# Hopping Transport in Molecularly Doped Polymers: On the Relation between Disorder and a Field-Dependent Mobility*

**D. H. Dunlap**

*Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico 87131*

For a variety of molecularly doped, pendant-, and main-chain polymers, and vapor-deposited molecular glasses, the mobility of photoinjected charges at high electric fields is described by the Poole–Frenkel law; $\mu = \mu_0 \exp(\gamma\sqrt{E})$. Apart from their organic constituents, the primary transport-related feature shared by these materials is the lack of a periodic structure. We review the relation between the $\sqrt{E}$-dependent mobilities and dispersive transport, as described by the theory of Scher and Montroll for hopping transport in a disordered medium. We show that with a small modification, the theory predicts dispersive transport below and nondispersive transport above a transition temperature $T_c$. We argue that the $\sqrt{E}$ dependence of the mobility and the universality of the current–time curves may be retained above and below $T_c$ if the bulk film behaves as a lattice of bonds of length $\mathcal{L}$, where $\mathcal{L}$ is intermediate between the dopant spacing and the thickness of the sample.

Journal of Imaging Science and Technology 40: 291–298 (1996)

## Introduction

**Observations.** Measurements of time-of-flight (TOF) mobilities of photoinjected charges in amorphous molecular films by Pai,[1] in 1970, showed that the mobility for a wide class of materials obeys the Poole–Frenkel law,[2] increasing exponentially with the square root of the electric field,[3]

$$\log \mu = \gamma\sqrt{E} + \text{const.} \tag{1}$$

In contrast to the present state of affairs, the early TOF current–time transients generally show an anomalous dispersion of the packet of photoinjected carriers. Both before and after the transit time $\tau$, the current $I$ decreases approximately algebraically with time $t$, indicating a continuous slowing and broadening of the carrier packet. Unless the transients are plotted on double-log paper, this combination of behaviors hides the distinction between the plateau and tail regions that are observed in similar experiments on molecular crystals.[4]

If the current decreases slowly and monotonically *before* the transit time, e.g., in an algebraic manner such that $I \sim t^{-(1-\alpha)}$, where the parameter $\alpha < 1$, it is possible for the TOF mobility to decrease with increasing film thickness $L$, as $L^{1-1/\alpha}$. This feature of highly dispersive transport may be appreciated without regard to a specific transport model. First, if none of the charges have yet to cross the sample, the current $I$ will be proportional to the velocity $v$ of the centroid of the carrier packet. Thus the observation that $I \sim t^{-(1-\alpha)}$ before transit implies that $v \sim t^{-(1-\alpha)}$. In a time $t$ the centroid of the carrier packet will move a distance $z$, such that

$$z = \int_0^t v(u)du \propto \int_0^t u^{-(1-\alpha)}du \propto t^{\alpha}. \tag{2}$$

It follows from Eq. 2 that $t \propto z^{1/\alpha}$. If we define the average drift velocity as the ratio $z/t$, we find the mobility

$$\mu = z/tE \propto z^{1-1/\alpha}. \tag{3}$$

Should it be the case that the experimentally determined transit time $\tau$ is proportional to the time $t$ in which the centroid of the carrier packet moves a distance $L$, it follows from Eq. 3 that the mobility will depend on sample thickness, such that $\mu \propto L^{1-1/\alpha}$. Such sample-length-dependent TOF mobilities are found in a variety of amorphous films, and they have been attributed to a broad distribution of hopping rates caused by spatial and energetic disorder in these materials.

Many of the essential effects of disorder on hopping transport in amorphous films are described in the context of a theory by Scher and Montroll (SM),[5] which relates the highly dispersive TOF transients to an algebraic decay of the pausing time distribution function for a continuous-time random walk,

$$\Psi(t) \sim 1/t^{1+\alpha}, \tag{4}$$

where the constant $\alpha$ is referred to as the disorder parameter. In this context the observed *universality* of the current–time curves is understood, one signature of which is the relative width of the transient tail,

$$W = (\tau_{1/2} - \tau_0)/\tau_{1/2}, \tag{5}$$

which is independent of electric field and sample thickness. In Eq. 5, $\tau_0$ is the time to reach the shoulder of the current–time curve, and $\tau_{1/2}$ is the time at which the current has decreased to half of its value at the shoulder. The SM theory predicts a field-dependent mobility as well, such that

$$\log \mu = (1/\alpha - 1)\log E + \text{const.} \tag{6}$$

For amorphous films such as the molecularly doped polymers, a strict logarithmic field dependence of $\log \mu$ has rarely

Original manuscript received February 9, 1996. Revised May 13, 1996.

* Presented in part at IS&T's 11th International Congress on Advances in Non-Impact Printing Technologies, October 29–November 3, 1995, Hilton Head, SC.

been observed in preference to the Poole–Frenkel law.[3,6] It has been shown, however, that a combination of the log $E$ dependence of Eq. 6 and other field dependencies arising from the detailed balance of the hopping rate closely resembles the $\sqrt{E}$ law over at least one and a half decades in $E$.[7] Moreover, when the algebraic decay of $\Psi(t)$ is caused by energetic disorder, the disorder parameter $\alpha$ increases with $T$, giving rise to an effective Poole–Frenkel factor that is in agreement with the empirical form, $\gamma = B(1/kT - 1/kT_0)$, suggested by Gill.[8,9] One could assert that, at least to a first approximation, all of the universal features of transport in molecularly doped polymers are associated with the algebraically decaying pausing time distribution of SM, were it not for the fact that one of the key predictions of the SM theory is no longer consistently observed in experiments; if it is observed at all, the anomalous dispersion of the current–time curves is observed only at low temperatures.

As the temperature is increased from 200 to 300 K, the current–time curves for molecularly doped polymers change character and become less dispersive. At higher temperatures, the TOF transients show clearly defined plateaus, and the mobility is found to be *independent* of length.[10–12] In the context of the SM theory, such a transition from dispersive to nondispersive transport comes about as a result of there being a narrower distribution of hopping rates at higher temperatures. When the distribution is so narrow that the first moment of $\Psi(t)$ is bounded, $\log \mu$ will no longer increase in proportion to $\log E$. Without this mechanism for anomalous field dependence, we should observe Ohmic behavior when the potential energy for a single hop over a distance $\rho$ in the direction of the field, $eE\rho$, is smaller than $kT$. For most molecularly doped polymers, however, the mobility remains strongly field-dependent in this low-field regime and continues to obey a Poole–Frenkel law.[11] In *p*-diethylaminobenzaldehyde diphenylhydrazone (DEH)-doped polycarbonate, for example, the $\sqrt{E}$ law was observed for fields as low as $0.8 \times 10^4$ V/cm at a temperature of 300 K.[13] This finding suggests that the field dependence of the mobility and the dispersive nature of the transport are consequences of independent mechanisms. In fact, the only evidence that high-temperature transport features might still be attributed to an algebraically decaying distribution of pausing times is the fact that universality of the current–time curves persists. The relative tail-width $W$ remains field independent, even at high temperatures.[11,12]

The failure of an algebraic pausing-time distribution to describe the transport properties of molecularly doped polymers does not necessarily imply that disorder effects are negligible. It is possible that the SM theory misses details that are essential in describing how the TOF transients can simultaneously have well-developed plateaus and anomalously broad tails, while at the same time the mobility is strongly field dependent. This angle has been actively pursued by Bässler and coworkers[14–17] via Monte-Carlo simulations of hopping in an energetically and spatially disordered environment. There is remarkable agreement between simulation and experiment as far as describing features of the current–time transients and their relation to the temperature dependence of $\mu$.[12,15,16] The agreement of simulations with the Poole–Frenkel law is not conclusive, however, for although simulations predict mobilities that follow the $\sqrt{E}$ law, they do so only for fields in the high $10^5$ to $10^7$ V/cm range.[17] Parris and Bookout[18] have developed a large-cell-renormalized effective medium theory that gives steady-state hopping conductivities at high fields in a topologically and energetically disordered array. They also find a $\sqrt{E}$-dependent mobility at high fields only, in agreement with the Monte-Carlo simulations of Borsenberger, Pautmeier, and Bässler.[17] Recent simulation studies by Gartsein and Conwell[19] have shown, however, that the field-dependent mobility will shift to lower fields when long-range correlations between dopant energies are introduced. The effect of these correlations on the current–time curves has not been reported.

**The Branching Length $\mathcal{L}$.** The discrepancies between theory and experiment suggest that if disorder is indeed the key to understanding transport in molecularly doped polymers, there must be an attribute of disorder that has not yet been adequately considered. Such an attribute should be compatible with the fact that the same field dependence of the mobility is observed, whether or not the current–time transients show a plateau. Such an attribute must also be subtle enough to have escaped detection in systematic approaches to the calculation of transport coefficients, such as Monte-Carlo simulations and effective medium theories. As a possible candidate we suggest the effect of large-scale fluctuations in the transport network, which arise as a result of the disparity in hopping rates. We will motivate and develop this remark in the context of a continuous-time random walk.

In the SM theory, the time to make $n$ hops is determined by the addition of $n$ times, which are drawn from a pausing-time distribution. The distribution of pausing times can be determined, in principle, by following the trajectory of each charge as it crosses a sample and plotting a histogram of the various dwell times encountered. Alternatively, one can determine the distribution of pausing times by working backwards from the experiment, requiring that $\Psi(t)$ be compatible with current–time transients. To describe the dispersive features seen at low temperatures and at the same time preserving analytic tractability, SM suggests that the tail of $\Psi(t)$ decays algebraically with the exponent $1 + \alpha$, as described by Eq. 4. For $\alpha < 1$, $\Psi(t)$ has no first moment. Transport is anomalous, and the mobility is field-dependent, because the sum of $n$ dwell times grows as $n^{1/\alpha}$. This approach leads to the scaling of $\mu$ with both $L$ and $E$, as described by Eqs. 3 and 6. If the dwell times are determined by energetic disorder, the *same* hops are made in less time as the temperature increases. This tendency is characterized by a disorder parameter $\alpha$, which increases with increasing temperature. A second phenomenon occurs as the temperature is increased, however; the ensemble of trajectories available to the carriers will broaden. At higher temperatures, energetically isolated paths that were seldom explored will compete more favorably with those that comprise the minimal percolating network. To characterize this tendency, we introduce a temperature-dependent branching length $\mathcal{L}$. We define the distance $\mathcal{L}$ to be a demarcation for the pausing-time distribution; for random walks over distances much smaller than $\mathcal{L}$, we assume that $\Psi(t)$ may be described by Eq. 4, in keeping with SM; on the other hand, for walks over distances much greater than $\mathcal{L}$, we modify $\Psi(t)$ to reflect the possibility of branching onto new paths.

The primary results that emerge from our analysis are as follows. We obtain a modified pausing-time distribution that predicts a transition at a temperature $T_c$ at which $\alpha = 1$. Below $T_c$, $\alpha$ lies between 0 and 1, and the current–time curves for $t < \tau$ and for $t > \tau$ are characterized in the usual manner by algebraically decaying asymptotes.

$$I(t)_{T < T_c} \sim \begin{cases} t^{-(1+\alpha)}, & t < \tau \\ t^{-(1+\alpha)}, & t > \tau \end{cases}. \tag{7a}$$

Above $T_c$, on the other hand, α is greater than 1. In this case the current for $t < \tau$ approaches a constant, and for $t > \tau$, it decays algebraically.

$$I(t)_{T > T_c} \sim \begin{cases} \text{const}, & t < \tau \\ t^{-(1+\alpha)}, & t > \tau \end{cases}. \tag{7b}$$

We show that the current–time curves maintain universality with respect to the electric field in both temperature regimes. In addition, we show that in spite of the modifications of the pausing-time distribution, the mobility retains a strong field dependence above and below $T_c$, which resembles Eq. 1 over a wide range of electric fields. We find that below $T_c$ the calculated mobility depends on the sample width L, but above $T_c$ it depends only on the intrinsic length $\mathcal{L}$. Our interpretation of the pausing-time distribution in terms of a length $\mathcal{L}$ is therefore in reasonable agreement with the experiments.

The remainder of this article is as follows. In the Background section we briefly review the essential features of the pausing-time distribution function that describe the TOF current–time transients and give rise to a field- and length-dependent mobility in the highly dispersive regime. This effect provides a motivation for the present investigation. Following this discussion, we introduce bonds of length $\mathcal{L}$ and describe their effect on the pausing-time distribution function. We obtain asymptotic expressions for the current–time curves, which lead to the essential results stated in Eq. 7, and summarize our findings in the last section.

## Background

**Field-Dependent Mobility.** In this section we will briefly review those aspects of the SM theory that lead to the unification of Eqs. 3, 5, and 6, which characterize some molecularly doped polymers in the dispersive transport regime. We make a number of simplifying assumptions and approximations to clarify the essential picture; further discussion may be found in Refs. 5, 7, and 9.

We begin with an estimate of the pausing-time distribution function $\Psi(t)$ for hopping in an array of dopant molecules with random energies distributed uniformly over a width σ. Let us consider only (spatial) nearest-neighbor hopping and only energetic disorder. We are interested in the long-time behavior of $\Psi(t)$, which is characterized by the lowest hopping rates. These hops are necessarily upward in energy from states with energy $\varepsilon \cong 0$. Therefore, we take the underlying hopping rate to be $R = v_0 \exp(-\beta\varepsilon)$, where $v_0$ is typical of the hopping rates one might find in an ordered molecular solid, $\varepsilon$ is the energy of one of the $M$ spatial neighbors, and $\beta = 1/kT$. For $\sigma/kT >> 1$, the $M$ rates are extremely disparate, and a particular hop is likely to be to the state that is closest in energy to a state at $\varepsilon = 0$. Thus we are interested in the distribution of *nearest-neighbor* energies,[20] $P(\varepsilon) = \frac{M}{\sigma}(1 - \varepsilon/\sigma)^{M-1}$. For large $M$ this is approximately an exponential;

$$P(\varepsilon) = \frac{M}{\sigma}\exp(-M\varepsilon/\sigma). \tag{8}$$

The exponential in Eq. 8 is contrived in the sense that $M$ is not truly an asymptotic parameter; we expect $M$ to range between 6 and 12. Nevertheless, the tendency for the distribution of nearest neighbors to approximate an exponential, regardless of the specific form of the underlying density of states suggests that these specific calculations may have broad applicability. We will therefore adopt the exponential form of Eq. 8 in what follows, both for simplicity and for illustrative purposes. An algebraic distribution of nearest-neighbor hopping rates $R$,

$$\eta(R) = \int d\varepsilon P_{nn}(\varepsilon)\delta(R - v_0 e^{-\beta\varepsilon}) \cong \int_0^\infty d\varepsilon\left[\frac{M}{\sigma}\exp(-M\varepsilon/\sigma)\delta(R - v_0 e^{-\beta\varepsilon})\right] = a v_0^{-a} R^{a-1}, \tag{9}$$

is obtained by integrating over Eq. 8. In Eq. 9, we have introduced a disorder parameter, $a = MkT/\sigma$ (We will make a connection between $a$ and the disorder parameter α of Eqs. 6 and 7 in the following section.) By averaging $R \exp(-Rt)$ over $\eta(R)$, we obtain a distribution of pausing times with an algebraic tail,

$$\Psi(t) = \int_0^{v_0} a v_0^{-a} R^{-a}\left(\mathrm{Re}^{-Rt}\right)\mathrm{d}R \sim \frac{a v_0 \Gamma(a+1)}{(v_0 t)^{a+1}}, \tag{10}$$

where Γ denotes the gamma function. For $a < 1$, it can be shown that, asymptotically (in $n$), the distribution of time to make $n$ hops is a universal function of the scaled variable $x = t/n^{1/a}$. It follows that the typical time to make $n$ hops,

$$t_n \sim n^{1/a}, \tag{11}$$

is proportional to $n^{1/a}$ for large $n$. The number of hops to cross a sample of thickness $L$,

$$n = L/\ell_1(E) \cong \frac{L}{(\rho^2\beta e/12)E}, \tag{12}$$

is calculated by dividing the sample thickness by the average progress made in the field direction in a single hop, $\ell_1(E)$. If we consider the rate for hopping to a variety of locations distributed uniformly on a sphere of radius $\rho$, we find that $\ell_1(E) = \rho[\coth(\beta eE\rho/2) - (2/\beta eE\rho)]$. Assuming that $\ell_1$ is linear in $E$ in a disordered medium, we have replaced $\ell_1(E)$ in Eq. 12 by its Taylor expansion to first order in $E$, $(\rho^2\beta e/12)E$. Combining Eqs. 11 and 12, we find the transit time,

$$\tau \cong \frac{1}{v_0}(12L/\rho^2\beta eE)^{1/a}. \tag{13}$$

Inserting Eq. 13 in Eq. 3, we obtain a field-dependent mobility such that

$$\ln\mu = \left(\frac{1}{a} - 1\right)\ln(\rho^2\beta eE/12L) + \ln(\rho^2\beta e v_0/12). \tag{14}$$

To compare this with a Poole–Frenkel law at small electric fields ($10^4$ V/cm < $E$ < $10^5$ V/cm), we expand the field-dependent term in Eq. 14 to first order in powers of $\sqrt{E}$ about $E = E_0$.

$$\left(\frac{1}{a} - 1\right)\ln(E) \cong 2(1/a - 1)\ln\sqrt{E_0} + 2(1/a - 1)\frac{d}{d\sqrt{E}} \times \ln\sqrt{E}\Big|_{E=E_0}\left(\sqrt{E} - \sqrt{E_0}\right). \tag{15}$$

Substituting $MkT/\sigma$ for $a$, we obtain

$$\ln\mu \cong \frac{2\sigma}{M\sqrt{E_0}}\left(\frac{1}{kT}-\frac{M}{\sigma}\right)\sqrt{E} - \frac{(\sigma/M)[\ln(12L/\rho^2\beta eE_0)+2]}{kT} + \ln(v_0 L/12E_0)+2. \quad (16)$$

For a disorder parameter $a$ = 0.6 at $T$ = 300 K, we require $\sigma/M$ = 0.042 eV. Let us select $\sqrt{E}_0 = 200(\mathrm{V/cm})^{1/2}$ to be the origin of the Taylor expansion in Eq. 15 and choose $L$ = 1 $\mu$m, $\rho$ = 10 Å, and $v_0 = 10^{12}\mathrm{s}^{-1}$. Equation 16 should be compared with Gill's function,

$$\ln\mu = B\left(\frac{1}{kT}-\frac{1}{kT_0}\right)\sqrt{E} - \frac{\Delta}{kT} + \mathrm{const}, \quad (17)$$

to identify, by inspection, the parameters

$$B = \frac{2\sigma}{M\sqrt{E_0}} = 4\times10^{-4}(e^2\mathrm{Vcm})^{1/2}, \quad (18)$$

$$T_0 = \sigma/kM = 500\,\mathrm{K}, \quad (19)$$

$$\Delta_{T=300\,\mathrm{K}} = (\sigma/M)[\ln(12L/\rho^2\beta eE_0)+2]_{T=300\,\mathrm{K}} = 0.55\,\mathrm{eV}, \quad (20)$$

and an extrapolated $(E \to 0)$ mobility at T = 300 K of

$$\mu_{E\to0,T=300\,\mathrm{K}} = 6.8\times10^{-4}\,\mathrm{cm}^2/\mathrm{V\,s}. \quad (21)$$

The Gill coefficients $B$, $T_0$, and $\Delta$ evaluated in Eqs. 18, 19, and 20, respectively, are typical of those found in experiments.

We will now extend our analysis of the field-dependent mobility to the range $E > 10^5$ V/cm, for which $\beta eE\rho > 1$. Let us first consider the possibility that $\ell_1(E)$ should be modified. In an ordered system at high fields, the average distance hopped in the direction of an applied field saturates, so that in each hop a carrier moves one lattice constant in the direction of the field; $\ell_1 = \rho\,[\coth(\beta eE\rho/2) - (2/\beta eE\rho)] \sim \rho$. On the other hand, in a disordered system, it should be more difficult to find a favorable site in the direction of the field. We argue, therefore, that at high fields $\ell_1$ is less likely to saturate and should retain its linearity with $E$. Let us also consider the field modification of the distribution of dwell times. As long as the field energy $\beta eE\rho \ll \sigma$, the slowest hopping rates will be enhanced by the exponential factor $\exp(\beta e\boldsymbol{E}\cdot\rho)$. Neglecting the anisotropy caused by the net drift, integration over the unit sphere gives an average field-enhancement factor $\sinh(\beta eE\rho)/\beta eE\rho$. This means that the long-time tails of the pausing-time distribution can be corrected for high fields by simply multiplying $v_0$ by $\sinh(\beta eE\rho)/\beta eE\rho$. With this modification, we find that

$$\ln\mu = \left(\frac{\sigma}{MkT}-1\right)\ln[\rho^2\beta eE/12L] + \ln[\sinh(\beta eE\rho)\rho v_0/12E]. \quad (22)$$

Equation 22 predicts that at low fields the mobility obeys a power law and at high fields it follows an exponential. Nevertheless, as discussed in Ref. 9, the mobility described by Eq. 22 closely resembles Gill's function (Eq. 17) for electric fields between $4\times10^4$ and $1.5\times10^6$ V/cm. It is in this manner that the $\sqrt{E}$-dependent mobility in the molecularly doped polymers appears to be closely related to the algebraically decaying pausing-time distribution of SM.

**Current–Time Curves.** The TOF current–time curves are determined by the distribution of charge as it drifts across the polymer film. The charge distribution is calculated under the assumption that after $n$ hops, the spatial distribution $f(z;n)$ approximates a Gaussian,

$$f(z;n) \sim \frac{1}{(2\pi n\rho^2)^{1/2}}\exp\left[\frac{(z-n\ell_1)^2}{2n\rho^2}\right], \quad (23)$$

for $n >> 1$. The time-dependent spatial distribution $g(z;t)$ may be calculated by multiplying $f(z;n)$ by the probability $p_n(t)$ that at time $t$ carrier has hopped $n$ times and summing over all possible numbers of hops. The Laplace transform of $p_n(t)$ is a product; $\tilde{p}_n(s) = \tilde{\Psi}^n(1-\tilde{\Psi})/s$. The Laplace transform of the spatial distribution function $\tilde{g}(z;s)$ is therefore

$$\tilde{g}(z;s) = \sum_{n=0}^{\infty} f(z;n)\tilde{p}_n(s) = \frac{(1-\tilde{\Psi})}{s}\sum_{n=0}^{\infty} f(z;n)\tilde{\Psi}^n. \quad (24)$$

The sum in Eq. 24 can be carried out in the Fourier and Laplace domains. For long wavelengths,

$$\tilde{g}(k;s) \sim \left[s + \frac{s\tilde{\Psi}}{1-\tilde{\Psi}}(\rho^2k^2/2 - ik\ell_1)\right]^{-1} \cong \frac{1}{s - i\tilde{\phi}\,k\,\ell_1}. \quad (25)$$

When dispersion is anomalous, the contribution of the term quadratic in $k$ to the width of the carrier packet is asymptotically small compared with the dispersion that arises from the drift. Therefore, in writing the second equality in Eq. 25, we have retained only the term linear in $k$. To simplify notation, we have introduced the memory function $\tilde{\phi} = s\tilde{\Psi}/(1-\tilde{\Psi})$.[21] The Fourier inversion of Eq. 25 gives an exponential,

$$\tilde{g}(z;s) = \frac{1}{\tilde{\phi}\,\ell_1}\exp(-sz/\tilde{\phi}\,\ell_1). \quad (26)$$

An integration over $z$ relates Eq. 26 to the Laplace transform of the TOF current,

$$\tilde{I}(s) = Ne - Ne\frac{s}{L}\int_0^L \mathrm{d}z\int_0^z \mathrm{d}x\tilde{g}(x;s) = \frac{Ne\tilde{\phi}\,\ell_1}{Ls}[1-\exp(-sL/\tilde{o}\,\ell_1)], \quad (27)$$

where $N$ is the number of photoinjected charges. The time dependence of the current may be determined asymptotically by inverting the leading term in an expansion of Eq. 27 for small Laplace variable $s$. To leading order in $s$, expressions for $\tilde{\Psi}$ and $\tilde{\phi}$ are as follows:

$$\tilde{\Psi}(s) = \left\langle\frac{R}{R+s}\right\rangle \sim 1 - b'(s/v_0)^a, \quad (28a)$$

$$\tilde{\phi}(s) \sim v_0(s/v_0)^{1-a}/b'. \quad (28b)$$

In Eqs. 28a and 28b, $b' = \pi a\csc(\pi a)$. To obtain an asymptotic expression for the current before the transit time, we consider the limit of Eq. 27 in which $L$ is large, so that $\exp(-sL/\tilde{\phi}\,\ell_1) << 1$. In this case,

$$\tilde{I}(s) \sim \frac{Ne\tilde{\phi}\ell_1}{Ls} = \frac{Ne\ell_1}{Lb}(s/v_0)^{-a}, \tag{29}$$

and therefore the current,

$$I(t) \sim \frac{Ne\ell_1 v_0}{Lb\Gamma(a)}(v_0 t)^{-(1-a)}, \tag{30}$$

decreases algebraically in time with an exponent $(1 - a)$. To obtain an asymptotic expression for the current after the transit time, we expand the exponential in Eq. 27 to second order in $Ls/\tilde{\phi}\ell_1$. We find

$$\tilde{I}(s) \sim -\frac{NeLs}{2\tilde{\phi}\ell_1} = -\frac{NeLb(s/v_0)^a}{2\ell_1}, \tag{31}$$

and therefore the current,

$$I(t) \sim \frac{NeLbav_0}{2\ell_1\Gamma(1-a)}(v_0 t)^{-(1-a)}, \tag{32}$$

decreases algebraically with the exponent $(1 + a)$. In summary, the disorder parameter $a$ plays an important role both in the field dependence of the mobility (see Eq. 14) and in the decay of the current with time, as observed at low temperatures for some TOF current–time curves. This clarifies the extent to which an algebraic pausing–time distribution links the field dependence of the mobility to anomalously dispersive current–time curves.

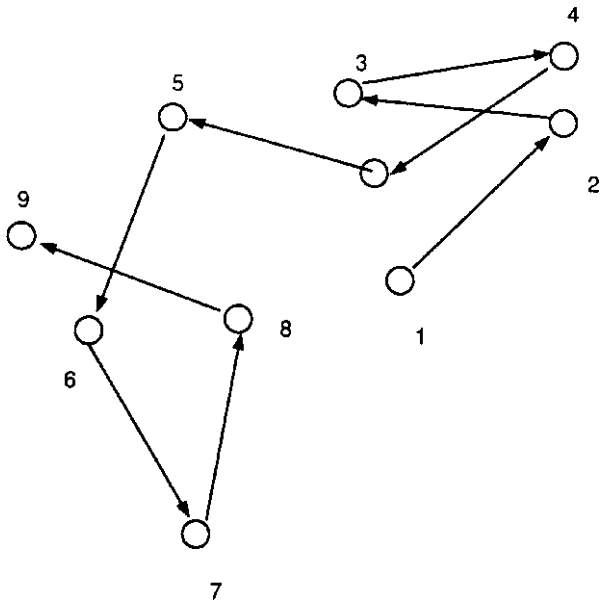


**Figure 1.** In the theory of SM, the transit time is calculated by the addition of dwell times $t$, which are drawn independently from a pausing-time distribution function with an algebraic tail, $\Psi(t) \sim t^{-(1+\alpha)}$. This process can be modeled as a bond-directed random walk on a chain in one dimension with hopping rates $R$ that are drawn at random from an algebraic distribution $\eta(R) \sim R^{\alpha-1}$. The bonds have been drawn pointing in a variety of directions to reinforce the idea that the spatial distribution corresponding to this sequence of hops is a Gaussian that drifts in the direction of the applied field.

### Modified Pausing-Time Distribution

In the Background, the spatial carrier distribution $\tilde{g}(z;s)$ was determined from the distribution $f(z;n)$ and the Laplace transform of the probability for making $n$ hops $\tilde{p}_n(s)$. Taking $\tilde{p}_n(s)$ to be the product $\tilde{\Psi}^n(1-\tilde{\Psi})/s$ implies that successive dwell times are to be chosen independently from the pausing-time distribution $\Psi$. Thus the temporal behavior of the random walk is calculated in the same manner as it would be for bond-directed hopping along a 1-D chain. This sequence is illustrated in Fig. 1. Describing $\Psi$ by Eq. 10 is asymptotically equivalent to selecting the rates $R$ connecting sites in the chain at random from the distribution $\eta(R)$ of Eq. 9.[9, 22]

A carrier will take about $m \approx \mathcal{L}/\ell_1$ hops in traversing a length $\mathcal{L}$. The time for this process, $t_{\mathcal{L}} \sim m^{1/a}/v_0$, is calculated by adding together $m$ times chosen at random from the pausing-time distribution $\Psi(t)$. When $\Psi$ decays algebraically according to Eq. 10 with $a < 1$, the sum of $m$ times is proportional to the dwell time corresponding to the slowest hop in the sequence. Specifically, it can be shown for large $m$ that the distribution of times for the *slowest* of the $m$ hops is a universal function of the same scaled time variable $x = t/m^{1/a}$ that characterizes the distribution of the *sum* of all $m$ dwell times. This means that the time for the slowest hop is a macroscopic fraction of the sum of the times for all $m$ hops, even as $m \to \infty$; the slowest hop is the rate-limiting step in the sequence, no matter how long the sequence. For our purposes here, we note that this limit indicates that in a sequence of $m$ hops, there is a high probability for encountering a slow hop with a rate of the order of $R_{\mathcal{L}} \approx v_0 m^{-1/a}$.

Faced with a difficult hop, a carrier may choose to follow an alternate path. Let us suppose that there are exactly two difficult paths along which the sequence of hops may proceed (rather than just one). Suppose, for example, that in one direction the rate is $R_{\mathcal{L}}$, while in the other direction the rate is $R'_{\mathcal{L}}$. We will choose these two rates independently from the distribution $\eta(R)$, just as we chose the other $m$ rates in the sequence, but with the restriction that $R_{\mathcal{L}}$ and $R'_{\mathcal{L}}$ are both smaller than $v_0 m^{-1/a}$. In the Laplace domain, the distribution of dwell times for this difficult hop,

$$\tilde{\Psi}_{\mathcal{L}}(s) = \left\langle \frac{R'_{\mathcal{L}} + R_{\mathcal{L}}}{s + R'_{\mathcal{L}} + R_{\mathcal{L}}} \right\rangle = \int_0^{v_0 m^{-1/a}} dR_{\mathcal{L}} \int_0^{v_0 m^{-1/a}} dR'_{\mathcal{L}} \left( \frac{amR_{\mathcal{L}}^{a-1}}{v_0^a} \right) \left( \frac{amR'^{a-1}_{\mathcal{L}}}{v_0^a} \right) \frac{R_{\mathcal{L}} + R'_{\mathcal{L}}}{s + R_{\mathcal{L}} + R'_{\mathcal{L}}}, \tag{33}$$

can be expressed as an integral over both $R_{\mathcal{L}}$ and $R'_{\mathcal{L}}$. The upper limits of the integrals have been reduced from $v_0$ to $v_0 m^{-1/a}$, so that the hop from this junction remains the rate-limiting step in the sequence of $m$ hops. The factors of $m$ in the numerator are for normalization of the distributions of $R_{\mathcal{L}}$ and $R'_{\mathcal{L}}$ on the reduced interval. Changing variables of integration in Eq. 33 to $R = R_{\mathcal{L}} m^{1/a}$ and $R' = R'_{\mathcal{L}} m^{1/a}$, we find

$$\tilde{\Psi}_{\mathcal{L}}(s) = \int_0^{v_0} dR \int_0^{v_0} dR' \left( \frac{aR^{a-1}}{v_0^a} \right) \left( \frac{aR'^{a-1}}{v_0^a} \right) \frac{R + R'}{s' + R + R'} = 1 - s' \frac{a^2}{v_0^{2a}} \int_0^{v_0} dR \int_0^{v_0} dR' \frac{R^{a-1} R'^{a-1}}{s' + R + R'}, \tag{34}$$

where we have introduced the scaled Laplace variable,

$$s' = m^{1/a} s. \tag{35}$$

By scaling the integration variables by $m^{1/a}$, the limits of integration in Eq. 33 have been restored to the full range $(0, v_0)$ in Eq. 34. Equation 34 expresses the distribution of times for the most difficult hop in a sequence of $m$ hops. Because the hop is a rate-limiting step, however, Eq. 34 also characterizes the distribution of the sum of $m$ times for crossing the length $\mathcal{L}$. The scaled rate $R_{\mathcal{L}} = m^{-1/a} R$ can therefore be thought of as the rate for crossing a "mesoscopic bond" of length $\mathcal{L}$ for a random walk on a set of coarse-grained sites. Each node connects onto two branches, however, so our sequence of hops is now equivalent to bond-directed hopping on a Cayley tree of connectivity 2. This sequence is illustrated in Fig. 2. The asymptotic expressions in the Background can be brought to the coarse-grained level by replacing $\tilde{\Psi}$ by $\tilde{\Psi}_{\mathcal{L}}$ and $s$ by $s'$ where the spatial distribution,

$$f_{\mathcal{L}}(z;n) \sim \frac{1}{\left(2\pi n m \rho^2\right)^{1/2}} \exp\left[\frac{(z - n\mathcal{L})^2}{2nm\rho^2}\right] \tag{36}$$

is now expressed in terms of the number $n$ of hops with length $\mathcal{L}$.

Integrating Eq. 34 to leading order in the scaled Laplace variable $s' = sm^{1/a}$, we find

$$\tilde{\Psi}_{\mathcal{L}}(s') = 1 - cs' - bs'^{2a} + \underline{\mathbf{O}}(s'^2), \tag{37}$$

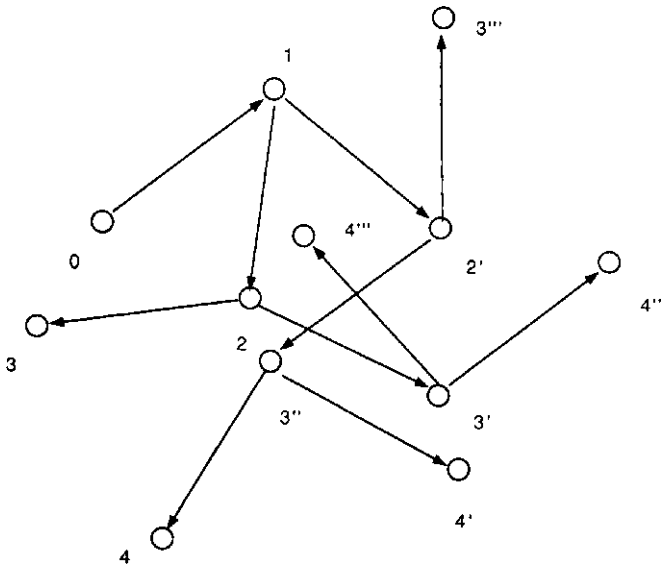


**Figure 2.** At the coarse-grained level, the process of drawing independent times from the pausing-time distribution function $\Psi_{\mathcal{L}}$ can be modeled as a bond-directed random walk with disordered hopping rates $R_{\mathcal{L}}$. At each node, however, we will allow a carrier the opportunity to choose between two paths. Thus the process is described by a Cayley tree of connectivity 2.

where the coefficients in Eq. 37 are functions of $a$,

$$\begin{aligned} c &= \frac{a^2}{2^{2(a-1)}(2a-1)} \int_0^{\pi/2} \mathrm{d}\theta \sin^{2a-1}(\theta) + D, \\ b &= \frac{a^2 \pi}{2^{2(a-1)} \sin(2\pi a)} \int_0^{\pi/2} \mathrm{d}\theta \sin^{2a-1}(\theta), \\ 1 &\le \frac{(2a-1)D}{2a^2\left[1 - \int_0^{\pi/2} \mathrm{d}\theta \cos^{2a}(\theta)\right]} \le 2, \end{aligned} \tag{38}$$

for $0 < 2a < 2$ except $2a = 1$. At this point we will define a coarse-grain memory function, $\tilde{\phi}_{\mathcal{L}}(s') = s'\tilde{\Psi}_{\mathcal{L}} / (1 - \tilde{\Psi}_{\mathcal{L}})$, and substitute $\tilde{\phi}_{\mathcal{L}}$ for $\tilde{\phi}$ in Eqs. 28 and 29, to obtain asymptotic expressions for the TOF current before and after the transit time $\tau$, respectively. For a small Laplace variable, $\tilde{\phi}_{\mathcal{L}}(s') \cong [c + bs'^{(2a-1)}]^{-1}$. If the dispersion parameter $a < 1/2$, then $\tilde{\phi}_{\mathcal{L}}(s') \cong s'^{(1-2a)} / b$. This form is identical to Eq. 28b, with $s'$ replacing $s$, $b$ replacing $b'$, and $2a$ replacing $a$. When $a < 1/2$, transport is clearly dispersive in the SM sense. The current–time asymptotes are found by analogy with Eqs. 29 and 31:

$$I(t)_{t<\tau} \sim \frac{Ne\,\ell_1^{\,2} v_0}{L\mathcal{L}\, b\Gamma(2a)} (v_0 t)^{-(1-2a)}, \tag{39a}$$

$$I(t)_{t>\tau} \sim \frac{NeL\mathcal{L}\, b 2a v_0}{2\ell_1^{\,2}\Gamma(1-2a)} (v_0 t)^{-(1+2a)}. \tag{39b}$$

We see from Eqs. 39a and 39b that, in the dispersive regime, the parameter $2a$ plays the role of $\alpha$ in Eq. 7. Therefore, to maintain contact with traditional analysis of dispersive transport, from here on we will replace our disorder parameter $a$ with $\alpha/2$;

$$\alpha \equiv 2a = 2MkT / \sigma. \tag{40}$$

A transition to a less dispersive regime occurs at the temperature $T_c$ for which $\alpha = 1$. Comparing Eq. 40 with Eq. 19, we note that $T_c$ is half of the compensation temperature $T_0$. For the choice of $\sigma/M = 0.042$ eV,

$$T_c = T_0/2 = 250 \text{ K}. \tag{41}$$

Above $T_c$ (for $1 < \alpha < 2$ ), the Laplace transform of the current before the shoulder is

$$\tilde{I}(s)_{t<\tau} \sim \frac{Ne\mathcal{L}}{L} \frac{\tilde{\phi}(s')}{s'} = \frac{Ne\mathcal{L} v_0}{cLs'} \left[1 - \frac{b}{c}(s'/v_0)^{\alpha-1}\right]. \tag{42}$$

Inverting Eq. 42, we find that the current approaches a steady state,

$$I(t)_{t<\tau} \sim \frac{Ne\mathcal{L} v_0}{cL} \left(\frac{\ell_1}{\mathcal{L}}\right)^{2/\alpha} \left[1 + \left|\frac{b}{c}\right| \left(\frac{\mathcal{L}}{\ell_1}\right)^{(2-2/\alpha)} \frac{(v_0 t)^{-(\alpha-1)}}{\Gamma(2-\alpha)}\right] \sim \text{const.} \tag{43}$$

After the shoulder, however, the current decays algebraically as in the dispersive regime. In the Laplace domain, the current

$$\tilde{I}(s)_{t>\tau} \sim -\frac{NeL}{2\mathcal{L}} \frac{s'}{\tilde{\phi}(s')} = -\frac{NeL}{2\mathcal{L}} [c(s'/v_0) + b(s'/v_0)^{\alpha}]. \tag{44}$$

Inversion of Eq. 44 demonstrates that the current,

$$I(t)_{t>\tau} \sim \frac{NeL\mathcal{L}v_0}{2\ell_1^2\alpha(\alpha-1)\Gamma(2-\alpha)}|b|(v_0t)^{-(\alpha+1)}, \qquad (45)$$

continues to decay algebraically with an exponent of $1 + \alpha$ for $t > \tau$, when $1 < \alpha < 2$.

To obtain the field dependence of the mobility, we examine the current for times $t < \tau$, in which case the current is proportional to the drift velocity, $I(t) = (Ne/L)\, v(t)$. From Eqs. 39a and 43 we obtain

$$v(t)_{T<T_c} = \frac{\ell_1^2 v_0}{\mathcal{L}\, b\Gamma(\alpha)}(v_0t)^{-(1-\alpha)} \qquad (46a)$$

and

$$v(t)_{T>T_c} = \frac{\mathcal{L}v_0}{c}\left(\frac{\ell_1}{\mathcal{L}}\right)^{2/\alpha}, \qquad (46b)$$

respectively. The transit times,

$$\tau_{T<T_c} = \frac{1}{v_0}\left[\frac{L\mathcal{L}\alpha b\Gamma(\alpha)}{\ell_1^2}\right]^{1/\alpha} \qquad (47a)$$

and

$$\tau_{T>T_c} = \frac{Lc}{\mathcal{L}v_0}\left[\frac{\mathcal{L}}{\ell_1}\right]^{2/\alpha}, \qquad (47b)$$

are calculated by integrating Eq. 2 with the substitution of Eqs. 46a and 46b for the velocity *v, and setting z=L*. Substitution of Eqs. 47a and 47b in Eq. 3 gives the mobility,

$$\mu_{T<T_c} = v_0\left[\frac{(\rho^2\beta e/2)^2 L}{\mathcal{L}b\alpha\Gamma(\alpha)}\right]^{1/\alpha}\left(\frac{E}{L}\right)^{2/\alpha-1}; \qquad (48a)$$

$$\mu_{T>T_c} = (\rho^2\beta e/2)^{2/\alpha}\,\frac{v_0}{c}\left(\frac{E}{\mathcal{L}}\right)^{2/\alpha-1}. \qquad (48b)$$

We see that below $T_c$ the mobility scales with the length of the sample, as $L^{1-1/\alpha}$. Above $T_c$, on the other hand, the mobility depends only on the intrinsic length $\mathcal{L}$. Both Eqs. 48a and 48b lead to a mobility of the form of Eq. 22, which closely describes a Poole–Frenkel behavior over a broad range of field. The connection between the Poole–Frenkel factor $\gamma$ and the dispersion parameter $\alpha$ that characterizes the current–time curves has changed, however; we see that $(2/\alpha - 1)$ in Eq. 48 is larger than $\exp(1/\alpha - 1)$, which one obtains from the SM theory in the absence of branching. Thus the mobility will remain a strong function of field even in the nondispersive ($\alpha \sim 1$) regime.

Universality of the current–time curves is preserved below the transition temperature. Substitution of the scaled time-variable $\xi = t/\tau$ in Eqs. 39a and 39b shows, for $T < T_c$, that the normalized current,

$$\left(\frac{I(\xi)_{t<\tau}}{I(\tau)_{t<\tau}}\right)_{T<T_c} \sim \xi^{-(1-\alpha)}, \qquad (49a)$$

$$\left(\frac{(I(\xi)_{t>t}}{I(\tau)_{t>\tau}}\right)_{T<T_c} \sim \xi^{-(1+\alpha)}, \qquad (49b)$$

is asymptotically independent of both the sample thickness and the electric field. For $T > T_c$, substitution of $\xi$ in Eqs. 43 through 45 gives a normalized current:

$$\left(\frac{I(\xi)_{t<\tau}}{I(\tau)_{t<\tau}}\right)_{T>T_c} \cong 1 + |D|\left(\frac{\mathcal{L}}{CL}\right)^{\alpha-1}\xi^{-(\alpha-1)}; \qquad (50a)$$

$$\left(\frac{(I(\xi)_{t>\tau}}{I(\tau)_{t>\tau}}\right)_{T>T_c} \sim \xi^{-(1+\alpha)}. \qquad (50b)$$

In Eq. 50a we have replaced $I(\tau)_{t<\tau}$ by $I(\infty)_{t<\tau}$, under the assumption that $b/c^{\alpha}(\mathcal{L}/L)^{\alpha-1} << 1$. We see that for $T > T_c$, universality of the asymptotes is maintained for different electric fields, but not for different sample thicknesses; Eq. 50a predicts that the plateau should tend to flatten out in thicker samples. We do not know if such a dependence of the plateau on sample thickness has been observed.

An estimate $\tilde{W}$ of the relative tail width $W$ is the ratio of the dispersion of the charge packet to its mean position, at time $\tau$. The mean-square displacement and the mean displacement can be calculated by taking the appropriate derivatives of Eq. 25 with respect to $k$, evaluated at the limit $k \to 0$. Below $T_c$ this is just the SM result for $\alpha < 1$,

$$\tilde{W}_{T<T_c} \sim [2\Gamma^2(1+\alpha)/\Gamma(1+2\alpha) - 1]^{1/2}, \qquad (51)$$

which shows independence of field and sample thickness. Above $T_c$ ($\alpha > 1$) we find that

$$\tilde{W}_{T>T_c} \sim \left[\frac{2b(\alpha-1)}{(4-\alpha)c}\right]^{1/2}\left(\frac{\mathcal{L}}{cL}\right)^{(\alpha-1)/2} \qquad (52)$$

is independent of field, but decreases with increasing sample length as $L^{-(\alpha-1)/2}$. This is in contrast to the observations of Schein et al. for DEH-doped polystyrene, (DEH:PS); no appreciable thickness dependence of $W$ was observed for variations in $L$ by a factor of 10.[11] On the other hand, Yuh and Stolka found a decrease of $W$ with sample thickness in TPD-doped polycarbonate, (TPD:PC), following $L^{-1/2}$.[23] With respect to Eq. 52, the former observation suggests that $\alpha$ is close to 1, whereas the latter suggests that $\alpha$ is nearly 2. Borsenberger and Baessler find a transition between these two behaviors as a function of temperature and sample thickness in TAPC-doped polystyrene, (TAPC:PS).[12] As the temperature or the sample thickness is increased, the dependence of $W$ on $L$ changes abruptly, from no $L$ dependence to $W \propto L^{-1/2}$.

## Summary

In the theory of SM, an algebraic pausing-time distribution contributes a field dependence to the TOF mobility, which resembles the Poole–Frenkel law for a disorder parameter $\alpha < 1$, and predicts Ohmic behavior for $\alpha > 1$. The same pausing-time distribution predicts nondispersive transport for which the current–time curves have anomalously broad tails if $\alpha > 1$, but predicts dispersive transport for $\alpha < 1$. Transport in molecularly doped polymers exhibits a transition between these two behaviors. The current–time curves are nondispersive at high temperatures and dispersive at low temperatures. There is no accompanying transition for the field-dependent mobility, however. Both above and below the dispersive transition, the mobility follows a Poole–Frenkel law. This behavior is

clearly inconsistent with the predictions of the SM theory. In this study we have explored a simple modification of the pausing-time distribution function, for which a field-dependent mobility and a nondispersive TOF transient are predicted to occur for the same value of α.

In modifying the pausing-time distribution, we have focused on the idea that deviations from dispersive transport occur as a result of an increased branching to new paths, which become more attractive to a charge carrier as the temperature is raised. To describe the temporal effects of branching in a tractable manner, we have expanded the directed random walk of SM to a Cayley tree of connectivity 2. This expanded random walk is based on the postulate that significant new branches should be encountered only after hopping a length $\ell < L$. To study the effect of branching, we estimated the size of the rare hopping rate $R_\ell$, which is on average encountered once in every segment of length $\ell$. We then imposed the condition that whenever a rate $R_\ell$ or smaller is encountered, a carrier is given the opportunity to select between two paths, rather than just one. This has the essential effect of doubling the value of the disorder parameter.

The primary results of this modification scheme are contained in Eqs. 48 through 52. The key is that the current–time curves are characterized by the exponent α, but the field-dependence of the mobility is now characterized by the exponent α/2. The point at which the current–time curves become nondispersive is at $\alpha = 1$. The point at which the theory no longer predicts a field-dependent mobility (at low fields) is at $\alpha = 2$. In the overlapping regime, $1 < \alpha < 2$, nondispersive transport and a field-dependent mobility coexist.

We find a transition from dispersive to nondispersive transport at a temperature $T_c$, which is half the compensation temperature $T_0$. On both sides of $T_c$ the asymptotes of the current–time curves show universality with respect to the field. Below $T_c$ we have dispersive transport, and $\mu$ depends on sample thickness. Above $T_c$ the current–time curve develops a plateau, and $\mu$ is independent of thickness. An estimate of the relative width $W$ of the current–time curves predicts $W$ to be thickness dependent above $T_c$, but independent of thickness below $T_c$. Above and below $T_c$ the field dependence of the mobility remains the same. These predictions are in qualitative agreement with experiments.

Finally, we make the following observation. In the literature, attempts have been made to fit the current–time curves before the shoulder to a power law $t^{-(1-\alpha)}$, even when they are considered to be nondispersive. Because the current always shows a slight decay before the shoulder, invariably it is found that the logarithmic slope $-(1 - \alpha)$ is very close to zero, implying that α is very close to 1.[24] In contrast, Eq. 43 suggests that in the nondispersive regime, the current before the shoulder should decay as $I(t) \sim I(\infty)[1 + At^{-(\alpha-1)}]$, asymptotically approaching a constant. If Eq. 43 is displayed on double-log paper, the slope before the shoulder will be approximately $-(\alpha - 1) \times A\tau^{-(\alpha-1)}$. Consequently, if Eq. 43 is obeyed, a measure of the logarithmic slope just before the shoulder will not be a good indicator of the dispersion parameter. It would be better instead to focus on the tail, where the logarithmic slope is predicted to be $-(1 + \alpha)$ both above and below $T_c$. In the nondispersive regime, this slope should begin at –2 and decrease to –3 as the temperature is increased. We note that such a variation of $1 + \alpha$ from $2 < 1 + \alpha < 3$ was found in measurements on DEH by Borsenberger, Pautmeier, and Bässler.[15]

**Acknowledgements**. I am grateful to Marty Abkowitz for pointing out discrepancies in the relation between the field-dependent mobilities and dispersive transport in molecularly doped polymers, and I am indebted to Ralph Young for extensive discussions and for his valuable assistance in the writing of this article.

## References

1. D. M. Pai, *J. Chem. Phys.* **52**: 2285 (1970).
2. J. Frenkel, *Phys. Rev.* **54**: 647 (1938).
3. See P. M. Borsenberger and D. S. Weiss, *Organic Photoreceptors for Imaging Systems,* Marcel Dekker Inc., New York, 1993, and references therein.
4. L. B. Schein, C. B. Duke, and A. R. McGhie, *Phys. Rev. Lett.* **40**: 197 (1970).
5. H. Scher and E. W. Montroll, *Phys. Rev. B*, **12**: 2455 (1975).
6. N. Crisa, *Phys. Stat. Sol. (b)* **116**: 269 (1983).
7. (a) G. Pfister, *Phys. Rev. B*, **16**: 3676 (1977); (b) G. Pfister and H. Scher, *Adv. Phys.* **27**: 747 (1978); (c) J. Mort and G. Pfister, *Polymer.-Plast. Technol. Eng.* **12**: 89 (1979).
8. W. D. Gill, *J. Appl. Phys.* **43**: 5033 (1972).
9. D. H. Dunlap, *Phys. Rev. B*, **52** (July 1 – 11 1995).
10. P. M. Borsenberger, *J. Appl. Phys.* **68**: 6263 (1990).
11. (a) L. B. Schein, J. C. Scott, L. Th. Pautmeier, and R. Young, *Mol. Cryst. Liq. Cryst.* **228**: 175 (1992); (b) L. B. Schein, *Phil. Mag. B*, **65**: 795 (1992).
12. P. M. Borsenberger and H. Bässler, *J. Appl. Phys.* **75**: 967 (1994).
13. L. B. Schein, A. Peled, and D. Glatz, *J. Appl. Phys.* **66**: 686 (1989).
14. (a) H. Bässler, *Int. J. Mod. Phys. B* **8**: 847 (1994); (b) H. Bässler, *Phys. Stat. Sol. (b)* **175**: 15 (1993).
15. P. M. Borsenberger, L. T. Pautmeier, and H. Bässler, *Phys. Rev. B* **46**: 12,145 (1992).
16. P. M. Borsenberger, L. T. Pautmeier, and H. Bässler, *Phys. Rev. B* **48**: 3066 (1993).
17. P. M. Borsenberger, L. Pautmeier, and H. Bässler, *J. Chem. Phys.* **94**: 5447 (1991).
18. (a) P. E. Parris and B. Bookout. to be published; (b) P. E. Parris in *Xerographic Photoreceptors and Photorefractive Polymers, Proc. SPIE* **2526**, 1995.
19. Yu. N. Gartsein and E. M. Conwell, *Chem. Phys. Lett.* (1995).
20. N. Apsley and H. P. Hughes, *Philos Mag.* **30**: 963 (1974).
21. V. M. Kenkre, E. W. Montroll, and M. F. Schlesinger, *J. Stat. Phys.* **9**: 45 (1973).
22. H. Schnoerer, D. Haarer, and A. Blumen, *Phys. Rev. B* **38**: 8097 (1988).
23. H. J. Yuh and M. Stolka, *Phil. Mag. B* **58**: 539 (1988).
24. J. C. Scott, L. Th. Pautmeier, and L. B. Schein, *Phys. Rev. B* **46**: 8603 (1992).