Transient transport in a dynamical two-chain model

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We use a dynamical two-chain model to study anomalous transport in chainlike systems (like polymers) with a statistical distribution of transition rates. Temporal disorder (resulting from energetic or spatial randomness) is taken into account in the framework of continuous-time random walks. The interchain and intrachain transitions are characterized by different waiting-time densities. The effective current along the chains is studied as a function of the interchain and intrachain waiting-time densities. The approach presented here allows an exact expression for the Laplace-transformed effective current and for higher moments of the effective probability distribution of the walker. The general scheme can be applied to a model consisting of N chains and also to higher-dimensional lattices.

I. INTRODUCTION

Photoconductivity in amorphous media is a topic of great importance both theoretically and experimentally, and also due to the central role of the effect in the xerographic process.[1,2]

As is well known, photoconductivity data often show a temporal transition from dispersive to nondispersive behavior.[1-3] The main feature of the recently developed experimental techniques is the possibility of monitoring the current over many orders of magnitude in time and intensity. Such measurements often reveal crossover effects in the transition form dispersive to nondispersive behavior.[1-5] Interestingly, these crossover effects can be understood in the context of transport theories in random media.[6]

The situation is even more complex when one considers charge carriers moving along and across many strands of polymers with different transition probabilities for jumps along or across the chains. Such a situation is encountered in the photoconductivity of doped quasilinear polymers such as polyacetylene, where charge carriers move on and between parallel, one-dimensional polymer chains with defects.[7]

As a contribution to the understanding of the complex situation that such models may lead to, a previous paper[5] studied transient transport in a hopping model with a power-law distribution of transition rates for carriers jumping along two parallel linear chains. In the present work we will display a variant dynamical model consisting of parallel chains by using the theory of continuous-time random walks (CTRW) with internal states.[6(b)]

We start by noticing that the CTRW theory was originally introduced into the physical literature to investigate the effects of disorder on charge-carrier transport.[2,8-11] From then on dispersive transport in disordered solids has been studied intensely using different generalizations of the CTRW approach. Recent investigations centered on continuous-time random walks with internal states,[6(b),12,13] so-called multistate CTRW (MCTRW), and on models with dynamical disorder.[14,15]

There are several parameters that may be affected by disorder, such as the intersite distances, the energy levels, or the internal states of the walker. In the analysis of the electric conductivity through strands of polymers, one therefore has to take into account many possibilities of walker-lattice interactions, which then lead to a complex picture. A simplifying feature is the fact that for a system of polymer strands the interchain and intrachain interactions differ significantly, so that one can use a model based on coupled chains.

In our approach we use a model consisting of N coupled, infinite chains as depicted in Fig. 1(a). Physically we imagine the walker to be at a certain time t on site s' on chain l and take $W_{ss'}(l)$ to be the transition rate from site s' to site s along the chain l. Note that we set the distance between two neighboring sites equal to 1, so that all lengths are in units of the intersite distance.

The walker can also make a jump from site s of chain l to the site s of a neighboring chain l', the jump being characterized by the rate $M_{l'l}$ (in the MCTRW this corresponds to a change of internal state). If the jumps along and across the chains are independent, we can view the walker as first jumping on a disordered chain characterized by random rates $W_{ss'}(l)$, taken from a given distribution. At some random time the walker changes to a neighboring chain (this fact is represented by the transition $l \rightarrow l'$); then during the next time interval the walker is on the chain l' characterized by *newly* distributed rates $W_{ss'}(l)$ (possibly taken from another distribution), and so on.

It should be remarked that the present model is different from that of Ref. 5, because here the distribution of rates $W_{ss'}(l)$ between sites is reset after every jump across the chains. The model analyzed here introduces an additional feature through the dynamical change of

rates $W_{ss'}(l)$.

Let thus $W_{ss'}(l)$ be the transition rates for a given, statistically disordered configuration. We now follow the spirit of the CTRW theory[2,6(b),8–12] and replace the set of $W_{ss'}(l)$ by a (decoupled) spatiotemporal transition probability density $\psi_l(s-s',t)$ [see Fig. 1(b)]. Disregarding for the moment jumps across the chains, and focusing on chain l only, we have

$$\psi_l(s-s',t)=\lambda_l(s-s')\psi_l(t) , \tag{1}$$

where the $\lambda_l(s-s')$ are the jumping probabilities from site s' to site s for a simple random walk on chain l and $\psi_l(t)$ is the waiting-time density associated with this chain. Note that $\psi_l(s-s',t)$ is translationally invariant and that $\sum_{s''}\lambda_l(s'')=1$. The probability that no jump along chain l has occurred up to time t after the last step will be denoted by $\phi_l(t)$:

$$\begin{aligned}\phi_l(t)&=1-\sum_{s''}\int_0^t\psi_l(s'',\tau)d\tau \\ &=1-\int_0^t\psi_l(\tau)d\tau .\end{aligned} \tag{2}$$

In the same spirit the jumps across chains, represented by $M_{l'l}$, can be characterized by general transition probability densities $\psi^f_{l'l}(t)$. Then the probability that the walker does not leave chain l during the time interval t since the last step is

$$\phi^f_l(t)=1-\sum_{l'}\int_0^t\psi^f_{l'l}(\tau)d\tau . \tag{3}$$

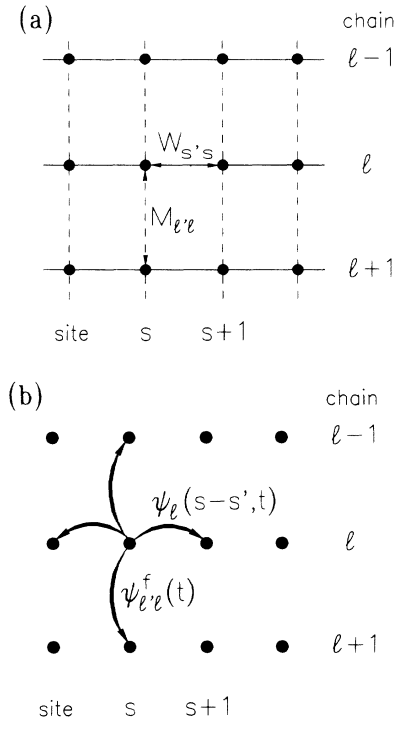

FIG. 1. (a) Illustration of the considered model, consisting of N parallel chains with jumping rates $W_{s's}(l)$ along, $M_{l'l}$ across, the chains. (b) The same model in CTRW description, using site-independent transition probability densities $\psi_l(s-s',t)$ and $\psi^f_{l'l}(t)$ instead of discrete jumping rates.

Using Eqs. (1) and (3), we can immediately write down the effective transition probability density $\eta_{ll}(s-s',t)$ associated to the jump of a walker on chain l from site s' to s after a waiting time t:

$$\eta_{ll}(s-s',t)=\lambda_l(s-s')\psi_l(t)\phi^f_l(t) . \tag{4a}$$

In the same way we can find the effective probability density $\eta_{l'l}(s-s',t)$ for transitions from site s on chain l to site s' on chain l':

$$\eta_{l'l}(s-s',t)=\delta_{ss'}\phi_l(t)\psi^f_{l'l}(t) \quad (\text{for } l\neq l') \tag{4b}$$

(note that we allow only such interchain jumps for which $s=s'$).

Now, the matrix $\eta=[\eta_{l'l}]$ satisfies the following normalization condition:

$$\sum_{s'}\sum_{l'}\int_0^\infty\eta_{l'l}(s'-s,t)dt=1 , \tag{4c}$$

which ensures that the walker will certainly leave any site at some time either by moving to another site s' of the same chain or by jumping to another chain l'.

The particular form of Eqs. (4a) and (4b) can be visualized as follows: The probability that a walker, arriving at t' on site s of chain l, performs its next step at time $t'+t$ along chain l is the combined probability of not having yet performed a jump to another chain up to time $t'+t$ and of moving to another site on chain l just at time $t'+t$. This explains the diagonal parts of the matrix η. The nondiagonal parts can be understood in a similar way.

We want to remark that the structure of Eqs. (4) is reminiscent of dynamical disorder models;[14–16] however, only if the waiting-time density $\psi_l(t)$ of the walker is exponential (Markovian CTRW) will we be able to associate our present MCTRW approach to an external-noise model (see the Appendix).

In what follows we are going to use the probability densities of Eqs. (4) to treat the problem of photoconductivity through strands of polymers. The outline of the paper is as follows: In Sec. II we derive expressions for the effective current along the chains and review some basic results of the MCTRW theory in order to obtain the higher moments of the effective probability distribution of the walk. In Sec. III we illustrate the model by presenting the results for two parallel chains. In Sec. IV we study analytically the long-time limit of the current and we display numerically evaluated plots of its full time-dependent behavior. We end the paper in Sec. V with a short discussion of crossover effects. The Appendix is devoted to an analysis of the connection of the present model to other models for dynamical disorder.

II. GENERAL APPROACH

A. The current

Let $R_l(s,t)$ be the probability that a walker arrives at site s on chain l just at time t. The functions $R_l(s,t)$ obey the following integral evolution equation:

$$R_l(s,t)=\sum_{s'}\sum_{l'}\int_0^t \eta_{ll'}(s-s',t-\tau)R_{l'}(s',\tau)d\tau+\delta(t)\delta_{s,0}c_l \ . \tag{5}$$

Here we assumed that the walker starts at time $t=0$ on site $s=0$. c_l is the probability that the walker initially occupies chain l ($\sum_l c_l=1$).

In the following, the Fourier and Laplace representations will be understood by their arguments, i.e.,

$$f(k)=\sum_s f(s)e^{iks}$$

and

$$g(u)=\int_0^\infty g(t)e^{-ut}dt \ .$$

Then we get from Eq. (5) the solution for $R_l(k,u)$:

$$R_l(k,u)=\sum_{l'}\Theta_{ll'}(k,u)c_{l'} \ , \tag{6a}$$

where $\Theta(k,u)=[\Theta_{ll'}(k,u)]$ is the inverse of the matrix $[1-\eta(k,u)]$:

$$\Theta(k,u)=[1-\eta(k,u)]^{-1} \ . \tag{6b}$$

The total effective current $I(t)$ along the chains can be written as

$$I(t)=\sum_s\sum_l\int_0^t\sum_{s''}s''\eta_{ll}(s'',t-\tau)R_l(s,\tau)d\tau \ . \tag{7a}$$

This formula can be understood as follows: A walker, which arrives at time $\tau<t$ on site s of chain l contributes to the current time t, if it jumps after a waiting time $t-\tau$ along the chain l. The contribution of each such jump to the current may be negative or positive, according to the direction in which the walker jumps, and is proportional to the length s'' of the step. Thus the total current along all chains is the sum over all integers s and s'' and over all chains l, integrated over all τ.

As usual, one has the Fourier-domain relations

$$f(k=0)=\sum_s f(s) \quad \text{and} \quad \frac{\partial}{\partial k}f(k)\bigg|_{k=0}=i\sum_s sf(s) \ .$$

Then the Fourier and Laplace representation of Eq. (7a) is

$$I(u)=(-i)\sum_l\left[\frac{\partial}{\partial k}\eta_{ll}(k,u)\right]R_l(k,u)\bigg|_{k=0} \ . \tag{7b}$$

This formula gives the full temporal behavior of the effective current in our dynamical N-chain model given in Eqs. (4). We note that if the interchain jumps to sites $s'\neq s$ are also allowed, the generalized form of Eq. (7b) is

$$I(u)=(-i)\sum_l\sum_{l'}\left[\frac{\partial}{\partial k}\eta_{ll'}(k,u)\right]R_{l'}(k,u)\bigg|_{k=0} \ . \tag{7c}$$

If more information about the process is needed, i.e, if higher moments of the positional distribution of the walker have to be evaluated, one can make use of the MCTRW formalism, as we now describe.

B. Higher Moments: The MCTRW approach

As in Ref. 12, we start with a general set of coupled CTRW to characterize a MCTRW; an example of such coupled equations is provided by Eq. (5). Now the probability $P_l(s,t)$ that the walker is at site s of chain l at time t is given by

$$P_l(s,t)=\int_0^t\Phi_l(t-\tau)R_l(s,\tau)d\tau \ , \tag{8}$$

where $\Phi_l(t)$ is the probability that in the interval $[0,t]$ *no* further jump occurred:

$$\Phi_l(t)=1-\sum_{s''}\sum_{l''}\int_0^t\eta_{l''l}(s'',\tau)d\tau \ . \tag{9}$$

As before, we start with our walkers from the origin; however, we allow them to be situated on different chains. The initial condition is then

$$P_l(s,0)=\delta_{s,0}c_l \ , \tag{10}$$

with $c_1+\cdots+c_N=1$ (N is the number of different chains). Notice that Eq. (8) is a convolution in time, which simplifies in the Laplace representation. Furthermore, for $\Phi_l(t)$ one has in the Laplace domain

$$\Phi_l(u)=\frac{1-\sum_{s''}\sum_{l''}\eta_{l''l}(s'',u)}{u} \ . \tag{11}$$

In the following we will use the vectorial notation

$$\mathbf{P}(k,u)=(P_1(k,u),\ldots,P_N(k,u))$$

and denote by $\mathbf{P}_0(k)$ the Fourier transform of the initial occupation probability $\mathbf{P}(s,t=0)$: $\mathbf{P}_0(k)=\mathbf{P}(k,t=0)$. In our case from Eq. (10) it follows that $\mathbf{P}_0(k)\equiv\mathbf{P}_0$ independent of k. The solution of the MCTRW in the Fourier and Laplace representation is then[12,13]

$$\mathbf{P}(k,u)=\mathbf{\Phi}(u)\cdot[1-\boldsymbol{\eta}(k,u)]^{-1}\cdot\mathbf{P}_0 \ , \tag{12}$$

where $\mathbf{\Phi}(u)=[\delta_{l'l}\Phi_l(u)]$ and $\boldsymbol{\eta}(k,u)=[\eta_{l'l}(k,u)]$. Then the probability that the walker is at time t on site s of chain l is given by the Fourier-Laplace inversion of the lth component of Eq. (12): $P_l(k,u)$. If we are only interested in the position of the walker at time t (independently of the chain),[17,18] we have to calculate the effective (marginal) probability distribution, defined through

$$\mathcal{P}(k,u)=\sum_l P_l(k,u) \ . \tag{13}$$

Marginal quantities represent an average in the sense that one does not distinguish between different chains. For the problem that we are interested in (a hopping model with jumps along and across chains), the effective distributions, Eq. (13), allow us to determine the current as the time derivative of the position of the walker independently of the actually occupied chain. We see that from the waiting-time density matrix $\boldsymbol{\eta}(k,u)$ the determination of many quantities of interest is reduced to a Laplace inversion. Thus from Eq. (12) all the moments of the distribution $\mathbf{P}(s,t)$ can be easily calculated.[13] One has

$$\{s_l^m(t)\} \equiv \sum_s s^m P_l(s,t)$$

$$= (-i)^m \mathcal{L}^{-1} \left[\frac{\partial^m}{\partial k^m} P_l(k,u) \right]_{k=0} , \tag{14}$$

where $\mathcal{L}^{-1}$ stands for the inverse Laplace transform.

Setting again $\Theta(k,u) \equiv [1-\eta(k,u)]^{-1}$, for example, the first and second moments can be written as

$$\{s_l(u)\} = -i \left[\Phi \cdot \Theta \cdot \frac{\partial \eta}{\partial k} \cdot \Theta \cdot \mathbf{P}_0 \Big|_{k=0} \right]_l , \tag{15a}$$

$$\{s_l^2(u)\} = -\left[\Phi \left[2\Theta \cdot \frac{\partial \eta}{\partial k} \cdot \Theta \cdot \frac{\partial \eta}{\partial k} \cdot \Theta + \Theta \cdot \frac{\partial^2 \eta}{\partial k^2} \cdot \Theta \right] \cdot \mathbf{P}_0 \Big|_{k=0} \right]_l . \tag{15b}$$

From now on and due to the fact that we are interested in the effective probability distribution, given by Eq. (13), we are going to use only the effective moments:

$$\langle s^m(t) \rangle \equiv \sum_l \{s_l^m(t)\} . \tag{16}$$

Thus, using the MCTRW approach, the effective current can alternatively be written as

$$I(u) = u \sum_l \{s_l(u)\} . \tag{17a}$$

It is now straightforward to show that Eq. (17a) is the same as Eq. (7c). Inserting Eq. (15a) into Eq. (17a) and using Eq. (6a), we get

$$I(u) = (-i)u \sum_l \left[\Phi \cdot \Theta \cdot \frac{\partial \eta}{\partial k} \cdot \mathbf{R}(k,u) \Big|_{k=0} \right]_l . \tag{17b}$$

From the normalization condition $\sum_l P_l(k=0,t)=1$, one has for the MCTRW propagator from Eq. (12)

$$\frac{1}{u} = \sum_l P_l(k=0,u) = \sum_l \left[\Phi \cdot \Theta \cdot \mathbf{P}_0 \Big|_{k=0} \right]_l . \tag{18}$$

The last expression holds for every initial condition $\mathbf{P}_0$. Hence $\sum_l \sum_{l'} \Phi_{ll'} \Theta_{l'l''}|_{k=0} = 1/u$ for all l''. From Eq. (17b) now Eq. (7c) immediately follows.

The advantage of the MCTRW approach lies, however, in the fact that even higher moments can be readily evaluated. For example, the generalized diffusion coefficient

$$D(t) = \tfrac{1}{2} \frac{d}{dt} (\langle s^2(t) \rangle - \langle s(t) \rangle^2) \tag{19}$$

can be obtained from Eqs. (15) and (16).

III. RESULTS FOR THE TWO-CHAIN MODEL

We now turn to the specification of the waiting-time density matrix η for a two-chain model. The structure of η, already presented in Eqs. (4a) and (4b), can be understood from earlier works on diffusion in the presence of external noise.[14] Using the translational invariance [the disorder along each chain is characterized by the waiting-time density $\psi_l(t)$ of the walker], one has for a two-chain model with biasing external field in the Fourier and time domains:

$$\eta(k,t) = \begin{bmatrix} \lambda_1(k)\psi_1(t)\phi_1^f(t) & \phi_2(t)\psi_{12}^f(t) \\ \phi_1(t)\psi_{21}^f(t) & \lambda_2(k)\psi_2(t)\phi_2^f(t) \end{bmatrix} . \tag{20}$$

The diagonal parts of η are transition probability densities, representing the motion of the walker along the chains. The nondiagonal parts are also densities but these elements represent jumps across the chains which, however, do not change the position of the walker (site s) with respect to the externally applied field.

For strong external electric fields, the motion of the charge carriers is dominated by jumps in the direction of the field, so that we can assume a biased model allowing only jumps in one direction, i.e.,

$$\lambda_l(s-s') = \delta_{s,s'+1} ,$$

independently of l. Then the structure function of the walk along each chain l is $\lambda_l(k) = e^{ik}$. With this condition and the definitions

$$\begin{aligned} \eta_{ll} &\equiv \eta_{ll}(u) = \mathcal{L}(\psi_l(t)\phi_l^f(t)) , \\ \eta_{l'l} &\equiv \eta_{l'l}(u) = \mathcal{L}(\phi_l(t)\psi_{l'l}^f(t)) , \end{aligned} \tag{21}$$

we get from Eqs. (6) and (7b) after the matrix inversion of $[1-\eta(k=0,u)]$ in matrix representation

$$I(u) = \frac{1}{(1-\eta_{11})(1-\eta_{22}) - \eta_{12}\eta_{21}} \left[\begin{bmatrix} 1-\eta_{22} & \eta_{12} \\ \eta_{21} & 1-\eta_{11} \end{bmatrix} \cdot \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \right] \cdot \begin{bmatrix} \eta_{11} \\ \eta_{22} \end{bmatrix} . \tag{22}$$

This finally results in

$$I(u) = \frac{c_1\eta_{11} + c_2\eta_{22} + c_1\eta_{22}\eta_{21} + c_2\eta_{12}\eta_{11} - \eta_{11}\eta_{22}}{1-\eta_{11}-\eta_{22}+\eta_{11}\eta_{22}-\eta_{12}\eta_{21}} , \tag{23}$$

where, as before, the constants c_l give the initial population of particles on the chains, so that here $c_1+c_2=1$. Note that the same result [Eq. (23)] can also be obtained by evaluating Eq. (17a).

The usual CTRW current can be obtained from Eq. (23) by decoupling the chains, i.e., setting $\psi_{l'l}^f = 0$. In this case one has

$$I(u) = \frac{c_1\eta_{11}(1-\eta_{22}) + c_2\eta_{22}(1-\eta_{11})}{(1-\eta_{11})(1-\eta_{22})} = c_1 \frac{\eta_{11}}{1-\eta_{11}} + c_2 \frac{\eta_{22}}{1-\eta_{22}} . \tag{24}$$

Furthermore, for $\psi^f_{l'l}=0$ one also has $\phi^f_l(t)\equiv 1$ for all t and thus $\eta_{11}(u)=\psi_1(u)$ and $\eta_{22}(u)=\psi_2(u)$. Equation (24) thus reproduces the Montroll-Scher-Lax result

$$I(u)=\psi(u)/[1-\psi(u)] ,$$

here weighted for the two separate chains according to their initial population.

In the context of CTRW Eq. (24) shows the transition from dispersive to nondispersive current by modeling the strength of disorder.[4] Remember that for a waiting-time density with a long-time tail, such as $\psi(t)\sim At^{-1-\alpha}$ $(t\to\infty)$, the usual CTRW expansion, Eq. (24), leads to the asymptotic behavior $I(t)\sim t^{-1+\alpha}$. Our expression for the effective current, Eq. (23), however, goes beyond the CTRW result because it takes into account the competition of jumps along *and* across the chains (i.e., the walker can waste additional time in interchain loops without changing the site).

From Eq. (23) we can learn several things: First, looking at Eqs. (21) and assuming that either the waiting-time density along the chains $\psi_l(t)$ or that across the chains $\psi^f_{l'l}(t)$ is Markovian [i.e., the waiting-time densities and also the $\phi^{(f)}_l(t)$ are exponential], the transition probabilities $\eta_{l'l}$ and η_{ll} may no longer have an algebraic long-time tail, due to the product in Eq. (21). Thus, even in the presence of strong disorder along each chain, i.e., $\psi_l(t)\sim t^{-1-\alpha_l}$, the effective current stays diffusive. This is so because each jump across the chains resets the watch for the motion along the chains and thus the long waiting times are cut off. Second, if the jumps across *and* along the chains both have a long-time tail, the asymptotic behavior of the current *along* the chains will also be strongly influenced by the jumps *across* the chains.

In Sec. IV we are going to display the long-time behavior for the effective current taking into consideration different waiting-time densities, both for the motion along and also across the chains.

IV. EVALUATION OF THE CURRENT

In this section we evaluate the effective current $I(t)$ and focus on its long-time behavior. Let us assume that along each chain we have a certain long-tailed waiting-time density $\psi_l(t)\sim A_l t^{-1-\alpha_l}$ (which might, for example, result from energetic or spatial disorder on chain l). For this we use the Weierstrass form

$$\psi_l(t)=\frac{1-a}{a}\sum_{k=1}^{\infty}(ab)^k e^{-b^k t} . \tag{25}$$

This form is a general time-fractal event-time density function,[19] and it has the advantage of being very flexible, so it can be easily Laplace transformed or evaluated numerically. Under the change $t\to bt$, Eq. (25) is scale invariant at longer times. So we get

$$\psi_l(bt)=\frac{\psi_l(t)}{ab}-\frac{1-a}{a}e^{-bt}\sim\frac{\psi_l(t)}{ab} , \tag{26}$$

from which for large t we obtain

$$\psi_l(t)\sim A_l t^{-1-\alpha_l} , \tag{27}$$

where $\alpha_l=\ln a/\ln b$.

Let us assume that jumps between the chains have also a similar form, possibly with a different coefficient β. We also set, for simplicity, $\psi^f_{l'l}=\psi^f_{ll'}\equiv\psi^f$. Thus,

$$\psi^f(t)\sim A_f t^{-1-\beta} . \tag{28}$$

From Eqs. (27) and (28) we obtain for $\phi_l(t)$ and $\phi^f_l(t)$

$$\phi_l(t)\sim\frac{A_l}{\alpha_l}t^{-\alpha_l}\quad\text{and}\quad\phi^f_l(t)\sim\frac{A_f}{\beta}t^{-\beta} . \tag{29}$$

In order to use our formula for the effective current, Eq. (23), we have to make the Laplace transform of the products of the $\psi(t)$ and $\phi(t)$ functions. An Abelian theorem states that if $0<\gamma<1$ and

$$f_\gamma(t)\sim A_\gamma t^{-1-\gamma}\quad\text{for } t\to\infty , \tag{30a}$$

one has

$$\mathcal{L}(f_\gamma(t))\equiv f_\gamma(u)\sim C-A_\gamma\frac{\Gamma(1-\gamma)}{\gamma}u^\gamma\quad\text{for } u\to 0 . \tag{30b}$$

Thus we get for the $\eta_{l'l}(u)$ elements in the limit $u\to 0$

$$\eta_{ll}\sim\Omega_{ll}-B_{ll}u^{\alpha_l+\beta} , \tag{31a}$$

$$\eta_{l'l}\sim\Omega_{l'l}-B_{l'l}u^{\alpha_l+\beta}\quad(l\neq l') , \tag{31b}$$

where

$$B_{ll}=\frac{A_l A_f}{\beta}\frac{\Gamma(1-\alpha_l-\beta)}{\alpha_l+\beta} ,$$
$$B_{l'l}=\frac{A_l A_f}{\alpha_l}\frac{\Gamma(1-\alpha_l-\beta)}{\alpha_l+\beta} . \tag{32}$$

Equations (31) hold for $\alpha_l+\beta<1$. Note that the constant

$$\Omega_{ll}=\int_0^\infty\eta_{ll}(t)dt=1-\Omega_{l'l}$$

has the meaning of the probability that the next step goes in the direction of chain l (independently of the time at which the next step occurs), whereas $\Omega_{l'l}$ is the probability that the next step goes from chain l to chain l'. Using Eqs. (31) in the formula for the effective current, Eq. (23), we have

$$I(u)\sim\frac{\Omega_{11}+\Omega_{22}-2\Omega_{11}\Omega_{22}}{\Omega_{ll'}(B_{ll}+B_{l'l})}u^{-\beta-\alpha_l}\quad(u\to 0) , \tag{33}$$

where l denotes the chain with $\alpha_l\le\alpha_{l'}$. Then for $\beta+\min(\alpha_l)<1$, the long-time behavior of $I(t)$ is as follows:

$$I(t)\sim\text{const}\times t^{\beta+\min(\alpha_l)-1}\quad(t\to\infty) . \tag{34}$$

We see that the long-time tail is governed by the motion between the chains (exponent β) and by the jumps along that chain in which the motion is most hindered [i.e., minimum of (α_l)]. The constant that appears in Eq. (34) carries information on the probabilities $\Omega_{l'l}$ and on the constants $B_{l'l}$. Then, if we fix the value of the smaller of the α_l, say, α_1, and vary α_2, we obtain the same long-time

form, but the prefactor will change; this will be manifest in a shift of the effective current. This and other interesting crossover effects will be displayed in the following, where we show the full time dependence of the effective current.

After this asymptotic analysis of the current, we now turn to the numerical evaluation of the temporal behavior of $I(t)$, in order to study the intermediate time regime. For $\psi_l(t)$ we use the Weierstrass form, Eq. (25), taking for α_l different values of $\ln a/\ln b$. The $\phi_l(t)$ functions can be obtained by a simple integration of Eq. (25) with respect to time:

$$\phi_l(t)=\frac{1-a}{a}\sum_{k=1}^{\infty} a^k e^{-b^k t} . \tag{35}$$

Similar expressions are used for the function $\psi^f_{l'l}(l)$ and $\phi^f_l(t)$. The $\eta_{l'l}(u)$ functions are given from Eqs. (21). Then the full time-dependent effective current is obtained by taking the inverse Laplace transform of $I(u)$; this step has to be performed numerically.

We first remark that the role of the parameters c_l which appear in Eq. (23) is not decisive. In Fig. 2 we plotted the currents for three different initial populations. As one can see from this figure, after a short transient regime the time dependence of $I(t)$ reaches the same shape regardless of the initial conditions. In the following figures we therefore only display the curves that correspond to the initial condition $c_1=c_2=\frac{1}{2}$, i.e., where the walker may start with equal probability on each chain.

Figure 3 shows the typical behavior of $I(t)$. In this plot we have set the exponents for the jumps between chains to the value $\beta=0.5$ and for jumps along chain number 2 to the value $\alpha_2=0.3$. By changing now α_1 from small $\alpha_1<\alpha_2$ to large values $\alpha_1>\alpha_2$, we readily demonstrate that the shape of the currents is always controlled by the minimum of α_1 and α_2. This agrees with Eq. (34), from which the asymptotic behavior of the current is given analytically by

$$I(t)\sim t^{\beta+\min(\alpha_l)-1} .$$

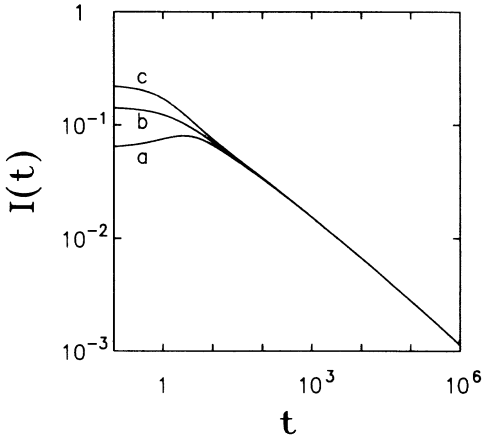

FIG. 2. Effective currents for $\alpha_1=0.1$, $\alpha_2=0.5$, and $\beta=0.5$, starting with different initial occupation probabilities: $c_1=1$, $c_2=0$ (curve a); $c_1=c_2=\frac{1}{2}$ (curve b); $c_1=0$, $c_2=1$ (curve c).

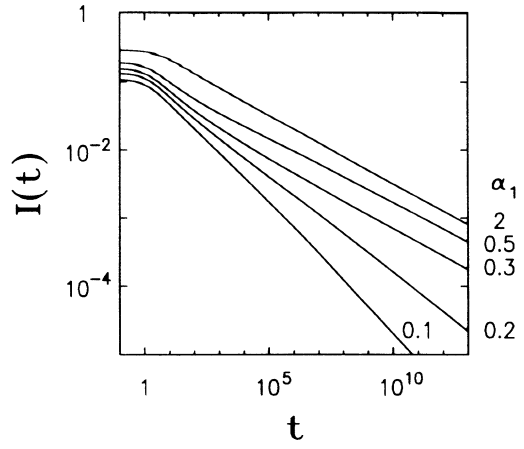

FIG. 3. Effective currents for $\alpha_2=0.3$ and $\beta=0.5$, where α_1 varies from 0.1 to 2. As long as $\alpha_1<\alpha_2$, the current decays asymptotically as $t^{\beta+\alpha_1-1}$, whereas for $\alpha_1>\alpha_2$ the decay follows the form $t^{\beta+\alpha_2-1}$.

Furthermore, for $\alpha_1>\alpha_2$ changes of α_1 do not influence the qualitative shape of the current and only produce a shift in its absolute magnitude. This is because changes of α_1 (for $\alpha_1>\alpha_2$) only vary the value of the prefactor in Eq. (33). Hence, even if one has normal diffusion along one chain (for example, $\alpha_1>1$), the behavior of the current is always controlled by the chain in which the motion is more hindered. This agrees with the original picture of the multiple-trapping model, where already the presence of some deep traps may lead to dispersive transport, even if the conductivity in the conduction band is good.

In Fig. 4 we have fixed the degree of dispersion in both chains to the same value ($\alpha_1=\alpha_2=0.5$). Then if we change the values of β, which characterizes the jumps between the chains, we see a crossover from dispersive current (which obtains for $\alpha+\beta<1$) to nondispersive

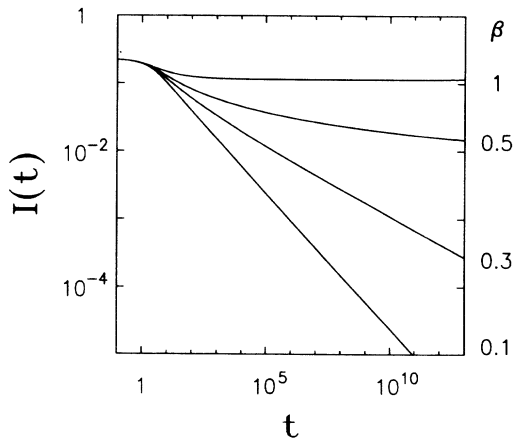

FIG. 4. Effective currents for $\alpha_1=\alpha_2=0.5$ where β varies from 0.1 to 1. As long as $\alpha+\beta<1$, the current decays asymptotically as $t^{\beta+\alpha-1}$, whereas for $\alpha+\beta>1$ the current approaches (after an initial transient decay) a constant for large t.

current, $I(t)\sim$const (which obtains for $\alpha+\beta>1$). This is in perfect agreement with Eq. (34). Note that, as also found in Ref. 4, for β such that $\alpha+\beta\approx 1$ the asymptotic form is reached only at very long times, the time to reach the asymptotic regime diverging for $\alpha+\beta\to 1$.

As a final remark, we observe that neither the model of Ref. 5 nor the present model can be seen as being a pure dynamical disorder model,[14–16] because in neither case does the generalized matrix master operator decouple in a walker (noise-dependent) operator and in a Van Kampen-type external-noise operator[20] (see the Appendix).

V. DISCUSSION

In this work we have used a dynamical quasi-one-dimensional model which accounts both for the statistical features of disorder encountered by the particles in their motion along the chains and also for fairly general mechanisms which lead to interchain coupling. We have analyzed the crossover from dispersive to regular transport in a one-dimensional model by studying the dynamical renewal produced by the reset in time caused by jumps across the chains. We note that we have presented only a special case: The general scheme can be applied to a model consisting of N chains and also to higher-dimensional lattices. For this we only need to introduce the adequate d-dimensional structure matrix $\lambda_l(s-s')$ and consider the corresponding $N\times N$ matrix η.

In the present dynamical model the anomalous diffusion is dominated both by the disorder along the chains and by the probability distribution for performing jumps across the chains. The approach presented here allows an exact expression both for the Laplace-transformed effective current and also for higher moments of the effective probability distribution. The mechanisms studied in this article should show up in photoconductivity experiments on doped quasilinear polymers, where charge carriers move on and between parallel one-dimensional polymer chains with defects. Experimental results would be helpful in order to establish the impact of the models presented here and those which we studied earlier.[5] The models are both simple enough to be studied analytically and rich enough to be able to mirror the influence of competitions between transitions along and across chains.

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APPENDIX

It is well known that the CTRW scheme is connected to the generalized master equation.[7] This idea can easily be extended to MCTRW. Following Ref. 12, the MCTRW probability P_l can be expressed as solutions of the following system of coupled generalized master equations (CGME):

$$\partial_t P_l(k,t)=\sum_{l''}\int_0^t \Lambda_{ll''}(k,t-\tau)P_{l''}(k,\tau)d\tau - \int_0^t P_l(k,\tau)\sum_{l''}\Lambda_{l''l}(k=0,t-\tau)d\tau\ , \tag{A1}$$

where the connection between η and $\Lambda=\Lambda_{l'l}(k,u)$ is given through

$$\Lambda_{ll'}(k,u)=\frac{u\eta_{ll'}(k,u)}{1-\sum_{l''}\eta_{l''l'}(k=0,u)}\ . \tag{A2}$$

So we can rearrange Eq. (A1) to show the explicit structure of its elements. Using Eq. (20), we see that only the diagonal elements of Λ are k dependent. For example, for the component $l=1$ we have

$$\partial_t P_1(k,t) = \int_0^t[\Lambda_{11}(k,t-\tau)-\Lambda_{11}(k=0,t-\tau)]P_1(k,\tau)d\tau + \int_0^t\left[\begin{bmatrix}-\Lambda_{21}(t-\tau) & \Lambda_{12}(t-\tau)\\ \Lambda_{21}(t-\tau) & -\Lambda_{12}(t-\tau)\end{bmatrix}\times\begin{bmatrix}P_1(k,\tau)\\ P_2(k,\tau)\end{bmatrix}\right]_1 d\tau\ . \tag{A3}$$

Note that this split shows a generalized walker kernel (noise dependent) plus a generalized master operator which works only on the internal states. This is a generalization of the van Kampen composite Markovian process.[20] But even when the noise kernel is k independent, the elements $\Lambda_{ll'}(t-\tau)$ $(l\neq l')$ carry information on the time scale of the walker, so formula (A3) is not a pure external-noise model. For instance, for our two-chain model we have

$$\Lambda_{l'l}(u)=\frac{u\mathcal{L}(\phi_l(t)\psi^f_{l'l}(t))}{1-\mathcal{L}(\phi_l(t)\psi^f_{l'l}(t))-\mathcal{L}(\lambda_l(0)\psi_l(t)\phi^f_l(t))}\ . \tag{A4}$$

Thus, if we use a Markovian CTRW ($\psi_l(t)=\alpha_l e^{-\alpha_l t}$), we will get

$$\Lambda_{l'l}(u)=\frac{\psi^f_{l'l}(u+\alpha_l)}{\phi^f_l(u+\alpha_l)}\quad (l\neq l')\ . \tag{A5}$$

So, if we put, for example, a Markovian external noise $\psi^f_{l'l}(t)=\gamma_{l'l}e^{-\gamma_{l'l}t}$, we will obtain

$$\Lambda_{l'l}(u)=\gamma_{l'l}\ , \tag{A6}$$

independently of the time scale α_l of the walker. In all other cases, however, the time scale of the walker (α_l) also influences, through Eq. (A5), the transitions between internal states. Thus the noise is not purely external for non-Markovian waiting-time densities $\psi_l(t)$ or $\psi^f_{l'l}(t)$.

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