Mechanism for carrier velocity saturation in pure organic crystals

V. M. Kenkre
Department of Physics and Astronomy and Center for Advanced Studies, University of New Mexico, Albuquerque, New Mexico 87131

P. E. Parris
Department of Physics, University of Missouri, Rolla, Missouri 65409

(Received 2 February 2002; published 28 May 2002)

We present a possible mechanism for the saturation of the velocity of photoinjected charge carriers in pure organic crystals, the analysis having been motivated by observations in pentacene. The mechanism is based on the strong wave vector dependence of the damping coefficient appearing in the appropriate effective mass equation. Our primary goal is to explore this mechanism in general terms rather than to apply it to a specific system such as pentacene. Our analysis is based on a Fokker-Planck equation treatment. We indicate how the damping coeffcient is related to relaxation times in usual Boltzmann equations and how it can be computed from Fermi golden rule transition rates.

DOI: 10.1103/PhysRevB.65.245106 PACS number(s): 72.10.−d, 72.20.−i, 72.60.+g

I. INTRODUCTION

Saturation of the velocity of injected charge carriers with increasing electric field has been observed in pure organic crystals such as pentacene.[1] In a recent publication[2] the present authors have analyzed this phenomenon and have shown that, contrary to what has been suggested in the literature,[1,3] drift velocity saturation cannot arise solely as a consequence of the nonparabolic nature of carrier bands. Two possible sources of the saturation have also been sketched in that analysis,[2] one based on the field dependence of the scattering and the other based on its wave vector dependence. Here, we report on specific realizations of the second idea, show what particular features of the quasimomentum dependence can lead to saturation of the velocity, and elucidate the effects of temperature on the phenomenon. Our considerations are based on the standard effective mass equation at zero temperature, augmented into a Langevin form through random noise terms at finite temperatures, and its associated Fokker-Planck equation with quasimomentum-dependent damping.

The effective mass equation for the evolution of the quasimomentum $\hbar k$ of a carrier valid at zero temperature is

$$\hbar \frac{dk}{dt} + \gamma_k v_k = qE, \tag{1}$$

where q is the carrier charge, E is the electric field, $v_k = (1/\hbar) d\varepsilon_k/dk$ is the group velocity of the carrier obtained from its band energy ε_k, and γ_k is the damping coefficient. At finite temperatures, we append a noise term to the right-hand side of Eq. (1) and, through standard procedures, obtain for the evolution of the probability distribution $f(k,t)$ a Fokker-Planck equation

$$\frac{\partial f(k,t)}{\partial t} = \frac{1}{\hbar^2} \frac{\partial}{\partial k} \left[\left(\gamma_k \frac{d\varepsilon_k}{dk} - \hbar q E \right) f(k,t) + \gamma_k k_B T \frac{\partial f(k,t)}{\partial k} \right], \tag{2}$$

where k_B is the Boltzmann constant and T the temperature. It is important to notice that, unlike in the treatment in the main body of Ref. 2, but as suggested at the end of that analysis, the damping coefficient γ_k here depends on the location k of the carrier in the Brillouin zone. Whereas it is clear from the analysis of Ref. 2 that no saturation occurs for a constant γ, the following simple argument shows how a class of k-dependent damping coefficients result quite naturally in saturation.

II. ESSENCE OF THE MECHANISM: $T=0$

Consider the zero-temperature case in which the quasi-Newtonian evolution (1) is appropriate. Assume an initial occupation by the carrier of a k state at or near the center of the Brillouin zone, and take the k dependence of the damping coefficient to be steep enough so that the carrier, in being accelerated towards the edge of zone, never reaches it and produces no Bloch oscillation, but comes to a steady state where the derivative of k in Eq. (1) vanishes. The location in the zone at which the carrier lies in the steady state has a k value which satisfies

$$\gamma_k v_k = qE. \tag{3}$$

The steady-state value of the velocity is v_k at that value of k. The field E that produces this velocity equals $1/q$ times the value of $\gamma_k v_k$ at that value of k. The k dependence of γ_k will thus be reflected in the field dependence of the velocity. As a result, the plot of v versus E will show a saturation if γ_k is sufficiently steep: small changes in k will result in large changes in γ_k and thereby of E. In other words, as a consequence of the steepness of γ_k, large changes in the field would be required to produce a discernible change in k and therefore in the velocity.

The velocity versus field curve is, thus, essentially the v_k versus $\gamma_k v_k$ curve. We have shown in Ref. 2 that saturation would occur if γ_k were to have the precise (singular) k dependence of the effective mass in a band. Such a dependence corresponds, for the case of a sinusoidal band $\varepsilon_k = -(W/2)\cos ka$, to the evolution equation

$$\frac{dv}{dt} + \frac{v}{\tau} = \frac{qE}{m^*} = \frac{qEa}{\hbar} \sqrt{v_0^2 - v^2}, \tag{4}$$

where a is the lattice constant and $v_0 = Wa$ is the maximum of the group velocity. As explained in Ref. 2, the evolution (4) can be obtained from the effective mass equation (1) by first putting the damping to zero, then dividing by the effective mass m^*, and finally putting the scattering back in through a term $-v/\tau$ where τ is a constant. Being proportional to the effective mass m^*, the corresponding γ_k displays a singularity in the middle of the zone: it rises to infinity at $ka = \pi/2$, jumps discontinuously to minus infinity, and then rises to a finite negative value at the zone edge.

We would now like to emphasize that the phenomenon of saturation does not require for its explanation such singular, discontinuous, or negative behavior. A steep rise of γ_k in the middle of the zone is all that is necessary. Thus, if γ_k is assumed to have the steepness characteristic of m^* but not its discontinuity or negative values, e.g., if

$$\gamma_k = \gamma_0 \left[1 + \frac{\lambda}{2} \left(\frac{1}{1+\lambda^2 (ka - \pi/2)^2} + \frac{1}{1+\lambda^2 (ka + \pi/2)^2} \right) \right], \tag{5}$$

saturation is assured. We display in Fig. 1 the k dependence of γ_k in the zone and the resulting saturation of the drift velocity with electric field. We assume a sinusoidal band for simplicity and express the velocity and the field in terms of dimensionless quantities v/v_0 and E/E_c where $E_c = \gamma_0 v_0 a/q$. The k dependence in the damping coefficient (5) has a ''resonance shape'' because it is derived from the k dependence of the effective mass (without its discontinuous and negative aspects). All that is necessary for saturation, however, is that γ_k rise steeply enough. An ''edge shape'' is therefore sufficient. Consider, for instance,

$$\gamma_k = \gamma_0 \{ 2 + \tanh[2(k - k_0)a] - \tanh[2(k + k_0)a] \}, \tag{6}$$

which rises very steeply in the neighborhood of k_0, as is illustrated in Fig. 2 for three values of $k_0 = \pi/4, \pi/2$, and $3\pi/4$, along with the consequent occurrence of saturation in the velocity-field plot.

The value of the field E and the location in the zone where the rise of γ_k is substantial together determine features of the saturation phenomenon. Because the velocity in the band v_k increases with k at the center of the zone but reaches a maximum in the middle of the zone (at $ka = \pi/2$ for a sinusoidal band) and then decreases for larger k values, a possibility exists that the v-E plot exhibits a rise followed *by a decrease* and a saturation at a value smaller than the peak. To illustrate this behavior, we use a tunable damping coefficient

$$\gamma_k = \gamma_0 (1 + \mu \tan^2[k/k_0]), \tag{7}$$

in which the location of the rise can be altered by changing the parameter k_0. We display in Fig. 3 two curves corresponding to $k_0 a = 1$ and $k_0 a = 3/2$. Saturation occurs at a velocity lower than the maximum in the latter case. While we know of no experiments that display such lower-than-peak saturation, this is an interesting consequence of the mechanism we propose, for systems in which the steep rise in of γ_k occurs far enough from the v_k peak region.

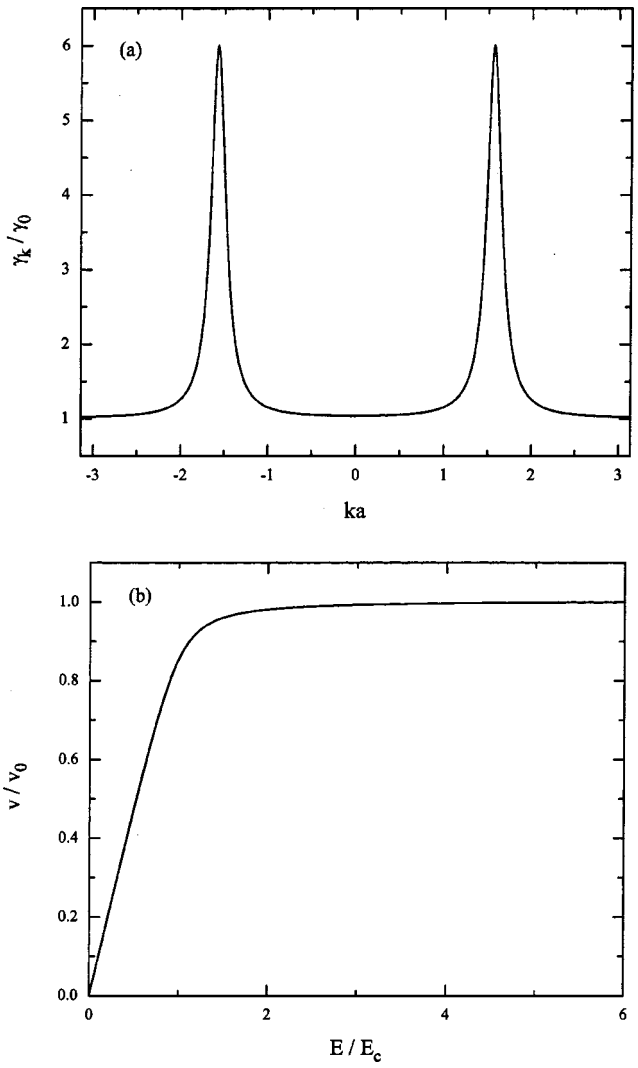

FIG. 1. Saturation of the carrier velocity with increasing field arising from the steep k dependence of the damping coefficient γ_k. This k dependence in the Brillouin zone, as given by Eq. (5), is shown in (a) while the corresponding zero-temperature carrier velocity is plotted in (b). Both velocity and field are scaled as explained in the text.

III. THERMAL EFFECTS ON SATURATION: $T > 0$

We thus see that, while saturation does not arise from the nonparabolic nature of bands, it can arise very simply from steep damping coefficients, at least at zero temperatures. Does finite temperature have any drastic effect on these conclusions? In order to answer this question, we turn to the Fokker-Planck equation (2) which describes the evolution of the distribution function $f(k,t)$, i.e., the probability density that the carrier occupies a state k at time t. In the steady state, $f(k,t)$ has a time-independent value (which we will denote below by f_k) and the contents of the square brackets on the right-hand side of Eq. (2) equal a k-independent quantity which may be evaluated in standard ways[6]. Details of this evaluation involve a straightforward extension of our analysis presented earlier[2,4] for the constant γ case. The resulting steady-state distribution f_k is given by

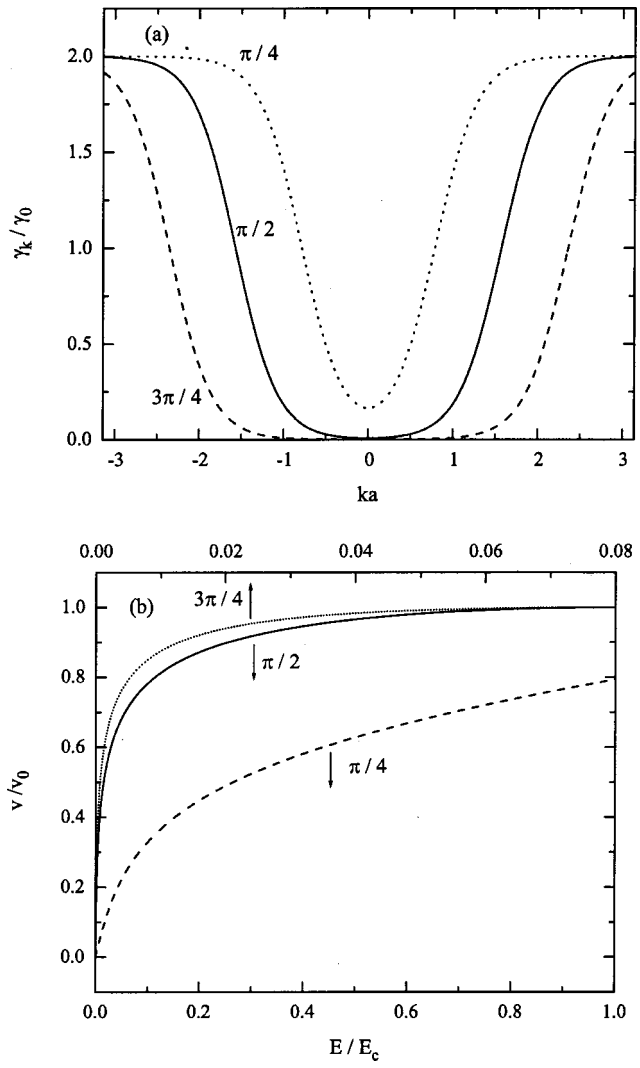

FIG. 2. Saturation as in Fig. 1 but shown here for an "edge" k dependence as given in Eq. (6). The k dependence of the damping coefficient is shown in (a) for three values of k_0a: $\pi/4$, $\pi/2$, and $3\pi/4$, respectively, which represent different locations in the Brillouin zone where the steep part of γ_k appears. The corresponding zero-temperature velocity-field plot is in (b) where the scale on the upper axis applies to the uppermost curve while that on the lower axis applies to the lower two curves as indicated by arrows.

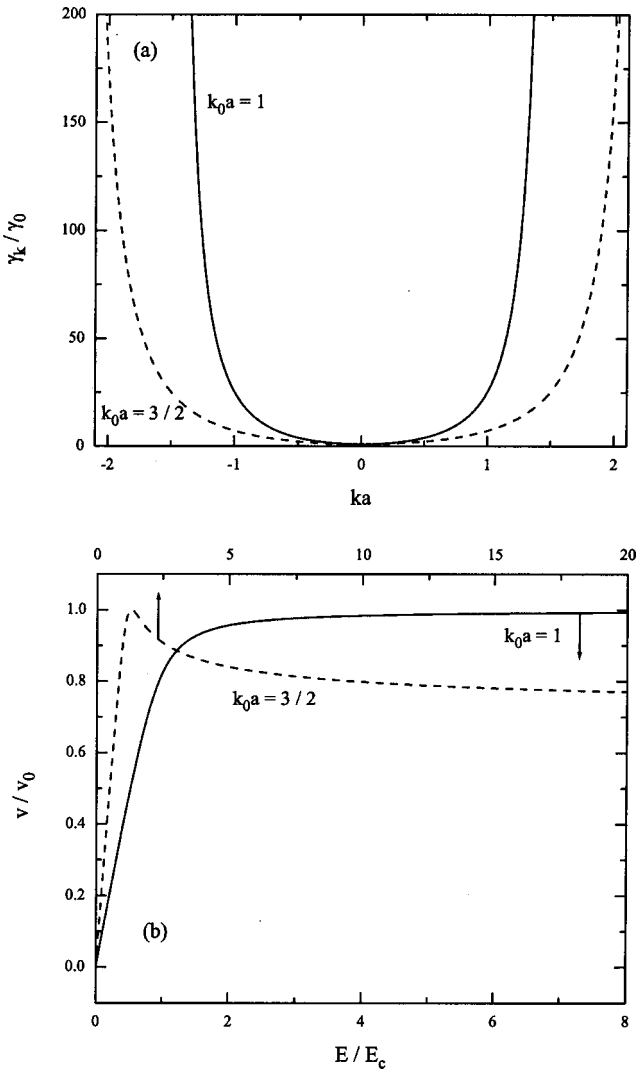

FIG. 3. Saturation below the peak velocity value as the result of the location in the zone of the steep part of γ_k. The k dependence of the damping coefficient in Eq. (7) is plotted in (a) for values of $k_0a=1$ and 3/2, as indicated. The corresponding zero-temperature velocity-field plots in (b) both display saturation, but for $k_0a=3/2$ the saturation occurs below the peak value. This is a prediction of our mechanism which, to our knowledge, has not yet been observed.

$$f_k=\frac{\int_0^{2\pi/a} dp h'_{k+p} e^{\beta(\varepsilon_{k+p}-\varepsilon_k)} e^{-\beta\hbar qE(h_{k+p}-h_k)}}{\int_{-\pi/a}^{\pi/a} dk \int_0^{2\pi/a} dp h'_{k+p} e^{\beta(\varepsilon_{k+p}-\varepsilon_k)} e^{-\beta\hbar qE(h_{k+p}-h_k)}}, \tag{8}$$

where a is the lattice constant, β is the inverse dimensionless temperature $1/k_BT$, and

$$h'_k=\frac{dh_k}{dk}=\frac{1}{\gamma_k}. \tag{9}$$

The steady-state velocity is obtained from f_k in Eq. (8):

$$v=\int_{-\pi/a}^{\pi/a} v_k f_k dk. \tag{10}$$

Numerical evaluation procedures allow us to obtain from Eqs. (8) and (10) the distribution and the velocity in the steady state.

In Fig. 4 we display field-dependent velocities for a system with damping coefficient given by Eq. (6) with $k_0a=\pi/2$. We notice that for the parameter values considered, saturation, which does occur at $T=0$, is destroyed at the finite temperature values shown. This destruction of saturation manifests itself in the well-known phenomenon of negative differential mobility. If, in the steady state, the carrier finds itself distributed in regions of the Brillouin zone in which v_k is less than the peak value in the zone, there is a

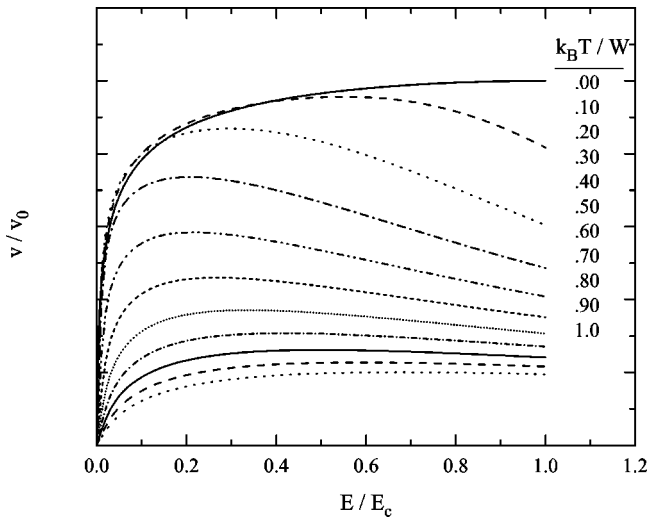

FIG. 4. Effect of nonzero temperature on the saturation pheonomenon, showing destruction of saturation and emergence of negative differential mobility. Plotted is the dependence of velocity on field, calculated numerically from the Fokker-Planck equation (2) for a damping coefficient as described by Eq. (6) with $k_0a=\pi/2$, for several different temperatures (scaled to W/k_B) as indicated.

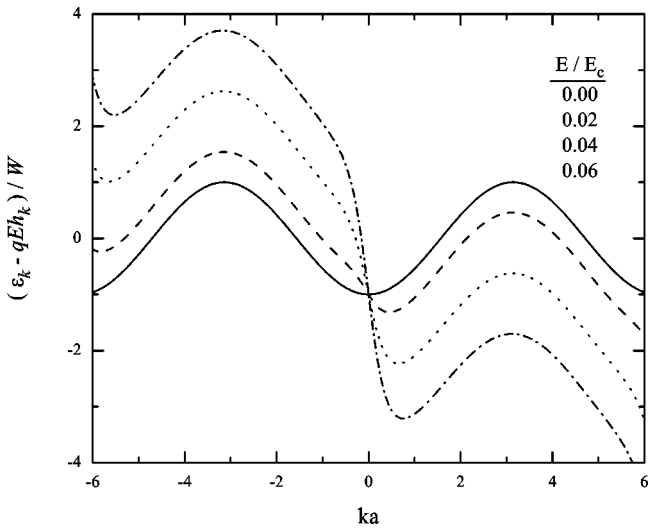

FIG. 5. Field-induced distortion of the effective potential seen by a carrier, showing considerable departure from the sinusoidal band shape. The damping coefficient γ_k is as described by Eq. (6) with $k_0a=\pi/2$. Several different values of the scaled field are shown. The effective potential facilitates, through a classical analogy (see text), the understanding of temperature effects on saturation. The minimum of the potential, located at $ka=0$ for zero field, moves to the right with increasing field, but due to the strong increase in γ_k with k, its relative motion slows down, leading to saturation. In this example, the minimum becomes sharper and less shallow as the field is increased, an effect which tends to focus the probability distribution at low temperatures.

tendency for the average velocity to be lowered. Such movement of the carrier into lower-velocity regions occurs as a result of the applied field for constant γ as has been shown in Ref. 2. Here, independently of the action of the field, thermal spreading distributes the carrier in those lower-velocity regions, causing destruction of the saturation.

In order to gain a clearer understanding of these thermal effects, we make use of an analogy between carrier motion in a band and the thermal motion of a classical particle in a potential. Consider the time evolution of the displacement x of a classical particle of mass M subjected to a potential $U(x)$ and to a damping force proportional to the particle velocity dx/dt through a proportionality factor $\alpha(x)$ which depends on position

$$M\frac{d^2x}{dt^2}+\alpha(x)\frac{dx}{dt}+\frac{dU(x)}{dx}=0. \tag{11}$$

Under very high damping, the inertial term is negligible and we have

$$\frac{dx}{dt}+\frac{1}{\alpha(x)}\frac{dU(x)}{dx}=0. \tag{12}$$

If we recast the effective mass equation (1) for the injected carrier in the form

$$\frac{dk}{dt}+\frac{\gamma_k}{\hbar^2}\frac{d}{dk}(\varepsilon_k-\hbar qEh_k)=0, \tag{13}$$

with h_k given by Eq. (9), and compare Eq. (12) with Eq. (13), we see that the motion of the carrier in the band can be understood intuitively in terms of the motion of the corresponding classical problem.[5] The ''potential'' to which the carrier is subjected in k space is $\varepsilon_k-\hbar qEh_k$. It has the periodic dependence characteristic of the band energy, modified by the damping coefficient and the strength of the applied field. If the damping coefficient is not dependent on k, the potential is $\varepsilon_k-qE\hbar k/\gamma$ and is, thus, a linearly displaced sinusoid for a tight-binding band. For k-dependent damping, which is of interest to the present investigation, the steepness characteristics of γ_k are reflected in the potential, and determine the extent of the thermal effects on saturation. In Fig. 5 we plot the effective potential seen by a carrier for a system with damping constant given by Eq. (6) with $k_0=\pi/2$. At $T=0$, the carrier settles down at the minimum of the potential. If the location of the minimum (in k space) has little sensitivity to changes in the field E as a result of the steepness of γ_k as shown in Sec. II, field saturation of the velocity occurs. As the temperature becomes nonzero, thermal fluctuations tend to move the carrier out of the minimum. Equivalently, the distribution function f_k, which at $T=0$ is a δ function localized at the potential minimum, spreads in the Brillouin zone because of thermal fluctuations. The velocity v, which at $T=0$ is simply the value of v_k at the potential minimum, now is an average, as in Eq. (10). As the population f_k grows in regions where v_k has values lower than the peak, the average velocity decreases, destroying the phenomenon of saturation.

Further quantitative insight may be gained by investigating the dependence of the width as well as the peak of the steady state distribution f_k on temperature, field strength, and characteristics of γ_k. For this purpose, we focus attention on the primary integral appearing in the steady-state solution (8)

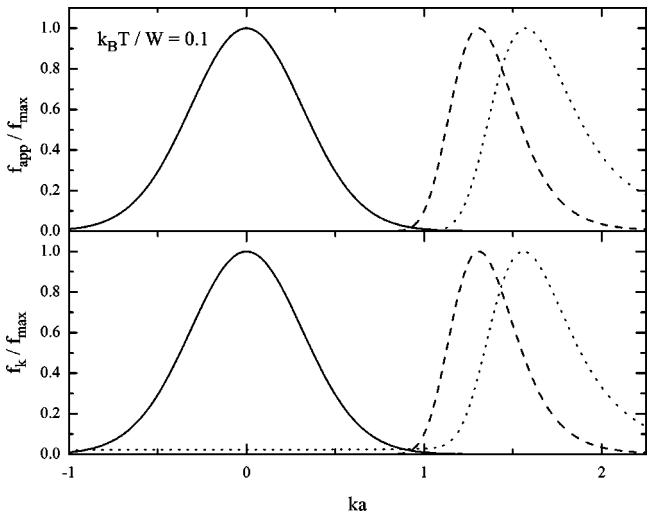

FIG. 6. Comparison of the approximate (top) and actual (bottom) expressions for f_k as given by Eqs. (15) and (8), respectively, for γ_k given by Eq. (6) with $k_0a=\pi/2$, $T=0.1(W/k_B)$, and increasing values of the scaled field $E/E_c=0$, 0.5, and 1, respectively, for the solid, dashed, and dotted curves shown. The approximation, which forms the basis of a classical analogy used to understand temperature effects, is seen to be excellent for the parameter values shown.

for the distribution function and, by making a change of integration variable $k+p\rightarrow p$, rewrite the integral as a product of two factors:

$$\int_0^{2\pi/a} dp h'_{k+p} e^{\beta(\varepsilon_{k+p}-\varepsilon_k)} e^{-\beta\hbar qE(h_{k+p}-h_k)} = e^{-\beta(\varepsilon_k-\hbar qEh_k)} \int_k^{k+2\pi/a} dp h'_p e^{\beta\varepsilon_p} e^{-\beta\hbar qEh_p}. \quad (14)$$

The second factor on the right-hand side of Eq. (14) is an integral which, being an average over a full Brillouin zone starting at wave vector k, is a weak function of k. Under the approximation that its (weak) dependence on k may be neglected, the distribution function in Eq. (8) is well represented by the simpler expression

$$f_k = \frac{e^{-\beta(\varepsilon_k-\hbar qEh_k)}}{\int_{-\pi}^{\pi} e^{-\beta(\varepsilon_{k'}-\hbar qEh_{k'})} dk'}. \quad (15)$$

Figure 6 compares the distribution as predicted by Eqs. (15) and (8) for a system with damping coefficient given by Eq. (6) to illustrate the validity of the approximation represented by Eq. (15).

For reasonable physical systems, damping rates γ_k are always positive and $h_k=\int_0^k \gamma_{k'}^{-1} dk'$ is a monotonically increasing function of $|k|$. The location k_p of the peak of f_k, found by putting the k derivative of the exponent in the numerator of Eq. (15) to zero, satisfies

$$(\gamma_k v_k)_{k=k_p} = qE, \quad (16)$$

which is precisely equivalent to the condition (3) at zero temperature obtained from the quasi-Newtonian treatment. At low temperatures, as anticipated, the distribution function f_k approaches a δ function centered at the zero-temperature equilibrium value of k, which marks the minimum of the potential. For finite temperatures, on the other hand, the distribution acquires a width about the peak. The mean velocity, obtained by averaging v_k over this finite width thus attains a temperature dependence. For the zero-temperature saturation to persist at finite temperatures, the width, of the peak must remain small. Indeed, at high enough temperatures, the spread of the distribution about its zero-temperature value will ultimately cause the velocity to decrease with increasing temperature.

To determine conditions favorable for saturation, we represent f_k as a Gaussian by expanding the exponent $\beta(\varepsilon_k-\hbar qEh_k)$ of the distribution function in Eq. (15) up to second order:

$$f_k \approx C e^{-\beta(\varepsilon_{k_p}-\hbar qEh_{k_p})} e^{-(k-k_p)^2/2\sigma^2}, \quad (17)$$

where C is the normalizing constant. The width σ of the distribution, whose extent is important for the retention or destruction of the saturation phenomenon occurring at $T=0$, is given by

$$\sigma^2 = \frac{m_p^* k_B T}{\hbar + qEm_p^* |h''_{k_p}|}, \quad (18)$$

where m_p^* is the effective mass $(1/\hbar^2)(d^2\varepsilon_k/dk^2)$ evaluated at the peak, and $|h''_k|=(1/\gamma_k^2)(d\gamma_k/dk)$. Equation (18) shows that the width of the peak in the distribution function increases linearly with the temperature. It also predicts a strong narrowing of the distribution with increasing field provided the rate of change of the inverse damping rates is sufficiently large. Specifically, such narrowing occurs when $qEm_0^*|h''_{k_p}|/\hbar \gg 1$, so that the second term in the denominator of Eq. (18) dominates the first, and, additionally, when $qE|h''_{k_0}| \gg k_B T$, so that the numerator dominates the denominator. This suggests that saturation will be stronger in systems for which the damping rate ''turns on'' very suddenly, so that $d\gamma_k/dk$ becomes large in a region where γ_k itself is fairly small.

As a tunable model system on which these ideas may be tested, we consider a system with a damping rate γ_k such that its reciprocal h'_k is the piecewise linear function:

$$\gamma_k^{-1} = h'_k = \begin{cases} \gamma_0^{-1} & \text{for } k_1 > |k| > 0, \\ \gamma_0^{-1}[1-(1-\eta)(k-k_1)/\Delta k)] & \text{for } k_1+\Delta k > |k| > k_1, \\ \eta\gamma_0^{-1} & \text{for } \pi/a > |k| > k_1+\Delta k. \end{cases} \quad (19)$$

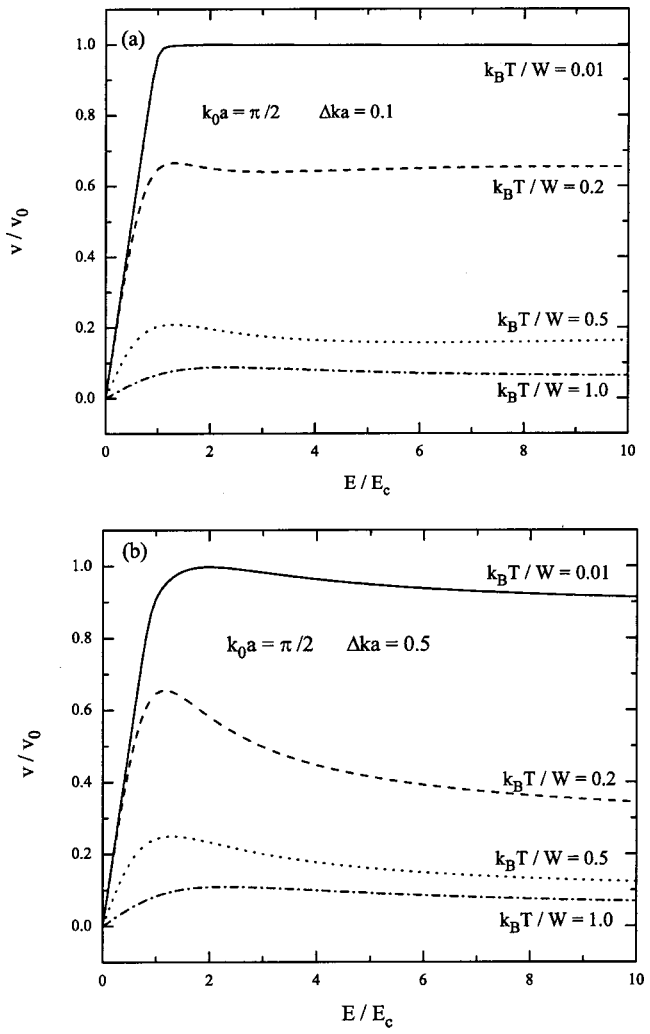

FIG. 7. Numerical calculation of the field-dependent drift velocity from the Fokker-Planck equation (2) for a damping coefficient as described by Eq. (19) with $k_0a=\pi/2$ and $\Delta ka=0.1$ and 0.5, for several different temperatures as indicated. For all curves the damping coefficient increases by a factor of 100 between $k=k_0$ and $k_0+\Delta k$. The zero-temperature velocity saturation is more resistant to thermal destruction for small Δk.

The parameter $\eta<1$ governs the change that occurs in the inverse damping rate between the zone center and edge, and the crossover interval in the zone where this change occurs extends from k_1 to $k_1+\Delta k$. Choosing η and Δk small maximizes the value of h_k'' in the peak region, since the derivative of Eq. (19) vanishes for k outside and equals the value $(1-\eta)/\Delta k$ inside the crossover interval where the change occurs. Thus, when the peak of the distribution takes a value between k_1 and $k_1+\Delta k$, the width given by Eq. (18) satisfies, for small Δk,

$$\sigma^2=\frac{m_0^* k_B T \Delta k}{qEm_0^*(1-\eta)}. \tag{20}$$

Variation of the parameter Δk controls the width and therefore the persistence or destruction of the saturation phenomenon. In Fig. 7 we present numerical calculations of the field-dependent drift velocity from the Fokker-Planck equation (2) for a damping coefficient as described by Eq. (19) with $k_0a=\pi/2$ and $\Delta ka=0.1$ and 0.5, for several different temperatures as indicated. For all curves shown, $\eta=0.01$, so that the damping coefficient increases by a factor of 100 between $k=k_0$ and $k_0+\Delta k$. We note that, as predicted, the velocity saturation observed at zero temperature is more resistant to thermal destruction when Δk is small.

IV. PRESCRIPTION TO COMPUTE γ_k AND CONCLUSIONS

The foregoing analysis has provided a possible mechanism, by no means unique, for the saturation of injected carrier velocity with increasing electric field in pure organic crystals. The basis is merely an appropriate k dependence of damping coefficients. In light of our previous discussion[2] of the earlier arguments of Warta and Karl,[3] one might be tempted to explain the observed velocity saturation in pentacene with the assumption that the source of the scattering is the spontaneous emission of optical phonons. Such scattering is indeed ineffective until the carrier energy exceeds that of the phonons emitted, and thus would suddenly ''turn on'' at a finite value of the electron wave vector. However, quantitative considerations disqualify this explanation in the case of pentacene, in which velocity saturation appears to occur at room temperature. Optical phonons in pentacene have frequencies of the order of 8–25 meV, which are thus easily absorbed and emitted at room temperature ($kT\sim 25$ meV). A sudden turn-on of the scattering rate would thus not be expected to occur. One must look to sources other than Shockley's[8] to bring about the mechanism we have discussed. The specification of the sources of mechanism lies beyond the scope of the present study which primarily indicates constraints on microscopic scattering mechanisms that are required by the oberved velocity saturation.

The investigation in the present paper has proceeded under the working assumption that the observed saturation is a real phenomenon. There is another intriguing possibility, recently suggested by Conwell and Basko,[9] that the saturation may be an artifact arising from an interpretation of current-voltage curves on the basis of a formula that inappropriately assumes a field-independent mobility. The explanation of saturation proposed in Ref. 9 requires the existence of a regime of negative differential mobility of the type predicted by our earlier analysis.[2] It is, however, completely different in spirit from the explanation proposed in the present paper. We hope that further work will be soon carried out to determine which (if either) of the mechanisms is applicable to experiments in pentacene.

It is important not to confuse γ_k with the inverse of the more familiar relaxation time τ_k which appears in standard Boltzmann equation treatments[7] of carrier transport in materials. We have pointed out in our earlier analysis[2] that identification of critical fields predicted by two separate theories, one based on a Boltzmann equation treatment with a constant relaxation time τ and the other based on a Fokker-Planck equation treatment with a constant rate γ, yields

$$\gamma = \frac{\hbar}{\tau a v_0} = \frac{m_0^*}{\tau}. \tag{21}$$

This means that γ is $1/\tau$ times the minimum value of the effective mass (at the zone edge). However, the relationship between the two quantities in the general k-dependent case appears not to be known. We present the following connection starting from a master equation

$$\frac{df(k,t)}{dt} = \sum_{k'} [Q_{kk'} f(k',t) - Q_{k'k} f(k,t)], \tag{22}$$

which, under two different respective approximations, results in the Fokker-Planck equation (2) involving γ_k, and the Boltzmann equation under the relaxation time ansatz involving τ_k. With the notation $Q_{kk'} = Q(k', k-k')$, we can write

$$\begin{aligned} Q_{kk'} f(k',t) &= Q(k+q,-q) f(k+q,t) \\ &\approx \left(1 + q\frac{\partial}{\partial k} + \frac{q^2}{2}\frac{\partial^2}{\partial k^2}\right)[Q(k,-q) f(k,t)] \end{aligned} \tag{23}$$

by stopping the Taylor expansion at second order if the rates decay quickly with increase in $q = k' - k$. Substitution in Eq. (22) and a sum over k', which is the same as a sum over q, yields

$$\begin{aligned} \sum_{k'} [Q_{kk'} f_{k'}(t) - Q_{k'k} f_k(t)] &= \frac{\partial f(k,t)}{\partial t} \\ &= -\frac{\partial}{\partial k}[F_k f_k(t)] + \frac{\partial^2}{\partial k^2}[S_k f_k(t)]. \end{aligned} \tag{24}$$

Here $F_k = \Sigma_{k'}(k'-k) Q_{k'k}$ is the first moment of the transition rates while $S_k = \Sigma_{k'}[(k'-k)^2/2] Q_{k'k}$ is the second moment. An additional relation

$$F_k - \frac{dS_k}{dk} = -\frac{S_k}{\hbar^2 k_B T}\frac{d\varepsilon_k}{dk} \tag{25}$$

between the moments of the transition rates and the band energy of the carrier follows from detailed balance. Rewriting Eq. (24) in the form (2), we obtain

$$\gamma_k = \frac{\hbar^2}{2k_B T} \sum_{k'} (k-k')^2 Q_{k'k}. \tag{26}$$

On the other hand, the well-known relaxation time approximation, when applied to Eq. (22) in its simplest version, yields

$$\tau_k = \frac{1}{\sum_{k'} Q_{k'k}}. \tag{27}$$

The conjunction of Eqs. (26) and (27) specifies a relationship between τ_k of the Boltzmann equation approach and the γ_k of the Fokker-Planck approach.[10]

Transition rates $Q_{k'k}$ are typically calculated using Fermi's golden rule as applied to the interaction of the carrier with scattering agents such as phonons or defects. Through Eq. (26) we have provided a usable prescription[11] for calculating the damping coefficient γ_k of the Fokker-Planck equation from the transition rates of the master equation. In a subsequent publication we plan to address connections between Fokker-Planck and Boltzmann approaches to practical transport theory.

ACKNOWLEDGMENTS

We thank Luca Giuggioli for discussions and acknowledge the partial support of this work by the National Science Foundation under Grant Nos. DMR-0097204 and DMR-0097210.

[1] Jan Hendrik Schön, Christian Kloc, and Bertram Batlogg, Phys. Rev. Lett. **86**, 3843 (2001); J. Schön, Ch. Kloc, and B. Batlogg, Phys. Rev. B **63**, 245201 (2001).

[2] V. M. Kenkre and P. E. Parris, Phys. Rev. B **65**, 205104 (2002).

[3] W. Warta and N. Karl, Phys. Rev. B **32**, 1172 (1985).

[4] P. E. Parris, M. Kuś, and V. M. Kenkre, Phys. Lett. A **289**, 188 (2001).

[5] Although γ_k is a measure of the damping in the effective mass equation (1), the role of the classical damping factor $\alpha(x)$ of Eq. (12) is played by its *reciprocal*, specifically by $\hbar^2/\gamma_k$. This reversal in the interpretation of γ_k arises from the formal analogy of the k evolution. Physically, $\hbar k$ is the (quasi)momentum. In the analogy, it plays the role of the classical displacement viewed in the extreme damping limit.

[6] See, e.g., L. E. Reichl, *A Modern Course in Statistical Physics*, 2nd ed. (Wiley, New York 1998); K. Lindenberg and B. J. West, *The Nonequilibrium Statistical Mechanics of Open and Closed Systems* (Wiley, New York, 1990).

[7] See, e.g., J. M. Ziman, *Electrons and Phonons* (Oxford University Press, New York, 1960); M. Dresden, Rev. Mod. Phys. **33**, 265 (1961).

[8] W. Shockley, Bell Syst. Tech. J. **30**, 990 (1951).

[9] E. M. Conwell and D. M. Basko (unpublished). The authors are grateful to E.M. Conwell for making their work available to them prior to publication.

[10] While Eqs. (26) and (27) exhibit the same dimensional relationship between γ_k and τ_k as given by Eq. (21), Eq. (26) connects γ_k directly to microscopic transition rates and the temperature.

[11] The prescription (26) requires that the transition rates in the master equation be of sufficiently short range since it assumes a smooth k variation of $Q(k,q)f(k)$. Such an assumption must break down at low temperatures when both $Q(k,q)$ and $f(k)$ tend to vary strongly in the neighborhood of $k=0$. This breakdown manifests itself in a divergence of the damping rate (26) at low temperatures. As $T \to 0$, it is expected that γ_k at $T=0$ is a finite quantity. This can be demonstrated explicitly for specific mechanisms directly from $Q(k,q)$.