Transport on a dynamically disordered lattice

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We consider diffusion on a lattice governed by a master equation in which the bond transition rates fluctuate dynamically between two different values with a relaxation time τ. The effective-medium bond transition rate in the Laplace domain is $\psi(z+1/\tau)$, where $\psi(z)$ is the known solution in the static limit $\tau\to\infty$. This solution exhibits no percolation transition for any finite τ, but it interpolates smoothly between the static solution and the solution in the limit of rapid fluctuations ($\tau=0$).

We consider here diffusive transport on a spatially and dynamically disordered lattice as described by the master equation

$$dP_i/dt=\sum_j w_{ij}(t)[P_j(t)-P_i(t)] \tag{1}$$

in which $P_i(t)$ is the probability that the walker is on site i at time t, and $w_{ij}(t)$ is the transition rate from site j to a nearest-neighbor site i at time t.

In previous work, the transition rates have been treated as spatially random but constant in time. The special case where any nearest neighbor w_{ij} equals 1 with probability p and vanishes with probability $q=1-p$ provides a classic model[1] of percolative transport, with a percolation threshold p_c determined by the specific lattice geometry.

We are concerned here with what happens when the transition rates are *temporally* random. That is, any individual w_{ij} can fluctuate in time between the values 1 and 0 with some characteristic relaxation time τ, and p and q are now the fractions of time spent in the two states.

With static disorder, the effective transition rate vanishes below the percolation threshold. With dynamic disorder, the effective transition rate behaves differently. In one dimension where $p_c=1$, for example, any static w that vanishes will completely suppress diffusion, but when the w's fluctuate dynamically between 0 and 1, spatial diffusion is still possible, because the "gates" open and close at random. If the relaxation time is long compared with the time scale for diffusive transport, the effective transition rate changes smoothly but rather abruptly in the neighborhood of p_c; but if the relaxation time is short, nothing dramatic happens at p_c.

In this paper the effects of dynamic disorder are found by means of a time-dependent version of the effective-medium approximation (EMA). The result can be stated very simply. Suppose that the *static* disorder problem has been solved in the EMA, giving the effective transition rate $w_e=\psi(z)$, where z is the Laplace transform variable conjugate to t. Steady-state migration is described by $\psi(0)$. Then the effective transition rate including dynamic disorder is $\psi(z+1/\tau)$, and steady-state migration is described by $\psi(1/\tau)$. Thus one can take advantage of previously obtained EMA solutions of the static disorder problem. To illustrate the consequences of dynamic disorder, w_e is calculated numerically for one-dimensional, square, and simple-cubic lattices, and the results are displayed graphically.

While our primary interest was in the problem described above, it appears that the procedure is somewhat more generally applicable. This is discussed in the Appendix.

To begin, following Kirkpatrick's scheme,[1] we rewrite Eq. (1) in matrix form

$$\frac{d}{dt}\mathbf{P}=-\mathbf{W}\cdot\mathbf{P}=-\sum_\alpha \sigma_\alpha(t)\mathbf{V}_\alpha\cdot\mathbf{P} \tag{2}$$

where the vector $\mathbf{P}$ is

$$\mathbf{P}=\sum_i P_i\,|\,i\rangle\ . \tag{3}$$

α refers to a particular nearest-neighbor bond (ij), the sum is over all bonds, and the matrix $\mathbf{V}_\alpha$ is given by

$$V_\alpha=(\,|\,i\rangle-|\,j\rangle)(\langle i\,|-\langle j\,|\,)\ . \tag{4}$$

Dynamic disorder is accounted for by a "Liouville master" equation, suggested by the treatment of gated diffusion by Szabo *et al.*[2] Consider first a single bond α. The probability that $\sigma_\alpha(t)=\sigma$ is $f_\alpha(\sigma,t)$. This satisfies a two-component master equation

$$\begin{aligned}\frac{\partial f_\alpha(0)}{\partial t}&=\frac{1}{\tau}[qf_\alpha(1)-pf_\alpha(0)]\ ,\\ \frac{\partial f_\alpha(1)}{\partial t}&=\frac{1}{\tau}[pf_\alpha(0)-qf_\alpha(1)]\ ,\end{aligned} \tag{5}$$

or, in more compact notation

$$\frac{\partial f_\alpha}{\partial t}=\Omega_\alpha f_\alpha=\frac{1}{\tau}[\,\rho(\sigma)\mathscr{P}_\alpha-\rho(1-\sigma)]f_\alpha\ , \tag{6}$$

which defines Ω_α. The operator $\mathscr{P}_\alpha$ replaces any function $A(\sigma_\alpha)$ by $A(1-\sigma_\alpha)$. The time τ is a characteristic relaxation time for approach to the equilibrium solution

$$f_\alpha(\sigma;\text{equilibrium})=\rho(\sigma)\ , \tag{7}$$

and $\rho(0)=q$ and $\rho(1)=p$. As is well known,[3] this master equation corresponds to a continuous time random walk between the states 0 and 1, with exponential waiting time distributions for the transitions.

The state of the entire system is specified by the two vectors $\mathbf{P}$ (for the possible states of the walker) and $\boldsymbol{\sigma}$ (for the possible bond states). The corresponding distribution function $f(\mathbf{P},\boldsymbol{\sigma},t)$ satisfies the Liouville master equation

$$\frac{\partial f}{\partial t}=\frac{\partial}{\partial \mathbf{P}}\cdot[\mathbf{W}\cdot\mathbf{P}f]+\Omega f\ , \tag{8}$$

where, if the bonds all fluctuate independently,

$$\Omega=\sum_{\alpha}\Omega_{\alpha}\ . \tag{9}$$

As an initial condition, we suppose that the walker states are known precisely, and that the bond states are in equilibrium (eq)

$$f(\mathbf{P},\boldsymbol{\sigma},0)=\delta(\mathbf{P}-\mathbf{P}_0)\rho_{\rm eq}(\boldsymbol{\sigma})\ , \tag{10}$$

with

$$\rho_{\rm eq}(\boldsymbol{\sigma})=\prod_{\alpha}\rho(\sigma_{\alpha})\ . \tag{11}$$

Our goal is to determine the average of $\mathbf{P}$ at time t. This average is performed in two steps. First, we look for the partial average $\mathbf{P}(\boldsymbol{\sigma},t)$ defined by

$$\mathbf{P}(\boldsymbol{\sigma},t)=\int d\mathbf{P}\,\mathbf{P}f(\mathbf{P},\boldsymbol{\sigma},t)\ . \tag{12}$$

On using (8), we find that the partial average obeys

$$\frac{\partial}{\partial t}\mathbf{P}=-\mathbf{W}\cdot\mathbf{P}+\Omega\mathbf{P}\ , \tag{13}$$

with the initial condition

$$\mathbf{P}(\boldsymbol{\sigma},0)=\mathbf{P}_0\rho_{\rm eq}(\boldsymbol{\sigma})\ . \tag{14}$$

The full average of $\mathbf{P}$ is given by $\sum_{\sigma}\mathbf{P}(\boldsymbol{\sigma},t)$.

It is convenient to introduce Laplace transforms. Without changing notations, functions of t will be replaced by functions of z. After a simple rearrangement, we find

$$\mathbf{P}(\boldsymbol{\sigma},z)=\mathbf{g}(\boldsymbol{\sigma},z)\cdot\mathbf{P}_0\ . \tag{15}$$

The partially averaged Green's function $\mathbf{g}(\boldsymbol{\sigma},z)$ is given formally by

$$\mathbf{g}(\boldsymbol{\sigma},z)=[z\mathbf{1}+\mathbf{W}(\boldsymbol{\sigma})-\Omega]^{-1}\rho_{\rm eq}(\boldsymbol{\sigma})\ . \tag{16}$$

The fully averaged Green's function is $\mathbf{g}(z)=\sum_{\sigma}\mathbf{g}(\boldsymbol{\sigma},z)$.

An exact calculation of $\mathbf{g}(\boldsymbol{\sigma},z)$ is at least as difficult as the general solution of the static bond disorder problem. But it is easy in the effective-medium approximation. The EMA can be formulated in a variety of equivalent ways; we choose the following one. We want to find an effective transition rate $\psi(z)$ such that the fully averaged $\mathbf{g}(z)$ is the same for the two media: (i) an effective medium in which $\mathbf{W}$ and Ω are replaced by

$$\mathbf{W}=\mathbf{W}_m=\psi(z)\sum_{\alpha}\mathbf{V}_{\alpha}\ ,\qquad \Omega=0\ , \tag{17}$$

and (ii) a medium in which all but one bond have the effective-medium behavior, and that bond is allowed to fluctuate in time,

$$\mathbf{W}=\psi(z)\sum_{\alpha(\neq 1)}\mathbf{V}_{\alpha}+\sigma_1\mathbf{V}_1\ ,\qquad \Omega=\Omega_1\ . \tag{18}$$

In case (ii) we suppress all indices and write

$$\boldsymbol{\Gamma}_{\sigma}=[z\mathbf{1}+\mathbf{W}_m+(\sigma-\psi)\mathbf{V}-\Omega(\sigma)]^{-1}\rho(\sigma)\ . \tag{19}$$

The effective-medium condition is that $\boldsymbol{\Gamma}_{\sigma}$ should reproduce the result of case (i)

$$\mathbf{g}(z)=(z\mathbf{1}+\mathbf{W}_m)^{-1}=\sum_{\sigma}\boldsymbol{\Gamma}_{\sigma}\ . \tag{20}$$

Equation (19) is equivalent to a pair of equations for $\boldsymbol{\Gamma}_0$ and $\boldsymbol{\Gamma}_1$

$$\left[\left(z+\frac{p}{\tau}\right)\mathbf{1}+\mathbf{W}_m-\psi\mathbf{V}\right]\cdot\boldsymbol{\Gamma}_0-\frac{q}{\tau}\boldsymbol{\Gamma}_1=q\mathbf{1}\ ,$$
$$\left[\left(z+\frac{q}{\tau}\right)\mathbf{1}+\mathbf{W}_m+(1-\psi)\mathbf{V}\right]\cdot\boldsymbol{\Gamma}_1-\frac{p}{\tau}\boldsymbol{\Gamma}_0=p\mathbf{1}\ . \tag{21}$$

By taking appropriate linear combinations, and using the effective-medium condition, we find

$$\psi\mathbf{V}\cdot\boldsymbol{\Gamma}_0-(1-\psi)\mathbf{V}\cdot\boldsymbol{\Gamma}_1=\mathbf{0}\ , \tag{22}$$

$$\left[\left(z+\frac{1}{\tau}\right)\mathbf{1}+\mathbf{W}_m-\psi\mathbf{V}\right]\cdot(p\boldsymbol{\Gamma}_0-q\boldsymbol{\Gamma}_1)-q\mathbf{V}\cdot\boldsymbol{\Gamma}_1=\mathbf{0}\ . \tag{23}$$

Now the matrix $\mathbf{V}_{\alpha}$, defined by Eq. (4), has the property that for an arbitrary matrix $\mathbf{H}$

$$\mathbf{V}_{\alpha}\cdot\mathbf{H}\cdot\mathbf{V}_{\alpha}=h_{\alpha}\mathbf{V}_{\alpha}\ , \tag{24}$$

where h_{α} is a scalar. We take the special choice

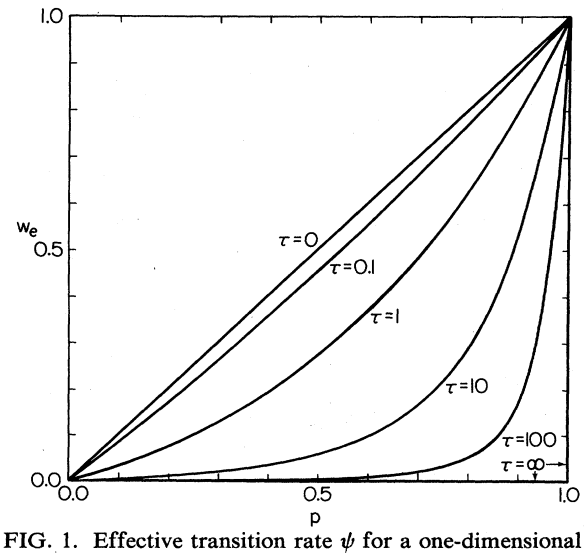

FIG. 1. Effective transition rate ψ for a one-dimensional lattice whose bond transition rates w_{ij} fluctuate between 0 and 1. Here τ is the characteristic time scale of the fluctuations, and p is the mean proportion of bonds with $w_{ij}=1$.

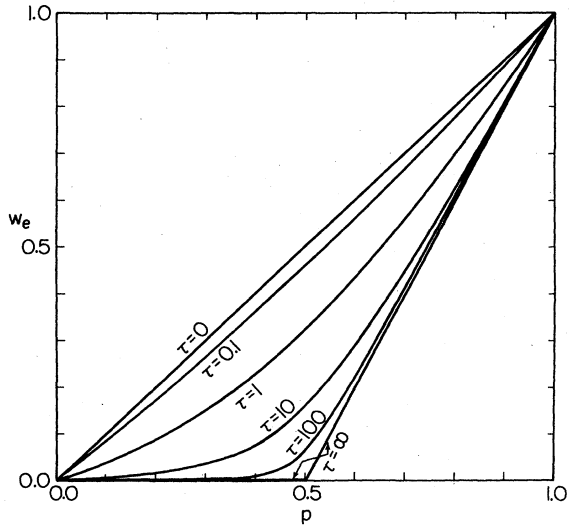

FIG. 2. Same as Fig. 1, but for a square lattice.

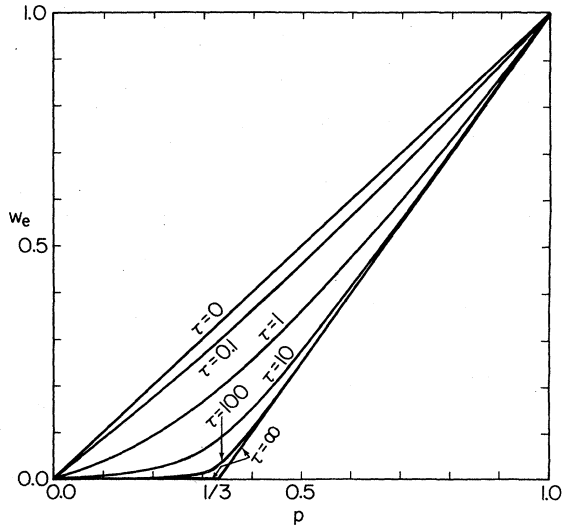

FIG. 3. Same as Fig 1, but for a simple-cubic lattice.

$$\mathbf{H}=\left[\left[z+\frac{1}{\tau}\right]\mathbf{1}+\mathbf{W}_m\right]^{-1}, \tag{25}$$

multiply Eq. (23) on the left by $\mathbf{VH}$, and use (24) to obtain

$$p(1-\psi h)\mathbf{V}\cdot\boldsymbol{\Gamma}_0-q(1+h-\psi h)\mathbf{V}\cdot\boldsymbol{\Gamma}_1=\mathbf{0}\ . \tag{26}$$

But (22) and (26) can have a nontrivial solution ($\mathbf{V}\cdot\boldsymbol{\Gamma}_0$ and $\mathbf{V}\cdot\boldsymbol{\Gamma}_1$ not both zero) only if the determinant of coefficients vanishes,

$$-q\psi(1+h-\psi h)+p(1-\psi)(1-\psi h)=0\ . \tag{27}$$

Because h is an explicit function of ψ, via (17), (24), and (25), this is the equation that determines the effective ψ. But the Laplace variable z appears explicitly in h only in the combination $z+1/\tau$. It follows that ψ is a function of $z+1/\tau$. Thus it is clear that if ψ is known in the limit of static disorder, $\tau\rightarrow\infty$, it takes the form $\psi(z+1/\tau)$ for arbitrary τ. This is what was claimed in the beginning of the paper.

The static disorder problem has been solved in the EMA, by Webman,[4] Odagaki and Lax,[5] and Summerfield,[6] and is discussed extensively by Sahimi *et al.*[7] If we take their results, replace z by $z+1/\tau$, and then take the stationary limit $z\rightarrow 0$, we obtain

$$\frac{p-w_e}{p_c(1-w_e)}=1-YG(0,1-Y)\ . \tag{28}$$

Here, p_c is $2/n_c$ where n_c is the coordination number of the lattice. This is the percolation threshold for static disorder in the EMA. The new variable Y is $(1+n_c w_e\tau)^{-1}$, and $G(0,z)$ is the ordinary lattice Green's function evaluated at the origin. Notations and normalizations differ among the various authors cited. We use the notation of Ref. 8. In one dimension, for example, the Green's function is

$$G(0,z)=(1-z^2)^{-1/2}\ . \tag{29}$$

For a square lattice in two dimensions $G(0,z)$ can be expressed in terms of the complete elliptic integral K. In three dimensions, the Chebyshev approximation presented in Ref. 9 is useful.

It is easy to see that the expected behavior

$$w_e=\frac{p-p_c}{1-p_c}\quad (p_c\le p\le 1) \tag{30}$$

is found in the static limit, and that

$$w_e=p \tag{31}$$

holds for the limit of rapid fluctuations $\tau\rightarrow 0$. It is also clear that w_e can vanish only at $p=0$; there is no percolation threshold.

In Figs. 1, 2, and 3 we have plotted w_e as a function of p for various values of τ, for the one-dimensional, square, and simple-cubic lattices. These show graphically the changes from large τ to small τ.

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APPENDIX

The procedure described in the main text can be used for the class of models defined by

$$\mathbf{W}=\mathbf{U}+\sum_\alpha \sigma_\alpha(t)\mathbf{A}_\alpha \tag{A1}$$

where $\mathbf{U}$ is a matrix with the translational symmetry of the lattice, the index α refers to a location on the lattice (e.g., a site or a bond), and the matrix $\mathbf{A}_\alpha$ has the representation

$$\mathbf{A}_\alpha=\mathbf{F}_\alpha\mathbf{F}_\alpha^\dagger \tag{A2}$$

where $\mathbf{F}_\alpha$ is a vector. Because the matrix $\mathbf{U}$ can be included in W_m, and $\mathbf{A}_\alpha$ still has the property [Eq. (24)], the preceding argument is still valid.

As an example, consider bond disorder where any w_{ij} can fluctuate between two nonzero values, for example, μ

and 1, with probabilities q and p. The appropriate choices of $\mathbf{U}$ and $\mathbf{A}_\alpha$ are

$$\mathbf{U}=\mu\sum_\alpha \mathbf{V}_\alpha\ ,$$
$$\mathbf{A}_\alpha=(1-\mu)\mathbf{V}_\alpha\ . \tag{A3}$$

The resulting steady state w_e is determined by

$$\frac{w_e(p+q\mu-w_e)}{p_c(1-w_e)(w_e-\mu)}=1-YG(0,1-Y)\ , \tag{A4}$$

with the same Y and $G(0,z)$ as before.

Note added. Druger, Ratner, and Nitzan have recently published a paper related to ours.[10] After describing some physical problems where a treatment of dynamic disorder might be useful, they propose a model that leads to results essentially the same as ours. In their model, the entire disordered lattice is randomly "renewed" at a constant rate. This contrasts with our model in which individual bonds are changed randomly in time. The result that we obtain in the EMA is exact for their model, but only approximate for ours. (This can be seen easily by looking at terms in the perturbation expansion that are omitted in the EMA.)

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