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Fokker–Planck analysis of the nonlinear field dependence of a carrier in a band at arbitrary temperatures

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Abstract

We present a Fokker–Planck equation in crystal momentum space which describes finite temperature transport of charge carriers performing band motion in a solid, and analyze through exact solutions the Ohmic and non-Ohmic behavior of the mobility.

Keywords: Nonlinear mobility; Bloch oscillations

Motivated in part by recent transport experiments on the motion of injected charges in ultrapure organic solids [1], and in part by the more general desire to understand nonlinear field dependence of the mobility in narrow band materials, we investigate here a simple model describing mutually noninteracting carriers of charge q moving in the presence of an electric field E through a one-dimensional tight binding band arising from nearest-neighbor matrix element V. The carriers interact with acoustic or optical phonons of energy much smaller than the electronic bandwidth ($\hbar\omega \ll V$). Neglecting interband scattering processes, and starting from a Fokker–Planck equation for the probability distribution $f(k,t)$ of finding the particle in a band state of wavevector k, we obtain an exact solution to the steady-state distribution f_k for arbitrary temperatures and driving fields, and use the solution to analyze the Ohmic and non-Ohmic behavior of the drift velocity as a function of field and temperature.

It follows from effective mass theory [2] that, in the absence of dissipation or scattering, a constant electric field E causes a continuous linear change $k \to k + qEt/\hbar$ in the crystal wavevector k of a charge carrier in a Bloch state associated with normal band motion. This ballistic motion in crystal momentum space results in Bloch oscillations [3], in which each carrier's wavevector cycles periodically through the Brillouin zone with period $\tau = 2\pi\hbar/qEa$, where a is the lattice constant. If there is no scattering, one has zero average group velocity and an absence of d.c. current. Scattering events involving absorption and emission of phonons randomly disrupt this cycle and allow a net drift velocity. Under the conditions envisioned here, with $\hbar\omega \ll V$, energy conservation demands that typical scattering events lead to only small changes in k. Correspondingly, in the presence of both the field and a scattering mechanism of this type, we take the evolution equation obeyed by $f(k,t)$ to be of the Fokker–

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Planck or Smoluchowski type,

$$\frac{\partial f}{\partial t} = \frac{\alpha}{\hbar^2}\frac{\partial}{\partial k}\left[\left(\frac{d\varepsilon_k}{dk} - \frac{\hbar qE}{\alpha}\right)f + \frac{1}{\beta}\frac{\partial f}{\partial k}\right], \tag{1}$$

where $\beta = 1/k_B T$ is the reciprocal thermal energy, ε_k the energy of the band state with wavevector k, and α a measure of the electron–phonon scattering rate, which in the simple treatment presented here is assumed to be independent of k. For nonzero α, the first term on the right-hand side of Eq. (1) reflects the tendency of the particle to relax to lower energies, and arises from phonon emission processes, while the last term corresponds to both absorption and emission events that allow the system to equilibrate. This last term vanishes at zero temperature ($\beta \to \infty$). At nonzero temperatures and zero field, this equation predicts the relaxation of any initial distribution to a Boltzmann band equilibrium, and is thus applicable to any concentration of classical carriers, or a sufficiently small concentration of quantum mechanical (fermionic) carriers, such as injected electrons or holes. At nonzero fields, the steady-state distribution $f_k = \lim_{t\to\infty} f(k,t)$ is altered from its symmetric equilibrium form resulting in a nonzero drift velocity

$$\langle v\rangle = \frac{1}{\hbar}\left\langle\frac{d\varepsilon_k}{dk}\right\rangle = \frac{1}{\hbar}\int_{-\pi/a}^{\pi/a} f_k \frac{d\varepsilon_k}{dk}\,dk. \tag{2}$$

Eqs. (1) and (2) apply for bandshapes that, except for the required periodicity in k-space, can be entirely arbitrary. The periodicity makes the evolution equation (1) obeyed by the particle momentum distribution *formally* identical to the equation analyzed by Kuś and Kenkre [4] (KK) in their investigation of a classical problem of microwave heating in ceramic materials [5], where a periodic potential in real space is provided by the atoms in the material. The KK analysis [4] begins with a second-order (Langevin) equation in time for the position x of a particle of charge q and mass m subjected to damping and Brownian motion characterized by friction coefficient γ, a periodic potential $U(x)$, and an electric field E. From the Fokker–Planck equation for the spatial probability distribution $P(x,t)$, the KK analysis then makes a high damping approximation to obtain the Smoluchowski equation

$$\frac{\partial P}{\partial t} = \frac{1}{m\gamma}\frac{\partial}{\partial x}\left[\left(\frac{dU}{dx} - qE\right)P + \frac{1}{\beta}\frac{\partial P}{\partial x}\right]. \tag{3}$$

Clearly, the position variable x, the quantity $m\gamma$, and the potential $U(x)$ in Eq. (3) in the analysis of Ref. [4] correspond in the present circumstance to the crystal momentum k, the quantity $\hbar^2/\alpha$, and the band energy ε_k appearing in Eq. (1). In what follows, we focus on the case of a 1D tight binding band, for which $\varepsilon_k = -2V\cos ka$, and for which the group velocity of a state with wavevector k is $v_k = v_0 \sin ka$, where $v_0 = 2Va/\hbar$ is the maximum possible band velocity. The sinusoidal form for the energy dispersion relation corresponds directly to the spatial sinusoidal potential $U(x) = U_0\cos(2\pi x/\ell)$ studied as a special case in the KK analysis [4]. Indeed, in spite of their very different underlying physics, the formal similarity of the two equations allows us to write down solutions for the steady-state probability distribution f_k immediately from those obtained in Ref. [4].

For example, the steady state solution of Eq. (1) subject to the boundary condition and normalization

$$f_{k+2\pi/a} = f_k, \qquad \int_{-\pi/a}^{\pi/a} dk\, f_k = 1, \tag{4}$$

appropriate to the Brillouin zone is found, as in Ref. [4], to give

$$\left(\frac{d\varepsilon_k}{dk} - \frac{\hbar qE}{\alpha} + \frac{1}{\beta}\frac{\partial}{\partial k}\right)f_k = -\frac{\hbar^2 J}{\alpha}, \tag{5}$$

where J is a k-independent constant that depends on E and β, and is related to the particle current through the Brillouin zone (not the spatial particle current). After integrating Eq. (5) it is straightforward to deduce using Eqs. (2) and (4) the relation

$$\langle v\rangle = \frac{1}{\hbar}\int_{-\pi/a}^{\pi/a} \frac{d\varepsilon_k}{dk} f_k\,dk = \frac{\hbar}{\alpha a}\left(\frac{qEa}{\hbar} - 2\pi J\right) \tag{6}$$

between the mean drift velocity and the previously introduced constant J. Note that, in this way, the present crystal momentum space analysis differs from the real space treatment of Ref. [4], in which the velocity of a particle moving in a periodic potential of period ℓ, normalized to one particle per spatial period, is obtained from Eq. (3) through the relation

$$\left\langle\frac{dx}{dt}\right\rangle = \lim_{t\to\infty}\int_0^{\ell} x\frac{\partial P(x,t)}{\partial t}\,dx$$

$$= \frac{1}{m\gamma} \int_0^{\ell} \left[\left(qE - \frac{dU}{dx} \right) P - \frac{1}{\beta} \frac{\partial P}{\partial x} \right] dx$$
$$= \frac{1}{m\gamma} \left(qE - \left\langle \frac{dU}{dx} \right\rangle \right) = J_{\mathrm{KK}}/\ell, \tag{7}$$

where J_{KK} is the constant particle current density in the spatially periodic system studied by Kuś and Kenkre.

In the present analysis, we integrate Eq. (5) subject to the periodic boundary condition and normalization of Eq. (4) to obtain the momentum distribution in the form [6]

$$f_k = \frac{J\beta\hbar^2}{\alpha(1 - e^{-2\pi\hbar\beta qE/\alpha a})} \times \int_k^{k+2\pi/a} dp\, e^{\beta(\varepsilon_p - \varepsilon_k) - \beta\hbar qE(p-k)/\alpha}. \tag{8}$$

An integration over values of k in the Brillouin zone and use of the normalization of f_k allows determination of the constant

$$J = \frac{\alpha}{\beta\hbar^2} \frac{1 - e^{-2\pi\hbar\beta qE/\alpha a}}{B}, \tag{9}$$

where

$$B = \int_0^{2\pi/a} dk\, e^{-\hbar k\beta qE/\alpha} \int_0^{2\pi/a} dp\, e^{\beta(\varepsilon_{p+k} - \varepsilon_p)}.$$

For the cosine band, the use of standard trigonometric identities allows the quantity B to be evaluated as a single integral

$$B = \int_0^{2\pi/a} dk\, e^{\hbar k\beta qE/\alpha} \times \int_0^{2\pi/a} dp\, e^{-2\beta V[\cos(p+k) - \cos(p)]}$$
$$= \frac{2\pi}{a} \int_0^{2\pi/a} dk\, e^{\hbar k\beta qE/\alpha} I_0(4\beta V \sin ka/2) \tag{10}$$

of the modified Bessel function $I_0(z)$. Eq. (10) can also be rewritten in terms of identities involving integrals of the Bessel function [7] and a closed-form evaluation of the momentum space particle current carried out:

$$J = \frac{\alpha a^2}{2\pi^2\beta\hbar^2} \frac{\sinh(\pi\hbar\beta qE/\alpha a)}{I_{-i\hbar\beta qE/\alpha a}(2\beta V) I_{i\hbar\beta qE/\alpha a}(2\beta V)}. \tag{11}$$

Using this result, we obtain from Eqs. (11) and (6) the following exact expression for the field and temperature dependence of the drift velocity:

$$\langle v \rangle = \frac{qE}{\alpha} - \frac{1}{\pi} \frac{a \sinh(\pi\hbar\beta qE/\alpha a)}{\beta\hbar I_{-i\hbar\beta qE/\alpha a}(2\beta V) I_{i\hbar\beta qE/\alpha a}(2\beta V)}, \tag{12}$$

where $I_\nu(z)$ is the modified Bessel function of order ν. We note that in the exact solution (12) the orders $\nu = \pm i\hbar\beta qE/\alpha a$ of the modified Bessel functions are strictly imaginary, proportional to the field E, and inversely proportional to the temperature and the scattering strength α.

Eq. (12) is the central result of this Letter. In Fig. 1 we plot the ratio of the drift velocity v to the maximum attainable band velocity $v_0 = 2Va/\hbar$ as a function of the applied electric field expressed as a dimensionless ratio E/E_0 of the actual electric field to the quantity $E_0 = 2V\alpha a/\hbar q$. The different curves in this figure correspond to different temperatures as expressed by the dimensionless parameter $2\beta V = 2V/k_B T$ that forms the argument of the Bessel functions in Eq. (12).

Basic features common to the theoretical curves presented include an Ohmic, linear increase of drift velocity at low fields and a decrease at very large fields. For low temperatures ($k_B T \ll 2V$) the peak separat-

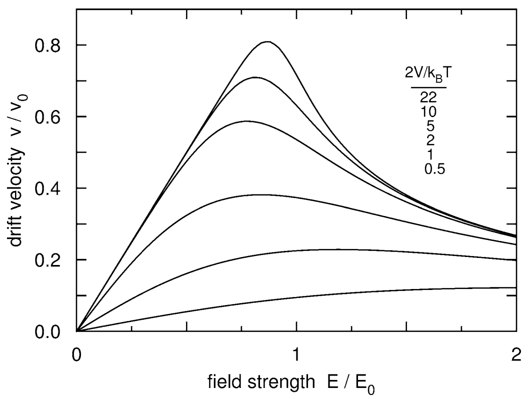

Fig. 1. Drift velocity v/v_0 as a function of applied field strength E/E_0 for different temperatures as labeled by the parameter $2V/k_B T$.

ing the field dependence in these two regimes is rather pronounced. At higher temperatures ($k_B T \gtrsim 2V$) the peak is broadened, and a substantial region develops where the drift velocity is nearly flat.

The position of the field where the maximum velocity is achieved is a complicated function of the temperature, occurring near E_0 for very low temperatures, moving to lower fields as the temperature increases, and then ultimately moving out to large fields for very high temperatures. At high temperatures the peak field appears to be a linear function of temperature.

In summary, we have investigated a model of carrier motion in narrow band materials which is simple enough to allow an exact solution, including the nonlinear field effects. A general tendency towards velocity saturation with field is not obtained in this model. Rather, the model predicts that the drift velocity should ultimately reach a peak and then decrease with increasing field. The regime of decreasing drift velocity with field arises, in this model, due to the fact that there is a minimum scattering time associated with the interaction with optical and/or acoustic phonons. At low fields, as the field increases, initially the particle distribution in k space is shifted more and more in the direction of the field and leads, therefore, to a drift velocity that increases with field. Ultimately, however, the field is able to drive the wavevector of the particle across the Brillouin zone and back (via Umklapp) into regions where the group velocity is negative. At some point the smearing out of the distribution throughout the Brillouin zone is more effective in decreasing the average drift velocity than is the increase associated with the the net displacement of the centroid of the distribution along the field direction.

As we have observed above, although the real-space Fokker–Planck equation (3) studied in the microwave heating problem is formally equivalent to the momentum space equation (1), it leads to different expressions for the steady-state particle velocity (cf. Eqs. (6) and (7)), due to the different physical basis behind each problem. Expressions required for the study of nonlinear field effects associated with Eq. (3) were given by KK in Ref. [4], but only linear versions were emphasized. Using the results of the present investigation, however, it is possible to obtain an exact expression for the drift velocity associated with the spatial Fokker–Planck equation (3), as well. Indeed, with the correspondence already outlined, it is straightforward

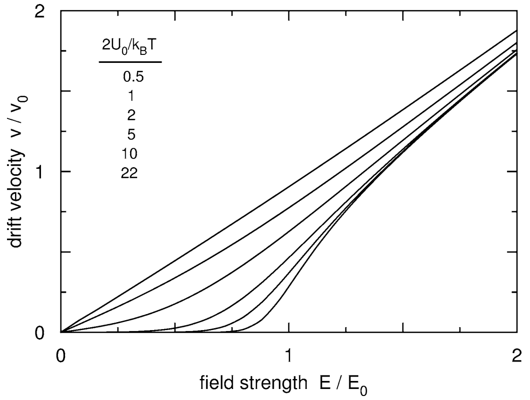

Fig. 2. Drift velocity v/v_0 for the classical problem of Eq. (3) as a function of applied field strength E/E_0, where $v_0 = 4U_0\pi/m\gamma\ell$ and $E_0 = 2m\gamma/q\ell\pi$, for different temperatures as labeled by the parameter $2U_0/k_B T$.

from Eqs. (7) and (11) to derive the following exact result:

$$\left\langle \frac{dx}{dt} \right\rangle = \frac{2}{\beta m\gamma\ell} \times \frac{\sinh(\beta qE\ell/2m\gamma)}{I_{-i\beta qE\ell/2\pi m\gamma}(2\beta U_0)\, I_{i\beta qE\ell/2\pi m\gamma}(2\beta U_0)} \tag{13}$$

for the mean particle velocity in the nonlinear diffusion problem of KK. This expression gives rise for large fields to a drift velocity that linearly increases with field (see Fig. 2) or, equivalently, to a mobility that saturates at high fields, as was noted in an earlier numerical analysis [6]. The effect of temperature for this classical system is opposite to that of the quantum system in Fig. 1: note the opposite ordering with temperature of the curves shown in the two figures. Despite the difference in appearance of Figs. 1 and 2, it is interesting to note that essentially much of the same mathematics applies to entirely different problems: quantum mechanical motion in a band, which is periodic in k-space, and classical motion in a potential, which is periodic in real space.

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