbing boundary conditions at the left and right endpoint, respectively. Here we have replaced the discrete indices f and i with the continuous variables x and x_i, respectively. F is an arbitrary function of x. Equation (18) has a discrete spectrum for any finite l. In the limit $l\to\infty$, the spectrum can either remain discrete or become continuous.

In the former case the smallest pole, which approaches zero as $l\to\infty$, dominates the decay for long-time and small s. We then find the appropriate one-pole approximation for $Q^l(x,s\mid x_i)$, insert it into Eq. (13), evaluate the sum, and find the asymptotic behavior for $\tilde{G}(x,s\mid x_i)$.

If the spectrum of Eq. (18) becomes continuous in the limit $l\to\infty$, the preceding approximation cannot be applied. Indeed, both Q^l and $\tilde{G}$ become asymptotically equivalent to free diffusion propagators, and all the "anomalous" behavior disappears. By varying the asymptotic behavior of $F(x)$ for $x\to\infty$ (which can be done by varying the temperature), transitions between the previously mentioned regimes become possible.

B. Eigenvalues of the diffusion operator in a generic potential

In this section and Sec. IV C we put $T=1$ for notational convenience. The transformation

$$f(x,t)=Q(x,t)e^{F(x)/2} \tag{19}$$

brings the Fokker-Planck equation (18) into its normal form

$$\frac{\partial}{\partial t}f(x,t)=\frac{\partial^2 f}{\partial x^2}+h(x)f(x,t)\ , \tag{20}$$

where the function $h(x)$ is related to the free energy $F(x)$ by the following formula:

$$h(x)=\frac{1}{2}\frac{d^2F}{dx^2}-\frac{1}{4}\left[\frac{dF}{dx}\right]^2 . \tag{21}$$

The relevant boundary conditions are

$$\frac{d}{dx}[f(x,t)e^{F(x)/2}]\bigg|_{x=0}=0 \tag{22}$$

and

$$f(l,t)=0\ , \tag{23}$$

which describe a perfectly reflecting and a perfectly absorbing boundary at $x=0$ and $x=l$, respectively. The Laplace transform of Eq. (20) reads

$$\frac{d^2 f}{dx^2}+[h(x)-s]f=-\delta(x-x')e^{F(x)}\ , \tag{24}$$

where x' is the initial position (level) of the random walker.

It is convenient to consider first the problem of diffusion on the half line $(0,\infty)$, and thereafter use the results to construct the solution in $(0,l)$. In the infinite domain, the right boundary condition must be replaced by the normalizability requirement

$$\int_0^\infty f(x,s)e^{-F(x)/2}dx<\infty\ . \tag{25}$$

Let the two homogeneous solutions of Eq. (24) satisfying Eq. (22) be $f_<(x,s)$ and Eq. (25) be $f_>(x,s)$. Their behavior in a neighborhood of $s=0$ is given by the following lemmas.

Lemma 1. Suppose that $dF/dx\to\infty$ for $x\to\infty$. Then

$$f_>(x,s)=\exp\left[-\frac{F(x)}{2}+\sum_{n=1}^{\infty}s^n\int_0^x u_n(x')dx'\right]\ , \tag{26}$$

with the functions $u_n(x)$ iteratively given by

$$u_1(x)=e^{F(x)}\int_x^\infty e^{-F(x')}dx' \tag{27}$$

and

$$u_n(x)=-e^{F(x)}\int_x^\infty e^{-F(x')}\sum_{q=1}^{n-1}u_q(x')u_{n-q}(x')dx'\ . \tag{28}$$

All the u_n's have bounded variation and vanish for $x\to\infty$.

The proof of this lemma is deferred to Appendix B.

Since $f_>(x,s)$ never vanishes, a second solution satisfying the left boundary condition is

$$f_<(x,s)=f_>(x,s)\left[c(s)\int_0^x f_>^{-2}(x',s)dx'+1\right]\ , \tag{29}$$

where [by insertion into Eq. (22)],

$$c(s)=-\frac{1}{2}\frac{d}{dx}[f_>(x,s)e^{+(F(x)/2-F(0)/2)}]^2\bigg|_{x=0}\ . \tag{30}$$

It follows from Eqs. (22) and (30) that if $f_>$ happens to fulfill the left boundary condition as well, then $c(s)=0$ and $f_<(x,s)=f_>(x,s)$. It also follows from Eq. (29) that the Wronskian of $f_<$ and $f_>$, $W(f_<,f_>)$, equals $-c(s)$. In summary, the zeros of $c(s)$ coincide with those of the Wronskian and with the eigenvalues of the problem in the half-infinite domain. If the diffusion problem has a stationary solution, there must be a zero eigenvalue. Since $f=e^{-F(x)/2}$ satisfies the left boundary condition, $s=0$ is an eigenvalue if $e^{-F(x)}$ is integrable. Thus we have the following lemma.

Lemma 2. If $F(x)\to\infty$ for $x\to\infty$, such that $\int e^{-F(x)}dx<\infty$, the diffusion equation has a stationary solution.

The logarithmic potential is thus excluded. The other eigenvalues are given by the other zeros of $c(s)$. If $dF/dx\to\infty$ for $x\to\infty$, both $f_<$ and $f_>$ are analytic in s, and so is $c(s)$. The set of the zeros of $c(s)$ has therefore no limit points. This proves the following.

Lemma 3. If $dF/dx\to\infty$ for $x\to\infty$, then the spectrum of the diffusion operator in $(0,\infty)$ is discrete.

We denote the eigenvalues by $\lambda_1^\infty,\lambda_2^\infty,\ldots,\lambda_n^\infty$, in order of increasing magnitude. The case $F(x)=ax$ is not treated in the previous analysis. However, it is immediately

clear that, since $h(x)=-a^2/4$ [cf. Eq. (20)], the problem is nearly the same as free diffusion, but with a shifted Laplace variable $s'=s+a^2/4$. We therefore conclude the following.

Lemma 4. For a potential which is asymptotically linear for large distances, $F(x)\sim ax$, the diffusion operator in $(0,\infty)$ has a continuous spectrum, given by the negative real half axis $(-\infty,-a^2/4)$, and an isolated eigenvalue at $s=0$.

Consider now the diffusion problem in $(0,l)$. The solutions satisfying the left and right boundary conditions will be denoted by $f^l_<(x,s)$ and $f^l_>(x,s)$. They are easily expressed in terms of the previously derived $f_>(x,s)$ and $f_<(x,s)$. We get, for $x\in(0,l)$, and $dF/dx\to\infty$ for $x\to\infty$,

$$f^l_>(x,s)=f_>(x,s)\left[1-\frac{\int_0^x f_>^{-2}(x',s)dx'}{\int_0^l f_>^{-2}(x',s)dx'}\right], \tag{31}$$

$$f^l_<(x,s)=f_<(x,s)\ . \tag{32}$$

The Wronskian $W(f^l_<,f^l_>)$ is then given by

$$W(f^l_<,f^l_>)=W(f_<,f_>)+\left[\int_0^l f_>^{-2}(x',s)dx'\right]^{-1}$$
$$=-c(s)+\left[\int_0^l f_>^{-2}(x',s)dx'\right]^{-1}. \tag{33}$$

Since the zeros of $W(f^l_<,f^l_>)$ are close to those of $c(s)$, Eq. (33) easily leads to the following lemma.

Lemma 5. Suppose that $dF/dx\to\infty$ for $x\to\infty$. The eigenvalues of the diffusion problem in $(0,l)$ depend continuously on l. For large l we have

$$\lambda^l_k=\lambda^\infty_k+\eta_k(l),\quad k=1,2,\ldots \tag{34}$$

where the correction term $\eta_k(l)$ is exponentially small, $\eta_k(l)=O(e^{-F(l)})$.

This is in accordance with the beautiful qualitative argument of Kramers[15] about the lowest eigenvalue for the problem of barrier crossing. Once more, the case $F(x)\sim ax$ requires separate treatment. Let $\sigma=s+a^2/4$. An easy calculation yields

$$f^l_>(x)=\sinh[\sigma^{1/2}(l-x)]\ , \tag{35}$$

$$f^l_<(x)=-\frac{a}{2\sigma^{1/2}}\sinh(\sigma^{1/2}x)+\cosh(\sigma^{1/2}x)\ . \tag{36}$$

The Wronskian is

$$W(f^l_<,f^l_>)=-\frac{a}{2}\sinh(\sigma^{1/2}l)+\cosh(\sigma^{1/2}l)\sigma^{1/2}\ . \tag{37}$$

The only zero of W for σ positive and s negative is given by

$$\sigma=\left[\frac{a}{2}-ae^{-al}\right]^2+O(e^{-2al}) \tag{38}$$

or

$$s=-a^2e^{-al}+O(e^{-2al})\ . \tag{39}$$

The least eigenvalue vanishes exponentially when the "barrier" height goes to infinity, again as predicted by Kramers's rule. Let us finally consider the situation when the potential increases more slowly than linearly. Then $dF/dx\to 0$, for $x\to\infty$, and the function $h(x)$ in Eq. (24) approaches zero. It follows that the asymptotic behavior is the same as free diffusion, with one difference: $s=0$ is an eigenvalue, which is embedded in the continuous spectrum, for a potential satisfying $\int_0^\infty e^{-F(x)}dx<\infty$. Our results are summarized in the following lemma.

Lemma 6. The spectrum of the diffusion operator in $(0,l)$, with reflecting and absorbing boundary conditions at the left and right endpoints, respectively, has, for finite l, a discrete spectrum. Let the eigenvalues be λ^l_0, $\lambda^l_1,\ldots,\lambda^l_n$, with $\lambda^l_k<\lambda^l_{k+1}$. The following holds true.

(1) If $F(x)$ increases asymptotically at least linearly with x, the least eigenvalue λ^l_0 approaches zero for $l\to\infty$ in a continuous manner, and remains bounded away from the rest of the spectrum, i.e., there exists a $\mu>0$ such that $|\lambda^l_0-\lambda^l_1|>\mu$ for $\forall l$.

(2) If $F(x)$ increases sublinearly but faster than logarithmically, λ^l_0 approaches zero, but also $|\lambda^l_0-\lambda^l_1|\to 0$ for $l\to 0$. In the limit $l=\infty$ the continuous spectrum is the whole negative real axis, except the point $s=0$, which is in the point spectrum (i.e., it is an eigenvalue).

(3) If $F(x)$ increases logarithmically, the situation is as under (2), except that $s=0$ belongs to the continuous rather than the point spectrum.

C. Least eigenvalue

The least eigenvalue λ^l_0 of the diffusion operator in $(0,l)$ is the zero of the Wronskian $W(f^l_<,f^l_>)$ which is the closest to the origin in the complex s plane. The Wronskian can be calculated by a slight modification of the method of steepest descent: First we approximate $f_>(x,s)$ by discarding all the terms in the exponent which are of order two or higher in s. Therefore

$$f_>(x,s)\sim\exp\left[-\frac{F(x)}{2}+s\int_0^x u_1(x)\right]. \tag{40}$$

We now have to evaluate $\int_0^l f_>^{-2}(x,s)dx$ [see Eq. (33)]. Supposing that $F(x)/2-s\int_0^x u_1(x')dx'$ is an increasing function of x, it has its maximum at $x=l$, the endpoint of the integration interval. Expanding the exponent to first order, we easily obtain the integral and hence the Wronskian. The zero of W closest to $s=0$ is then easily found to be at

$$s=-\lambda^l_0=-\frac{e^{-F(l)}F'(l)}{\int_0^\infty e^{-F(x)}dx}+O(e^{-2F(l)})\ . \tag{41}$$

Note that it does not matter in this approximation whether one chooses l or ∞ as the upper limit in the integral. Equation (21) agrees with Eq. (20) when $F(x)=ax$. It has the following nice interpretation: the rate of escape from the barrier is proportional to the probability of being at l in the infinite system, which is

$$e^{-F(l)}/\int_0^\infty e^{-F(x')}dx'$$

times the drift velocity $F'(l)$. This is the well-known Kramers argument. The residue of the propagator at $s=-\lambda_0$ is found by a simple calculation to be

$$\frac{e^{-F(x)}}{\int_0^\infty e^{-F(x)}dx}+O(e^{-2F(l)}) . \tag{42}$$

We then see that the probability distribution in the time domain is given for long times as

$$Q^l(x,t)=e^{-\lambda_0^l t}\frac{e^{-F(x)}}{\int_0^\infty e^{-F(x')}dx'} . \tag{43}$$

D. Linear potential: Recurrence and transience

We now go back to our original problem of the random walk on a tree. The problem was mapped into that of diffusion on a line, with a potential $F(x)=E(x)+T\ln(z/k)x$ [cf. Eq. (17)], where z is the branching ratio of the tree, k is a positive constant, E is the energy, and x the height. The branching ratio z can depend on x in an arbitrary manner. Reintroducing the temperature in our expression, rescaling the time (i.e., the Laplace parameter s), and omitting all unimportant (i.e., constant) factors, we find

$$Q^l(f,s\mid i)=\frac{A^f}{s+A^l} , \tag{44}$$

with

$$A=e^{-[\Delta/T-\ln(k/z)]}<1 . \tag{45}$$

Here we have adopted the same notation as in Ref. 14.

The linear case for the free energy has a special peculiarity: a transience-recurrence transition. Here we will just recall the major steps for showing that and refer the reader to Ref. 14 for a more detailed description. Inserting (44) into (13) we find up to constant factors

$$\sum_{l=k_0}^{\infty} Q^l(f,s\mid i)z^{-l}=(1-A)A^f\left\{s^{-\ln z/\ln A-1}\sum_{l=0}^{\infty}(-1)^l\left[\frac{A^{-l\epsilon_z\epsilon}}{1-A^l/z}+(1-\delta_{l+1,n})\frac{A^{(l+1)\epsilon_z\epsilon}}{(A^{l+1}z)^{-1}-1}\right]\right.$$
$$\left.+\sum_{l=0}^{\infty}(-1)^l s^l\left[\left[\frac{\ln s}{\ln A}-\epsilon(s)-k_0\right]\delta_{l+1,n}-\frac{(A^{l+1}z)^{-k_0}}{(A^{l+1}z)^{-1}-1}(1-\delta_{l+1,n})\right]\right\} , \tag{46}$$

where we have introduced a parameter

$$n=-\frac{\ln z}{\ln A}=\frac{T\ln z}{\Delta+T\ln(z/k)} , \tag{47}$$

which is, in general, a noninteger quantity. Accordingly, the Kroneker δ's which appear in Eq. (24) are zero, except for special values of the temperature, at which logarithmic terms appear.

We now disregard the s dependence of $\epsilon(s)$ in Eq. (46), and denote the singular part of the propagator by $s^{-\beta}$. This defines the exponent

$$\beta(T)=\left[\frac{\ln z}{\ln A}+1\right]=\frac{\Delta-T\ln k}{\Delta+T\ln(z/k)} . \tag{48}$$

Let $T_1=\Delta/\ln(k)$. Now for $0<T<T_1$, β is positive, $\tilde{G}\to\infty$ for $s\to 0$, and the walk on the tree is recurrent. For $T_1<T$, β is negative, $\tilde{G}\to\text{const}<\infty$ for $s\to 0$, and the walk is transient.

V. INHOMOGENEOUS TREES

In Secs. II–IV we treated trees with a uniform branching ratio z. For notational convenience we wrote down the equations for a branching ratio which did not depend on the level k. All the basic ideas we used can still be applied in the case where z only depends on the level k, but is uniform on every level. In the following we sketch an argument which allows us to calculate $\tilde{G}(f,s\mid i)$ even in situations where z is random variable for every node. We assume that all the z's are independently distributed according to the same distribution. Before we start our argument we want to point out that random trees have already attracted some interest.[16,17]

If we now cut off subtrees at level l, then these subtrees are different, but statistically they are equal in the sense that the average number of nodes at level j $D^l(j)$ is the same and

$$D^l(j)=\langle z\rangle^{l-j} . \tag{49}$$

It is convenient to split off this random part from the free energy F,

$$F^l(j)=\tilde{F}(j)+T\ln D^l(j) , \tag{50}$$

where $F^l(j)$ is now the (averaged) free energy in a subtree of height l and $\tilde{F}(j)$ contains the rest; here we take

$$\tilde{F}(j)=(\Delta-T\ln k)j \tag{51}$$

linear. We note that this is in a sense the most interesting case. Indeed if $\tilde{F}$ is sublinear, then F^l is still asymptotically linear due to Eqs. (49) and (50). If $\tilde{F}$ increases faster than linearly, the random part of the free energy is negligible for large l values.

Note that by replacing z by $\langle z\rangle$ in Eq. (17) we have, for $E(j)=\Delta j$,

$$F^l(j)=F(j)+lT\ln\langle z\rangle . \tag{52}$$

We now proceed to show that the basic result for the homogeneous tree carries over to the inhomogeneous one with $\langle z\rangle$ replacing z.

Let n_i and n_f be the initial and final nodes, and f and i their respective level. We can derive a formula for the propagator $\tilde{G}(n_f,s\mid n_i)$ by arguments similar to those leading to Eq. (13). We first introduce the probability $\hat{P}^l$

that a walker starting at n_i has never left a subtree of height l. The probability that the walker has exactly reached level l on its random walk is then given by $\hat{P}^l - \hat{P}^{l-1}$. This probability will then quickly equilibrate in the subtree of height l according to the appropriate Boltzmann distribution. That means the fraction $e^{-\tilde{F}(f)}/Z^l$ is in node n_f, with

$$Z^l = \sum_{j=i}^{\infty} e^{-F^l(j)/T} . \tag{53}$$

In this way we get the probability for all paths leading from n_i to n_f and reaching exactly level l as their maximal level. Summing now over all level $l \geq k_0$, where k_0 is the level of the closest ancestor of n_i and n_f, we find

$$\tilde{G}(n_f, s \mid n_i) = \sum_{l=k_0}^{\infty} (\hat{P}^l - \hat{P}^{l-1}) \frac{e^{-\tilde{F}(f)/T}}{Z^l} . \tag{54}$$

The $\hat{P}^l$'s are given for the interesting long-time limit by Kramers's formula as

$$\hat{P}^l = \frac{1}{s + \lambda_0^l} , \tag{55}$$

where λ_0^l in the least eigenvalue for the random walk on a level l subtree. This time scale is given by the slow probability flux out of the subtree, as can be seen from Eq. (41) for a continuous walk.

We now note that

$$\frac{e^{-\tilde{F}(f)/T}}{Z^l} = \frac{e^{-F^l(f)/T}}{Z^l} \langle z \rangle^{-l} = \frac{e^{-F(f)/T}}{Z} \langle z \rangle^{-l} , \tag{56}$$

where

$$Z = \sum_{j=1}^{\infty} e^{-F(j)/T} . \tag{57}$$

The l-independent factor can then be taken outside the sum and, by reshuffling the terms, we get

$$\begin{aligned} \tilde{G}(n_f, s \mid n_i) &= (1 - \langle z \rangle^{-1}) \frac{e^{-F(f)/T}}{Z} \sum_{l=k_0}^{\infty} \langle z \rangle^{-l} \hat{P}^l \\ &= (1 - \langle z \rangle^{-1}) \frac{e^{-F(f)/T}}{Z} \sum_{l=k_0}^{\infty} \frac{\langle z \rangle^{-l}}{s + \lambda_0^l} . \end{aligned} \tag{58}$$

Here we have neglected $\hat{P}^{k_0 - 1}$, which is not important at long times. Equation (58) differs from the corresponding equation for the homogeneous tree only by containing $\langle z \rangle$ rather than z; see Eq. (4) of Ref. 14. In Eqs. (54) and (58) we have approximated the average of the propagator over the ensemble of possible trees with an expression obtained by using the average of the least eigenvalue in Kramers's argument. In other words, fluctuations in the partition function Z^l have been neglected. This is reasonable since our preceding argument deals only with the average of the propagator. A thorough analysis of the fluctuations has yet to be accomplished.

VI. CONCLUSION

In this paper we show how an arbitrary diffusion process in a potential field can be mapped by a coarse graining into a dynamics on a tree. Roughly speaking, the coarse graining consists of lumping all the states of the system which can be reached from a given state with a certain energy change into one mode of the tree.

The procedure only uses the connectivity of the dynamics. The choice of diffusion in R^d as an example was only made for convenience. Other Markov processes, like simulated annealing of any combinatorial problem with a Metropolis dynamics, can also be treated in the same fashion, provided the energy is a slowly varying function. In other words, the energy change associated with a single move should be small compared to the typical energy difference between two connected nodes of the tree. Otherwise, the concept of an energy surface as used here is no longer meaningful.

The coarse-graining procedure is interesting and helpful if the resulting dynamics on the tree is Markovian, i.e., a random walk. This is the case, at least approximately, if the original problem has a high density of local energy minima. Exactly this situation is expected for relaxation in frustrated physical systems, like spin glasses, and in the simulated annealing description of hard combinatorial problems.

Having argued for the applicability of the concept of random walks on a tree to a wide class of problems, we develop in a rigorous and general fashion the theory for homogeneously branching trees. The algebraic relaxation with the temperature-dependent exponents, which has previously been found by many authors, is shown to depend on the asymptotic behavior of an appropriately defined energy function: This function, however, cannot freely be chosen to define the model, being subject to certain restrictions in order to keep the mathematics self-consistent. The energy must go to infinity at least linearly with the height of the tree, in order to give meaningful exponents.

Finally, we give heuristical arguments supporting the thesis that nonhomogeneously branching trees can be treated in the same way as homogeneous ones by replacing the branching rate with its average.

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APPENDIX A

In this appendix we treat the question of islands in the first construction or of daughter nodes with higher energy than the parent node in the second construction. The reason for both phenomena are local maxima in the energy surface. This is a most unlikely event for the low-energy parts of the state space. Usually for any given state one will always find a neighboring state with higher energy. As an illustration consider an Ising spin glass, where for a low-energy state nearly any spin flip will increase the energy.

Apart from the preceding arguments there are simple technical remedies for those situations. For the first tree construction one has just to enlarge $S_L(h)$ with all the islands it has in it. For the second tree construction the holes with the higher energy should become part of the parent, keeping the energy of the parent unchanged. As a system random walking in state space can enter and leave a local maximum only through the node representing the surrounding area, the previously described procedure is the appropriate method to coarse grain the local maxima away.

APPENDIX B: PROOF OF LEMMA 1

We wish to solve the equation

$$f''+[h(x)-s]f=0 , \tag{B1}$$

where $h(x)=F''(x)/2-[F'(x)/2]^2$ and s is a small parameter. Equation (B1) can be mapped into the Riccati equation

$$v^2+v'=-h(x)+s \tag{B2}$$

by the transformation

$$f=\exp\left[\int^x v(x')dx'\right] . \tag{B3}$$

This is the first step in the derivation of the Green-Liouville (or WKB) approximation,[18] the next step usually being the zeroth-order approximation $v=\sqrt{-h(x)+s}$. We can do better, however, by exploiting the fact that one solution of Eq. (B1) is, for $s=0$, given by $f(x)=\exp[-F(x)/2]$. We therefore write the ansatz

$$v(x)=-\frac{1}{2}\frac{dF}{dx}+u(x,s) , \tag{B4}$$

where the unknown function $u(x,s)$ obeys

$$u^2+u'-\frac{dF}{dx}u=s . \tag{B5}$$

A formal series solution is given by

$$u(x,s)=\sum_{n=1}^{\infty} s^n u_n(x) . \tag{B6}$$

By insertion of Eq. (B6) into Eq. (B5) and comparison of the coefficient to each power of s, we easily obtain

$$u_1'(x)-\frac{dF}{dx}u_1(x)=1 \tag{B7}$$

and

$$u_n'(x)-\frac{dF}{dx}u_n(x)=-\sum_{q=1}^{n-1} u_q(x)u_{n-q}(x) , \tag{B8}$$

which is solved recursively by the formula

$$u_1(x)=-e^{F(x)}\int_x^{\infty} e^{-F(x')}dx' \tag{B9}$$

and

$$u_n(x)=e^{F(x)}\int_x^{\infty} e^{-F(x')}\left[\sum_{q=1}^{n-1} u_q(x')u_{n-q}(x')\right]dx' . \tag{B10}$$

An application of the L'Hospital rule shows that, for $x\to\infty$, $u_1(x)\to-(dF/dx)^{-1}$, which by assumption vanishes. By Eq. (B9), u_1 is negative. Furthermore,

$$\begin{aligned} u_1'(x)&=-\frac{dF}{dx}e^{F(x)}\int_x^{\infty} e^{-F(x')}dx'+1 \\ &\geq e^{F(x)}\int_x^{\infty}\frac{d}{dx'}e^{-F(x')}dx'+1=0 . \end{aligned} \tag{B11}$$

Hence u_1 is monotonously increasing to zero. From Eq. (B10) we see that u_2 is positive. We also find that by Eq. (B8),

$$\begin{aligned} u_2'(x)&=\frac{dF}{dx}e^{F(x)}\int_x^{\infty} e^{-F(x')}u_1(x')^2dx'-u_1^2(x) \\ &\leq u_1^2(x)\left[F'e^{F(x)}\int_x^{\infty} e^{-F(x')}dx'-1\right]\leq 0 . \end{aligned} \tag{B12}$$

We now show by induction on n that u_q is negative and increasing for odd q, positive and decreasing for even q. The assertion holds for $q=1$ and 2. Assume that it holds for all $q<n$.

When n is even, the indices $n-q$ are odd for odd q and even for even q. By assumption each $u_{n-q}(x)u_q(x)$ is then positive and decreasing. We than have, by arguments similar to those leading Eq. (B12),

$$u_n'\leq\sum_{q-1}^{n-1} u_{n-q}(x)u_q(x)\left[F'(x)e^{F(x)}\int_x^{\infty} e^{-F(x')}dx'-1\right]\leq 0 . \tag{B13}$$

Hence u_n is positive and decreasing for n even. The same line of reasoning applied to n odd completes the induction proof. It is now easily proven that the partial sums

$$P(x,s,m)=\sum_{q=1}^{m} s^q u_q(x) \tag{B14}$$

satisfy, for $m\geq 2$ and regarding only terms up to order m, the equation

$$\frac{dP}{dx}(x,s,m)=\frac{dF}{dx}P(x,s,m)+s-P^2(x,s,m-1) , \tag{B15}$$

while, for $m=1$, $P(x,s,1)=u_1(x)s$. The integral version of Eq. (B15) is

$$P(x,s,m)=su_1(x)+e^{F(x)}\int_x^{\infty} e^{-F(x')}P^2(x',s,m-1)dx' , \tag{B16}$$

which gives the following bound for $P(s,m)=\sup_{\forall x}|P(x,s,m)|$:

$$\begin{aligned} P(s,m)&\leq P(s,1)[s+P^2(s,m-1)] \\ &=|u_1(0)|[s+P^2(s,m-1)] . \end{aligned} \tag{B17}$$

It now follows that $P(s,m)$ approaches a finite limit for

$m \to \infty$ if the function $f: x \to |u_1(0)|(s+x^2)$ has an attractive fixed point with a basin of attraction including the point $x_0 = P(s,1) = s|u_1(0)|$. A calculation shows that

$$x^* = \frac{1}{2}\left[\frac{1}{|u_1(0)|} - \left[\frac{1}{|u_1(0)|^2} - 4s\right]^{1/2}\right] \tag{B18}$$

is a real, attractive fixed point for

$$|s| < \frac{1}{4|u_1(0)|^2} . \tag{B19}$$

The other fixed point is a repellor. We have thus proved that, for $|s| < 1/4|u_1(0)|^{-2}$, the series (B6) is uniformly convergent. To complete the proof, we have to show that $\sum_{q=1}^{\infty} s^q u_q'(x)$ is uniformly convergent. This follows from the fact that $(dF/dx)P(x,s,m)$ is a bounded function of x, which by Eq. (B15) again implies that $(dP/dx)(x,s,m)$ can be bounded by a constant (independent of x).

To prove the boundedness of $(dF/dx)P(x,s,m)$, we note that, by multiplying Eq. (B16) with dF/dx,

$$\left|\frac{dF}{dx}P(x,s,m)\right| \le s + P^2(s, m-1) . \tag{B20}$$

Insertion into Eq. (B15) yields

$$\sup_{\forall x}\left|\frac{dP}{dx}(x,s,m)\right| \le 2[|s| + P^2(s, m-1)] \tag{B21}$$

which approaches a constant less than for $m \to \infty$. Q.E.D.

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