Effective diffusion coefficient for two-band systems

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The effective longitudinal diffusion coefficient for two-band systems is determined. Emphasis is put on the nonlinear transport regime realized at high electric fields. Particular results are obtained for bipolar transport in two-band semiconductors and vertical transport in semiconductor superlattices. An additional contribution to the effective diffusion coefficient is identified, which results from different drift velocities in the respective bands (minibands). © *2005 American Institute of Physics*. [DOI: 10.1063/1.1863435]

Diffusion coefficients enter the famous drift-diffusion equations of semiconductor physics and are, therefore, important quantities that characterize electronic transport. The study of fluctuation phenomena in nonequilibrium systems has been demonstrated to be a powerful tool of semiconductor diagnostics. The fluctuation-diffusion relation proposed by Price[1] connects the tensor of spectral densities of current fluctuations in a uniform and stationary electron gas with the one of the electron diffusion coefficient.[2] This relation has been proven to be very useful in providing information on hot-electron diffusion from noise measurements.

From a theoretical point of view, the calculation of hot-electron noise and diffusivity possess an independent task within a kinetic theory beyond the determination of the drift velocity. There are still challenging problems to be addressed. This refers in particular to the microscopic description of quantum diffusion in multiband (multiminiband) semiconductors,[3] the application of this approach to the bipolar transport,[4] and the diffusion in heterostructures,[5] as well as superlattices.[6] An essential step in such a study is the identification of the experimentally relevant diffusion coefficient.

To illustrate our approach, first let us treat a simple textbook example for a two-band system, namely the almost intrinsic semiconductor material, in which the perturbed electron and hole concentrations ($n=n_0+\Delta n$ and $p=p_0+\Delta p$) weakly deviate from the respective equilibrium concentrations (n_0 and p_0). Unless $\Delta n=\Delta p$, a space-charge is set up giving rise to quite large internal electric fields. Combining the equation of continuity with Poisson's equation and restricting the spatial dependence to the field direction, we obtain[7]

$$\frac{\partial \Delta n}{\partial t}=\mu_e E\frac{\partial \Delta n}{\partial x}+D_e\frac{\partial^2 \Delta n}{\partial x^2}-\frac{\Delta n}{\tau_n}-\frac{\sigma_e}{\varepsilon}(\Delta n-\Delta p), \tag{1}$$

$$\frac{\partial \Delta p}{\partial t}=-\mu_h E\frac{\partial \Delta p}{\partial x}+D_h\frac{\partial^2 \Delta p}{\partial x^2}-\frac{\Delta p}{\tau_p}+\frac{\sigma_h}{\varepsilon}(\Delta n-\Delta p), \tag{2}$$

where $\sigma_e=en\mu_e$ and $\sigma_h=ep\mu_h$ denote the electron and hole conductivities, respectively, which do not depend on the electric field in the Ohmic regime. Similarly, $D_e(D_h)$, $\mu_e(\mu_h)$, and $\tau_n(\tau_p)$ denote the diffusion coefficient, mobility, and scattering time of electrons (holes), respectively. The electric field is expressed by E, whereas ε denotes the dielectric constant. Please note that the drift velocities of electrons and holes are given by $v_e=-\mu_e E$ and $v_h=\mu_h E$. Equations (1) and (2) can be easily solved by applying a Laplace and Fourier transformation with respect to the time dependence t and the spatial coordinate x, respectively. We analyze the pole structure of the solution by treating the limit of long wavelengths ($q\to 0$) and small Laplace variables ($s\to 0$). Focusing on almost intrinsic materials ($\tau_n\approx\tau_p$) and keeping in the expansion of the pole only contributions up to second order in q, we are able to identify the effective drift velocity

$$v_{\text{eff}}=\frac{\mu_h\sigma_e-\mu_e\sigma_h}{\sigma_e+\sigma_h}E=\frac{n-p}{n/\mu_h+p/\mu_e}E, \tag{3}$$

and the effective diffusion coefficient

$$D_{\text{eff}}=\frac{D_e\sigma_h+D_h\sigma_e}{\sigma_e+\sigma_h}+\varepsilon\frac{\sigma_e\sigma_h}{(\sigma_e+\sigma_h)^3}[(\mu_e+\mu_h)E]^2. \tag{4}$$

The result in Eq. (3) represents the known expression for the drift velocity of an electron-hole excitation.[7] This quantity may change its sign depending on the character of the minority carrier concentration. In contrast, we encounter on the right-hand side of Eq. (4) an additional contribution to the effective diffusion coefficient, which is proportional to E^2 and which is not related to the quantities $D_{e,h}$ of single bands. This excess contribution to the diffusion coefficient describes spreading of an initial carrier inhomogeneity due to different drift mobilities of electrons and holes. When the Einstein relation becomes applicable, the additional contribution in Eq. (4) can be used to introduce an effective electron temperature T_{eff},

$$D_{\text{eff}}=\frac{k_B T_{\text{eff}}}{e}\frac{n+p}{n/\mu_h+p/\mu_e}, \tag{5}$$

with

$$k_B T_{\text{eff}}=k_B T+\varepsilon\frac{np}{n+p}\left[\frac{(1/\mu_e+1/\mu_h)E}{n/\mu_h+p/\mu_e}\right]^2. \tag{6}$$

Without the second term in Eq. (4), we have $T_{\text{eff}}=T$. By a simultaneous measurement of the field-dependent concentrations n and p, the mobilities μ_e and μ_h, and the effective diffusion coefficient D_{eff}, the prediction of an additional diffusion mechanism can be verified and qualitatively deter-

mined from Eqs. (5) and (6) by comparing the temperature T with the parameter T_{eff}.

The calculational scheme outlined above is not only applicable for bipolar systems, but can also be used for unipolar transport. Let us determine the effective diffusion coefficient induced by interminiband transitions in a semiconductor superlattice of period d. Assuming a constant internal electrical field, the carrier concentration n_ν of the νth miniband is calculated from the continuity equation

$$\frac{\partial n_\nu(r,t)}{\partial t} = D_{\nu\nu'}\Delta n_{\nu'} - \mathrm{v}_{\nu\nu'}\nabla \mathrm{n}_{\nu'} + \omega_{\nu\nu'}\mathrm{n}_{\nu'}, \tag{7}$$

with $D_{\nu\nu'}$ and $v_{\nu\nu'}$ being the diffusion coefficients and drift velocities, respectively. Carrier generation and recombination are characterized by $\omega_{\nu\nu'}$. As described above, we treat a one-dimensional two-miniband system and perform a Laplace and Fourier transformation with respect to the variables t and x, respectively. The resulting set of linear equations

$$\begin{aligned} -sn_1(q,s) &= q^2D_{11}n_1 + q^2D_{12}n_2 + iqv_{11}n_1 + iqv_{12}n_2 \\ &\quad + n_1/\tau_{12} - n_2/\tau_{21} - n_1(q,t=0), \\ -sn_2(q,s) &= q^2D_{21}n_1 + q^2D_{22}n_2 + iqv_{21}n_1 + iqv_{22}n_2 \\ &\quad - n_1/\tau_{12} + n_2/\tau_{21} - n_2(q,t=0), \end{aligned}$$

in which we introduced the initial carrier densities $n_{1,2}(q,t=0)$ and the interminiband scattering times τ_{12} and τ_{21}, is easily solved. The solution is treated in the long-wavelength limit ($q\to 0$) and for $s\to 0$. We obtain

$$n_{1,2}(q,s) = \frac{F_{1,2}n_{1,2}(q,t=0)}{s + iqv_{\mathrm{eff}} + q^2D_{\mathrm{eff}}} \tag{8}$$

with miniband occupation numbers

$$F_1 = \frac{\tau_{12}}{\tau_{12}+\tau_{21}}, \quad F_2 = \frac{\tau_{21}}{\tau_{12}+\tau_{21}} \tag{9}$$

and the effective drift velocity

$$v_{\mathrm{eff}} = \sum_{\nu,\nu'} v_{\nu\nu'}F_{\nu'}. \tag{10}$$

v_{eff} has the meaning of an averaged value of the drift velocities $v_{\nu\nu'}$. The effective diffusion coefficient in Eq. (8) is expressed by

$$\begin{aligned} D_{\mathrm{eff}}(E) &= \sum_{\nu,\nu'} D_{\nu\nu'}(E)F_{\nu'} + \frac{(\tau_{12}\tau_{21})^2}{(\tau_{12}+\tau_{21})^3}\{[v_{11}(E) \\ &\quad - v_{22}(E)]^2 - [v_{12}(E) - v_{21}(E)]^2\}. \end{aligned} \tag{11}$$

This field-dependent quantity encompasses an additional contribution to the diffusion coefficient, which vanishes whenever the diagonal and off-diagonal elements of the velocity tensor match each other ($v_{11}=v_{22}$ and $v_{12}=v_{21}$). For a superlattice exhibiting negative differential conductivity, the second term on the right-hand side of Eq. (11) may give rise to a nonmonotonous field dependence. This contribution to the diffusion coefficient has a simple physical origin. For the time being, let us neglect intrinsic diffusion $D_{\nu\nu'}=0$ and interminiband transitions $\omega_{\nu\nu'}=0$. We consider the evolution of a carrier ensemble composed of particles in both minibands, which has initially at $t=0$ a δ-functionlike character. Under the condition $v_{11}>v_{22}$ and $v_{12}=v_{21}=0$, the peak splits into two parts moving with different velocities by maintaining their δ-functionlike shapes. Next, we allow interminiband transitions ($\omega_{\nu\nu'}\neq 0$), which leads to a spreading of the carrier packets. Transitions between the minibands cause fast moving particles to move slowly and vice versa. Consequently, the whole interval $\Delta x=(v_{11}-v_{22})t$ becomes occupied by carriers. When a sufficiently long time t has passed, the particles accumulate at $v_{\mathrm{eff}}t$, which is a point inside the interval Δx ($v_{22}<v_{\mathrm{eff}}<v_{11}$). From the exact solution of Eq. (7), the width Δx_p of the packet can be estimated. We obtain

$$\Delta x_p \approx \sqrt{t}\frac{\tau_{12}\tau_{21}}{(\tau_{12}+\tau_{21})^{3/2}}(v_{11}-v_{22}),$$

which, according to the definition of the diffusion coefficient $\Delta D=(\Delta x_p)^2/t|_{t\to\infty}$, reproduces the additional contribution on the right-hand side of Eq. (11).

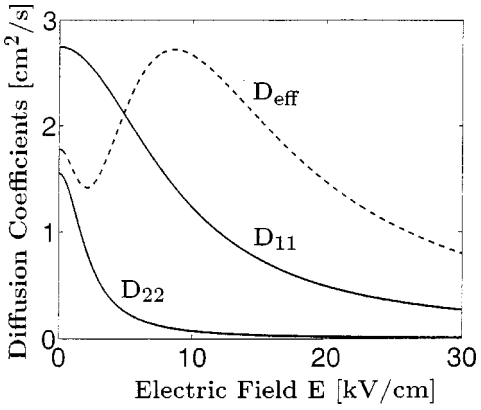

FIG. 1. Electric field dependence of the effective diffusion coefficient D_{eff} (dashed line) compared with the partial contributions D_{11} and D_{22} (solid lines) of the minibands. For the calculation, we used: $d=15$ nm, $\Delta_1=3.85$ meV, $\Delta_2=21.26$ meV, $\tau_1=0.2$ ps, $\tau_2=0.05$ ps, and $T=300$ K. The interminiband scattering times are assumed to be given by $\tau_{21}=0.1$ ns and $\tau_{12}=\tau_{21}\exp(\varepsilon_g/k_BT)$ with $\varepsilon_g=74.5$ meV.

In order to illustrate qualitative features of the field dependence of the effective diffusion coefficient, we now discuss a numerical example using the simple Esaki–Tsu model for the miniband drift velocities[8]

$$v_{\nu\nu} = \frac{\Delta_\nu d}{2\hbar}\frac{\Omega\tau_\nu}{1+(\Omega\tau_\nu)^2}\frac{I_1(\Delta_\nu/(2k_BT))}{I_0(\Delta_\nu/(2k_BT))}F_\nu, \tag{12}$$

and the corresponding diffusion coefficients

$$D_{\nu\nu} = \frac{v_{\nu\nu}d}{2}\coth\left(\frac{\hbar\Omega}{2k_BT}\right), \tag{13}$$

which are valid both in the ultraquantum limit and the Ohmic regime.[3] In Eqs. (12) and (13), $\Omega=eEd/\hbar$ denotes the Bloch frequency, while Δ_ν and τ_ν represent the widths of the superlattice minibands and the intraminiband scattering times, respectively. I_0 and I_1 are modified Bessel functions. As an example let us treat a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice, which is composed of 10 nm thick GaAs quantum wells separated by 5 nm thick AlGaAs barriers. Inserting the corresponding miniband widths ($\Delta_1=3.85$ meV, $\Delta_2=21.26$ meV) and typical intrasubband scattering times ($\tau_1=0.2$ ps, $\tau_2=0.05$ ps) into Eq. (11), we obtain a nonmonotonous electric field dependence of the effective diffusion coefficient D_{eff} as illustrated in Fig. 1 by the dashed line. A maximum in D_{eff} at $E\approx 8.65$ kV/cm and a minimum, which occurs for $v_{11}(E)$

$=v_{22}(E)$, are due to the additional, velocity-dependent diffusion contribution on the right-hand side of Eq. (11). The nonmonotonous field dependence of D_{eff} is observed, when the drift velocities of carriers in different subbands strongly differ from each other for certain field strengths. This conclusion is qualitatively confirmed by experimental results obtained on GaAs/(Ga,Al)As quantum wells[5] and superlattices.[6] A more quantitative comparison of our theoretical result with experimental data[5,6] would require a detailed consideration of the energy spectrum and scattering mechanisms, which goes beyond the scope of this paper.

In summary, we considered the effective longitudinal diffusion coefficient of two-band models in the nonlinear transport regime and identified an additional contribution, which results from different drift velocities in the two bands (minibands). In particular, for heterostructures and semiconductor superlattices, maxima and minima are expected to appear in the electric-field dependence of the diffusion coefficient, which can be determined on the basis of the Price relation by measuring the noise temperature. Measurements of the transient transport[9] provide a different possibility to experimentally detect the predicted additional contribution to the diffusion coefficient.

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