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# Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics

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## Hierarchical Transport Processes in Photoconduction

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#### HIERARCHICAL TRANSPORT PROCESSES IN PHOTOCONDUCTION

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Abstract In this work we evaluate current flows under anomalous diffusion conditions. We use Lévy walks: continuous-time random walks (CTRW) with coupled spatial and temporal memories. Renewed interest in CTRW was triggered by recent advances in photoconductivity.

The effects of disorder on the current flow have been investigated extensively during the last years. In recent works<sup>1,2</sup> we studied transient transport on a linear chain with different distributions of trap energies (i.e. release rates), utilizing the continuous-time random-walk model (CTRW).<sup>3-5</sup> The renewed interest in CTRWs was kindled by recent experimental data from transient photoconductivity measurements, which show crossovers from dispersive to nondispersive behavior.<sup>6</sup>

In this work we focus on extending currents' evaluations to more general conditions of anomalous transport by also treating enhanced diffusion, such as found in turbulent motion. A powerful description for such processes are CTRWs with coupled spatio-temporal kernels.<sup>7</sup>

In the CTRW formalism the probability P(r,t) of finding a particle at r at time t, provided it started at t=0 from r=0 is:

$$P(\mathbf{r},t) = \sum_{\mathbf{r}'} \int_{0}^{t} P(\mathbf{r}',\tau) \psi(\mathbf{r}-\mathbf{r}', t-\tau) d\tau + \Phi(t) \delta_{\mathbf{r},\mathbf{0}}. \qquad (1)$$

In Eq. (1)  $\psi(\mathbf{r},t)$  is the probability distribution of making a step of length  $\mathbf{r}$  in the time interval t to t+dt, and  $\Phi(t)$  is the survival probability at the initial site,  $\Phi(t) = 1 - \int_0^t \psi(\tau) d\tau$ , with  $\psi(t) = \sum_{\mathbf{r}} \psi(\mathbf{r},t)$ .

In Fourier-Laplace space P(k,u) is readily expressible as a function of  $\psi(k,u)$ :

$$P(k,u) = \frac{1 - \psi(u)}{u} \frac{1}{1 - \psi(k,u)}$$
 (2)

from which the current follows as:

$$I(u) = -iu \frac{\partial}{\partial \mathbf{k}} P(\mathbf{k}, u) \Big|_{\mathbf{k}=0} = \frac{-i}{1-\psi(u)} \frac{\partial \psi(\mathbf{k}, u)}{\partial \mathbf{k}} \Big|_{\mathbf{k}=0}$$
(3)

As shown in former works<sup>7,8</sup> the form:

$$\psi(\mathbf{r},t) = A r^{-\mu} \delta(r - t^{\nu}) \tag{4}$$

provides a very good means to describe anomalous diffusion. We now utilize this expression to calculate I(t) by focusing on motion in the direction of the field. A straightforward analysis of Eqs. (2) and (3) shows that the regime k < u of  $\psi(k,u)$  is of interest. We find, parallelling Ref. 9, the following asymptotic behaviors:

$$1-\psi(u) \sim u^{7}$$
 , with  $\gamma = \min(\mu\nu - 1, 1)$  (5)

and

$$\psi(k,u) - \psi(u) - iku^{\delta}, \text{ with } \delta = \min(\mu\nu - \nu - 1,0)$$
 (6)

This leads to the following final forms for the current:

$$I(t) \sim t^{\nu-1}$$
 for  $1 < \nu \mu < \min(2, 1+\nu)$  (7a)

$$I(t) \sim t^{\nu\mu-2}$$
 for  $1+\nu < \nu\mu < 2$  (7b)

$$I(t) \sim t^{1-(\mu-1)\nu}$$
 for  $2 < \nu\mu < 1+\nu$  (7c)

$$I(t) - const for \nu\mu > max(2,1+\nu) (7d)$$

To ascertain the domain of validity of Eqs. (7) we have performed simulations for CTRWs with coupled memory terms. In Fig. 1 we show the I(t)-behavior, plotted in log-log scales. The upper part of the figure gives the current for an enhanced situation,  $\nu = 2$ . The lower part of the figure depicts the current under a dispersive condition,  $\nu = 1/2$ . We note

that at long times the numerical results follow straight lines satisfactorily close, fact which validates our asymptotic analysis.

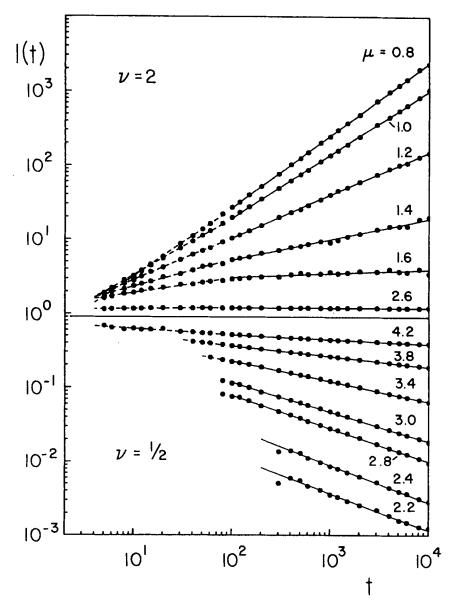


FIGURE 1 The current flow I(t) vs. time on log-log scales. In the upper part of the figure  $\nu=2$ , in the lower part  $\nu=1/2$ , the values of  $\mu$  are as indicated. The dots are simulation results, the full lines denote linear least-squares fits and the dashed lines are guides to the eye.

The numerical results for  $\nu=1/2$ , 3/2 and 2 are summarized in Fig. 2. The fitted slopes agree well with the analytical results, Eqs. (7), which are also given in the figure as solid lines. Here the transition regimes  $3 < \mu < 4$  for  $\nu=1/2$ ,  $4/3 < \mu < 5/3$  for  $\nu=3/2$  and  $1 < \mu < 3/2$  for  $\nu=2$  are clearly visible. In all three cases, for small  $\mu$ , the limiting  $\epsilon$ -values,  $\epsilon=-1/2$  for dispersive current and  $\epsilon=1/2$ ,  $\epsilon=1$  for enhanced current, are reached within the time of the numerical experiment. Whereas the numerical results follow in general the theory, the transitions between the different regions occur smoother than theoretically evaluated. This opens the way for a crossover analysis of the type performed by us for photoconducting materials. One should note that now dispersive transport is nothing but a special case - Eq. (7a) with  $\nu < 1$ ,  $1/\nu < \mu < 2/\nu$  - of the general CTRW -coupled-memory formalism.

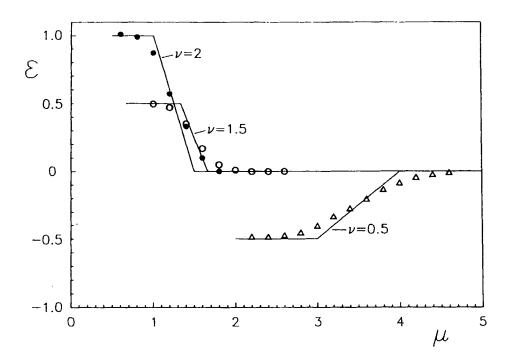


FIGURE 2 Asymptotic behavior of the current; the symbols denote the numerically determined exponents for  $\nu = 1/2$ , 3/2, and 2. The solid lines give the analytically expected behavior, Eqs. (7).

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