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Transient transport in a quasi-one-dimensional hopping model with a power-law distribution of transition rates

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We study transport in a quasi-one-dimensional system consisting of two or more parallel linear chains with finite interchain transition rates s. The transition rates r along the chains are stochastically distributed according to $\rho(r)\sim r^{\alpha-1}$. In all cases we have nonuniversal behavior and crossover effects. For fixed s we find that at times $t\ll s^{-1}$ transport is dominated by α, whereas for $t\gg s^{-1}$ transport is dominated by $n\alpha$, n being the number of parallel chains. If s is also randomly distributed according to $\rho(s)\sim s^{\beta-1}$, transport is governed by $\alpha+\min(\alpha,\beta)$ for all times.

The effects of disorder in one-dimensional systems have been investigated extensively during the last years.[1-3] There are several parameters that may be affected by disorder: intersite distances, energy levels, barrier heights, transition rates, or combinations of all these.

In recent works[4,5] we studied transient transport on a linear chain with different distributions of trap energies (or transition rates), utilizing the continuous-time random-walk model (CTRW) formalism.[6-9] The basic ingredient of this theory is the waiting-time distribution $\psi(t)$, which is the probability per time unit of leaving a site at time t after occupying this site at $t=0$. For a power-law distribution of transition rates of the form

$$\rho(r)=\alpha r^{\alpha-1} \quad (0<r<1,\ \alpha>0)\,, \tag{1}$$

where r is given in units of the attempt-to-escape frequency ν_0, one has

$$\psi(t)\sim t^{-1-\alpha}\,, \tag{2}$$

and we recover for α well inside the region [0,1] the findings of Scher and Montroll:[9]

$$I(t)\sim t^{\alpha-1} \quad (0<\alpha<1)\,, \tag{3}$$

where $I(t)$ is the current before the transit time (or, say for an infinite chain) and $\sim$ stands for the asymptotic limit for $t\to\infty$.

Experimental data from recent transient photoconductivity measurements show a temporal transition from dispersive to nondispersive behavior.[10] The new feature of these experiments is the possibility of monitoring the current over eight or nine decades in time and intensity. A way to explain the transition from dispersive to nondispersive behavior is to invoke crossover effects. Indeed, for α near its critical value $\alpha_c=1$, the asymptotic behavior of $I(t)$ is very different from Eq. (3) and rather follows the form $I(t)\sim 1/\ln t$ (see Ref. 8). A detailed analysis of the situation around $\alpha_c=1$ is given in Refs. 4 and 5.

To extend this analysis to more realistic situations than one-dimensional chains we study in this paper how the transient transport properties are altered in the case of a set of quasi-one-dimensional systems consisting of two or more connected parallel linear chains. The situation for two chains is depicted in Fig. 1(a). The transition rates r_i and w_i are assumed to be random variables, both distributed according to Eq. (1) with the same parameter α, whereas the s_i are discrete ($s_i=s$ for all i) for the present. Later we will also discuss the case that the s_i are stochastically distributed following Eq. (1). We expect this model to be of interest in the analysis of the electric conductivity through strands of rigid polymers, where the interchain and the intrachain site couplings may be widely different.

Let us first start with the geometry of Fig. 1(a) and center on the transport in the direction of the chains. We now project the quasi-one-dimensional system of Fig. 1(a) on a single line by reinterpreting pairs of sites on the two chains as one site of the new line [Fig. 1(b)]. Following the CTRW idea, for the new chain we define a waiting-time distribution $\psi(t)$ as being the probability per time unit of performing a step in chain direction at time t after the last step in this direction; the distribution $\psi(t)$ obtains as an average over the random variables r, w and, if necessary, s. Since this averaging process is site independent, it follows that also $\psi(t)$ is site independent. Therefore, once we have calculated $\psi(t)$, we can follow the standard pro-

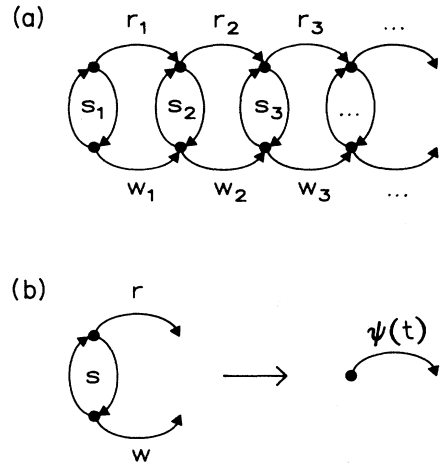

FIG. 1. (a) Quasi-one-dimensional system consisting of two parallel linear chains. A particle can move from site i of any chain to site $i+1$ of the same chain with the transition rate r_i or w_i, or it can move to site i of the neighboring chain with transition rate s_i. The r_i, w_i, and s_i are random variables. (b) The system of two parallel chains is reduced to one chain by replacing the sites in the same column with a single site and calculating a waiting-time distribution $\psi(t)$ (averaged over r, w, and s).

cedure (see our previous discussion[4,5]) and calculate the resulting current $I(t)$ by numerical Laplace inversion of

$$I(u)=\frac{\psi(u)}{1-\psi(u)}. \tag{4}$$

To obtain Eq. (4) we assume the particle to start at site 1, the chain length being infinite. Here and in the following we denote by $f(u)$ the Laplace transform of $f(t)$, i.e., $f(u)=\mathcal{L}[f(t)]$.

Let us now focus on the calculation of $\psi(u)$. Consider the basic element of the quasi-one-dimensional system [Fig. 1(b)], which element consists of one pair of sites, i.e., one column. Let the particle arrive at $t=0$ on this column, p and q being the probabilities that it first reaches the upper or lower site, respectively. Evidently, $p+q=1$ holds. Furthermore, let $\Psi_r(t)$ and $\Psi_w(t)$ be the probabilities that the particle occupies the upper or lower site at time t after the arrival on this column. Then one can establish the following differential equations:

$$\begin{aligned}\frac{\partial\Psi_r(t)}{\partial t}&=-(r+s)\Psi_r(t)+s\Psi_w(t),\\ \frac{\partial\Psi_w(t)}{\partial t}&=-(w+s)\Psi_w(t)+s\Psi_r(t).\end{aligned} \tag{5}$$

These are easily solved via Laplace transformation, using the initial conditions $\Psi_r(0)=p$ and $\Psi_w(0)=q$. This yields for the Laplace transform of the total occupation probability of the considered column, which is given by $\Psi(t)=\Psi_r(t)+\Psi_w(t)$:

$$\Psi(u)=\frac{2s+u+qr+pw}{(u+s+r)(u+s+w)-s^2}. \tag{6}$$

Now we can deduce the waiting-time distribution $\psi(t)$, which is the negative time derivative of $\Psi(t)$,[11] averaged over r, w, and, if necessary, s. For the Laplace transforms one then gets

$$\begin{aligned}\psi(u)&=\langle 1-u\Psi(u)\rangle_{r,w(,s)}\\ &=\left\langle\frac{u(pr+qw)+s(r+w)+rw}{(u+s+r)(u+s+w)-s^2}\right\rangle_{r,w(,s)}.\end{aligned} \tag{7}$$

As r and w are identically distributed, Eq. (7) simplifies to

$$\psi(u)=\left\langle\frac{r(u+2s)+rw}{(u+s+r)(u+s+w)-s^2}\right\rangle_{r,w(,s)}. \tag{8}$$

Thus $\psi(u)$ is independent of the initial probabilities p and q and also of the site number, since the distribution of transition rates is the same for all columns. Equation (8) is the basis for our further discussion.

First, consider the two extreme cases $s=0$ (decoupled chains) and $s\to\infty$ (perfect coupling). In the first case Eq. (8) reduces to

$$\psi(u)=\left\langle\frac{r}{u+r}\right\rangle_r, \tag{9}$$

which was already discussed in Ref. 4, yielding $\psi(t)\sim t^{-1-\alpha}$ and $I(t)\sim t^{\alpha-1}$ $(0<\alpha<1)$. In the second case one gets from Eq. (8) in the limit $s\to\infty$,

$$\psi(u)=\left\langle\frac{r}{u+\frac{1}{2}(r+w)}\right\rangle_{r,w}. \tag{10}$$

This can be easily Laplace inverted and averaged over r and w:

$$\begin{aligned}\psi(t)&=\langle re^{-(r+w)t/2}\rangle_{r,w}=\langle re^{-rt/2}\rangle_r\langle e^{-wt/2}\rangle_w\\ &=\alpha^2\gamma(\alpha+1,\tfrac{1}{2}t)\gamma(\alpha,\tfrac{1}{2}t)(\tfrac{1}{2}t)^{-1-2\alpha},\end{aligned} \tag{11}$$

where $\gamma(\alpha,t)$ is the incomplete gamma function.[12] As $\lim_{t\to\infty}\gamma(\alpha,t)=\Gamma(\alpha)$, we obtain $\psi(t)\sim t^{-1-2\alpha}$ for the asymptotic behavior of $\psi(t)$. Therefore, in this case the motion is no longer governed by the parameter α but by 2α. This result can be generalized to a system of n connected parallel chains, where motion is then governed by $n\alpha$. For the current this results for $t\to\infty$ in $I(t)\sim t^{n\alpha-1}$ for $0<\alpha<n^{-1}$ and $I(t)\sim$const for $\alpha>n^{-1}$. Hence, the critical value for α, below which transport gets anomalous, decreases from 1 to n^{-1} when one considers n parallel chains.

A similar result has recently been derived by Havlin, Bunde, Weissman, and Aharony[13] for the transport exponents $\bar{\zeta}$ (resistivity exponent) and d_w (diffusion exponent). They also found that α has to be replaced by $n\alpha$, when a system of n parallel, perfectly connected linear chains is considered. (When comparing, note that in the notation of Ref. 13, $1-\alpha$ corresponds to our α.) Hence, the critical value α_c, separating the regimes of normal and anomalous transport is $\alpha_c=n^{-1}$ (in our notation).

For finite values of s there occurs a crossover. At times t that are much smaller than s^{-1} (the mean time for moving from one chain to the other) the particle acts as if it moves on a single chain, whereas for times t much greater than s^{-1} it behaves as if the chains were perfectly connected. This is demonstrated in Figs. 2 and 3. By Laplace inverting and averaging Eqs. (8) and (4) we calculated

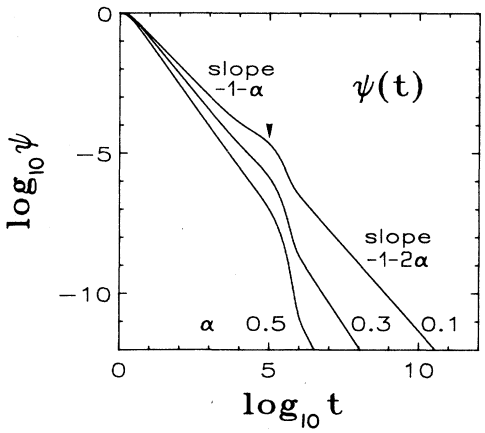

FIG. 2. Double-logarithmic plot of $\psi(t)$ for $s=10^{-5}$ and $\alpha=0.1$, 0.3, or 0.5, respectively. For clarity of presentation we have set all three $\psi(t)$ equal at $t=1$.

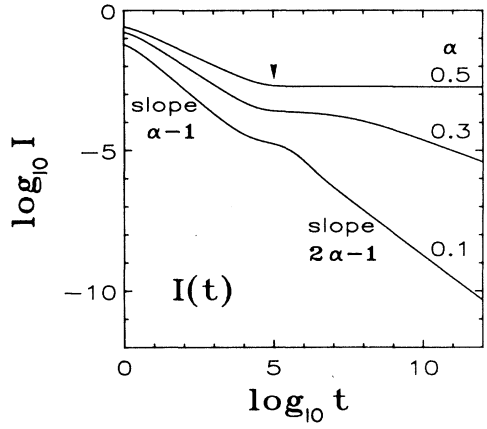

FIG. 3. Double-logarithmic plot of $I(t)$ for $s=10^{-5}$ and $\alpha=0.1$, 0.3, or 0.5, respectively.

numerically both $\psi(t)$ and $I(t)$. In double-logarithmic presentation $\psi(t)$ exhibits a crossover from slope $-1-\alpha$ for $t \ll s^{-1}$ to a slope $-1-2\alpha$ for $t \gg s^{-1}$, as predicted above, and, similarly, the slope of the current changes from $\alpha-1$ to $2\alpha-1$ $(0<\alpha<\frac{1}{2})$ or $0(\frac{1}{2}\leq\alpha<1)$ in double-logarithmic presentation. Similar results are expected, if the number of parallel chains exceeds 2.

Let us now turn our attention to the case where not only r and w but also s is a random variable, obeying the power-law distribution

$$\rho(s)=\beta s^{\beta-1} \quad (0<s<1, \beta>0) . \tag{12}$$

Calculating $\psi(t)$ for different values of α and β we obtain for the geometry in Fig. 1 the following results. (i) For $\alpha \leq \beta$ the time dependence of $\psi(t)$ follows $\psi(t) \sim t^{-1-2\alpha}$. (ii) For $\alpha>\beta$ the time dependence of $\psi(t)$ follows $\psi(t) \sim t^{-1-\alpha-\beta}$. These results can be understood as follows. The smaller the parameter α or β of the power-law distribution of transition rates is, the more the transport in this direction is hindered. A particle sitting on any site of the quasi-one-dimensional system has two possibilities to move to the next column; it may jump directly to the next column with transition rate r or w (the distribution of both governed by α) or it may intermediately move to the other site in the same column with transition rate s, whose distribution is governed by β, and then jump to the next column (with w or r, respectively). The first way of moving in chain direction is always governed by the distribution of r and w, i.e., by the parameter α, whereas the second way is governed by the most difficult step, which is the step with the smaller power in the distribution of transition rates. Therefore, one may expect the exponent of t in the asymptotic behavior of $\psi(t)$ to be $-1-\alpha-\min(\alpha,\beta)$, a result which is in full agreement with our numerical computations.

Hence, in order to describe motion along two connected parallel chains with a power-law distribution of interchain and intrachain transitions rates one has to replace the parameter α in Eqs. (2) and (3) by $\alpha+\min(\alpha,\beta)$.

So far, we have shown interesting new aspects of transient transport in quasi-one-dimensional systems with power-law distributions of transition rates. Although the mechanism studied here has a simple structure, it may well play an important part in the understanding of transport through fiberlike complex systems. Thus we expect the mechanism to show up in the photoconductivity of doped quasilinear polymers such as polydiacetylene, where carriers move on and between parallel, one-dimensional polymer chains with defects.

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