Zener antiresonance in the quantum diffusion of semiconductor superlattices

2004 J. Phys.: Condens. Matter 16 4441

(http://iopscience.iop.org/0953-8984/16/25/005)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) 4441–4454 PII: S0953-8984(04)76960-X

Zener antiresonance in the quantum diffusion of semiconductor superlattices

P Kleinert[1] **and V V Bryksin**[2]

[1] Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany
[2] Physical Technical Institute, Politekhnicheskaya 26, 194021 St Petersburg, Russia

Received 26 February 2004
Published 11 June 2004
Online at stacks.iop.org/JPhysCM/16/4441
doi:10.1088/0953-8984/16/25/005

Abstract

The well-known theory of quantum transport is extended to an approach that allows the description of quantum diffusion in strongly biased multi-band semiconductors and semiconductor superlattices. The longitudinal diffusion coefficient is identified and expressed by a quantity that satisfies a different quantum-kinetic equation than the carrier distribution function, from which the drift velocity is calculated. Results are obtained for a simple two-band model at the interband (intersubband) tunnelling resonance. In contrast to the drift velocity, the diffusion coefficient may exhibit a Zener antiresonance.

1. Introduction

Recently, there has been considerable theoretical and experimental progress in studying electric-field-induced intersubband transitions in modulation-doped semiconductor heterostructures. Following the early suggestion of Kazarinov and Suris [1], mid-infrared emitters, in particular quantum cascade lasers, have been studied and routinely fabricated (for a review, see, for example [2]). These devices exploit intersubband transitions between conduction band states of biased heterostructures. Population inversion and gain are observed due to a field-mediated carrier redistribution, in which intersubband tunnelling plays the most important role. The extensive technological efforts have been accompanied by many theoretical studies of field-induced intersubband effects and its influence on quantum transport. Unfortunately, these studies have not been accomplished to the same extent for fluctuation phenomena in nonequilibrium multi-band systems. Treatments of this kind would additionally contribute to an understanding of the relationship between microscopic processes and their macroscopic manifestation. It is well known that noise and diffusion of hot carriers are sensitive to all microscopic details and provide complementary information about high-field properties of heterostructures.

Except for complete numerical approaches, there is, to our knowledge, no systematic treatment of diffusion phenomena in strongly biased semiconductors. We fill this gap by

0953-8984/04/254441+14$30.00

addressing the influence of field-induced intersubband transitions on the longitudinal diffusion coefficient and the related noise properties. Considering this interesting problem, at first glance a question arises: Is it really necessary to develop a completely new theory for the field-dependent diffusion coefficient, or can we benefit from achievements made in ordinary transport theory for the current density? Because of the famous Einstein relation, which is valid at low electric-field strengths, it is tempting to assume that the mobility (drift velocity) as well as the diffusion coefficient are always governed by the same statistical quantity, namely the nonequilibrium carrier distribution function $f(\mathbf{k}, t)$. To our surprise, the validity of such a conclusion has to be strongly questioned. Studies of the stationary transport in bulk systems rely on the description of a uniform carrier distribution far away from the contacts. This situation has to be compared with the definition of the diffusion coefficient in terms of spreading, in which the evolution of 'excess carriers' is monitored. A description of spreading requires the treatment of the occupation probability $f(\mathbf{k}, \mathbf{r}, t)$, which depends not only on the quasi-momentum $\mathbf{k}$ at a given time t, but also on the position $\mathbf{r}$ of the carrier or its related wavevector $\boldsymbol{\kappa}$ $[f(\mathbf{k}, \boldsymbol{\kappa}, t)]$. Strictly speaking, a rigorous kinetic theory of diffusion processes in semiconductors starts by considering the spreading of an initial δ-like inhomogeneity of the carrier density. The special choice of a δ-like inhomogeneity is not restrictive for the steady state. Such an approach avoids the artificial and unphysical distinction between excess carriers and carriers of a uniform background, as proposed in [3]. In our description of diffusion effects under high-field conditions, it is not the distribution function $f(\mathbf{k}, t)$ itself, but the quantity $\nabla_{\boldsymbol{\kappa}} f(\mathbf{k}, \boldsymbol{\kappa}, t)|_{\boldsymbol{\kappa}=0}$ that is of fundamental importance. This function satisfies a different kinetic equation than the distribution function $f(\mathbf{k}, t)$, from which the drift velocity is obtained. We shall arrive at the conclusion that for arbitrary electric-field strengths, the drift velocity and the diffusion coefficient are not related to each other by the simple Einstein relation. Rather, it is necessary to derive and solve a specific kinetic equation for a novel quantity, when studying diffusion phenomena in strong electric fields. Recently, such an approach has been proposed for one-band systems [4]. We shall extend this scheme to multi-band (multi-subband) models, while focusing on interband (intersubband) tunnelling.

2. Basic theory

Most theoretical approaches perform numerical Monte Carlo simulations [3, 5–7] to determine the frequency dispersion of the differential mobility, diffusivity, and noise as a function of an applied electric field of arbitrary strength. In addition, the physical interpretation of numerical data is provided by analytical formulae derived from complementary theoretical approaches based on the Boltzmann equation [6]. We shall derive an alternative, rigorous quantum-mechanical approach to study the field-dependent longitudinal diffusion coefficient of multi-band systems, valid for a nondegenerate electron gas described within the one-particle picture. Our starting point constitutes the 'spreading method', which allows a phenomenological definition of the diffusion coefficient. Within this approach, Fick's law is used to determine the conditional probability $P_{\nu\nu'}(\mathbf{r} - \mathbf{r}_0|t)$ to find an electron at a given time t at the lattice site $\mathbf{r}$ in the ν'th band, provided that it occupied the state $\mathbf{r}_0$, ν' at an earlier time $t = 0$. The Laplace-transformed probability propagator satisfies the phenomenological conservation law

$$sP_{\nu\nu'}(\mathbf{r} - \mathbf{r}_0|s) = \delta_{\nu\nu'}\delta(\mathbf{r} - \mathbf{r}_0) + \sum_{\mu} \frac{\partial}{\partial z} P_{\nu\mu}(\mathbf{r} - \mathbf{r}_0|s) v_{\mu\nu'}(s)$$
$$+ \sum_{\mu} \frac{\partial^2}{\partial z^2} P_{\nu\mu}(\mathbf{r} - \mathbf{r}_0|s) D_{\mu\nu'}(s) + \sum_{\mu} P_{\nu\mu}(\mathbf{r} - \mathbf{r}_0|s)\omega_{\mu\nu'}(s), \tag{1}$$

which is used to define macroscopic observables. The spatial changes of P are restricted to the z axis, which is oriented parallel to the electric field $\mathbf{E}$. The components of the drift velocity, the diffusion coefficient, and the rates for carrier generation and recombination are denoted by $v_{\nu\mu}(s)$, $D_{\nu\mu}(s)$, and $\omega_{\nu\mu}(s)$, respectively. For simplicity, we consider an initial δ-like 'excess carrier' distribution. This special choice does not put any restrictions on the steady state.

As seen from equation (1), the transport coefficients are expressed by the moments of the conditional probability propagator. This quantity results from a Bethe–Salpeter equation, which is closed when formulated for more general objects that depend on four band indices $P^{\nu_1\nu_3}_{\nu_2\nu_4}$ (with $P_{\nu\nu'} \equiv P^{\nu\nu'}_{\nu\nu'}$) (see [8]). In Fourier space, the moments of the generalized probability propagator are defined as

$$^{(n)}P^{\nu_1\nu_3}_{\nu_2\nu_4}(s) = \sum_{\mathbf{k},\mathbf{k}'} {}^{(n)}P^{\nu_1\nu_3}_{\nu_2\nu_4}(\mathbf{k},\mathbf{k}'|s) = \sum_{\mathbf{k},\mathbf{k}'} \frac{\partial^n}{\partial\kappa_z^n} P^{\nu_1\nu_3}_{\nu_2\nu_4}(\mathbf{k},\mathbf{k}',\boldsymbol{\kappa}|s)|_{\kappa=0}. \tag{2}$$

Let us continue by deriving the set of equations for the lowest-order moments by multiplying equation (1) by $(z - z_0)^n$ and by an integration by parts. The result

$$s\,{}^{(0)}P_{\nu\nu'}(s) = \delta_{\nu\nu'} + \sum_{\mu} {}^{(0)}P_{\nu\mu}(s)\omega_{\mu\nu'}(s), \tag{3}$$

$$s\,{}^{(1)}P_{\nu\nu'}(s) = \mathrm{i}\sum_{\mu} {}^{(0)}P_{\nu\mu}(s)v_{\mu\nu'}(s) + \sum_{\mu} {}^{(1)}P_{\nu\mu}(s)\omega_{\mu\nu'}(s), \tag{4}$$

$$s\,{}^{(2)}P_{\nu\nu'}(s) = \sum_{\mu} {}^{(2)}P_{\nu\mu}(s)\omega_{\mu\nu'}(s) + 2\mathrm{i}\sum_{\mu} {}^{(1)}P_{\nu\mu}(s)v_{\mu\nu'}(s) - 2\sum_{\mu} {}^{(0)}P_{\nu\mu}(s)D_{\mu\nu'}(s), \tag{5}$$

provides the basis for our microscopic approach to calculate the transport coefficients. According to [9], the conditional probability propagator P is expressed by the vacuum expectation value

$$P^{\alpha_1\alpha_3}_{\alpha_2\alpha_4}(s) = \frac{1}{Z}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st}\,\mathrm{Sp}_{\mathrm{ph}}\{\mathrm{e}^{-H_{\mathrm{ph}}/k_{\mathrm{B}}T}\langle 0|a_{\alpha_2}\mathrm{e}^{\mathrm{i}Ht/\hbar}a^\dagger_{\alpha_4}a_{\alpha_3}\mathrm{e}^{-\mathrm{i}Ht/\hbar}a^\dagger_{\alpha_1}|0\rangle\}, \tag{6}$$

averaged over the vibrational subsystem described by the Hamiltonian H_{ph}. For our general approach, it is not necessary to specify the phonon contribution. Fermionic creation and annihilation operators classified by quantum numbers α_i are denoted by $a^\dagger_{\alpha_i}$ and a_{α_i}. The partition function is given by $Z = \mathrm{Tr}\exp(-H_{\mathrm{ph}}/k_{\mathrm{B}}T)$. Please note that the total Hamiltonian encompasses the free electronic and phononic part as well as the interaction term H_{int} and the contribution of the electric field. By applying an equation-of-motion analysis, the kinetic equation for the probability propagator P is derived in the similar way as was done in [4]. We do not take into account the Coulomb interaction between the carriers, and focus, therefore, on the one-electron picture. This is the main approximation in our approach. Within the $\mathbf{k}$-representation, we obtain the following kinetic equation (see [8]):

$$\begin{aligned}\sum_{\nu,\nu'}[s\delta_{\nu_3\nu'}\delta_{\nu\nu_4} + \hat{I}^{\nu'\nu_3}_{\nu\nu_4}(\mathbf{k}',\boldsymbol{\kappa})]P^{\nu_1\nu'}_{\nu_2\nu}(\mathbf{k},\mathbf{k}',\kappa|s) &= \delta_{\mathbf{k},\mathbf{k}'}\delta_{\nu_1\nu_3}\delta_{\nu_2\nu_4}\\ &+ \sum_{\mathbf{k}_1}\sum_{\mu,\mu'} P^{\nu_1\mu'}_{\nu_2\mu}(\mathbf{k},\mathbf{k}_1,\boldsymbol{\kappa}|s)W^{\mu'\nu_3}_{\mu\nu_4}(\mathbf{k}_1,\mathbf{k}',\boldsymbol{\kappa}|s),\end{aligned} \tag{7}$$

in which the field-dependent scattering probability W collects scattering-in and scattering-out contributions for all intra- and interband transitions. Details of the band structure enter the operator

$$\begin{aligned}\hat{I}^{\nu'\nu_3}_{\nu\nu_4}(\mathbf{k}',\boldsymbol{\kappa}) &= \left\{\frac{\mathrm{i}}{\hbar}\left[\varepsilon_{\nu_3}\left(\mathbf{k}' - \frac{\boldsymbol{\kappa}}{2}\right) - \varepsilon_{\nu_4}\left(\mathbf{k}' + \frac{\boldsymbol{\kappa}}{2}\right)\right] + \frac{e\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}'}\right\}\delta_{\nu_3\nu'}\delta_{\nu\nu_4}\\ &+ \frac{\mathrm{i}}{\hbar}e\mathbf{E}\cdot\left[\mathbf{Q}_{\nu\nu_4}\left(\mathbf{k}' + \frac{\kappa}{2}\right)\delta_{\nu'\nu_3} - \mathbf{Q}_{\nu_3\nu'}\left(\mathbf{k}' - \frac{\kappa}{2}\right)\delta_{\nu\nu_4}\right],\end{aligned} \tag{8}$$

in which $\varepsilon_\nu(\mathbf{k})$ denotes the tight-binding dispersion relation of the νth subband and $\mathbf{Q}_{\nu\nu'}(\mathbf{k})$ the dipole matrix elements. Within the $\mathbf{k}$ representation of the Hamiltonian, the electric field $\mathbf{E}$ explicitly enters the kinetic equation (7). In this picture, the off-diagonal elements of the propagator P become relevant, when tunnelling plays an important role.

From equation (7), the following sum rule is derived:

$$s\sum_{\mathbf{k}'}\sum_{\nu'} P^{\nu_1\nu'}_{\nu_2\nu'}(\mathbf{k},\mathbf{k}',\boldsymbol{\kappa}=0|s) = \delta_{\nu_1\nu_2}, \tag{9}$$

which is a consequence of our one-electron approach (in which $\sum_\alpha a^\dagger_\alpha a_\alpha = 1$ is satisfied). According to the set of equations (3)–(5), the transport coefficients are obtained from the moments of the probability propagator P, which is calculated on the basis of a microscopic theory. The kinetic equations for these quantities are easily derived from the definition in equation (2) and from (7). By simple algebraic manipulations, we confirm that the formal solutions of the equations for the lowest-order moments are given by

$$\begin{aligned} {}^{(1)}P^{\nu_1\nu_3}_{\nu_2\nu_4}(\mathbf{k},\mathbf{k}'|s) = \sum_{\mathbf{k}_1}\sum_{\mu,\mu'}\Bigg\{ & -\sum_{\nu,\nu'} {}^{(1)}\hat{I}^{\nu'\mu'}_{\nu\mu}(\mathbf{k}_1)\, {}^{(0)}P^{\nu_1\nu'}_{\nu_2\nu}(\mathbf{k},\mathbf{k}_1|s) \\ & + \sum_{\mathbf{k}_2}\sum_{\nu_1',\nu_2'} {}^{(0)}P^{\nu_1\nu_1'}_{\nu_2\nu_2'}(\mathbf{k},\mathbf{k}_2|s)\, {}^{(1)}W^{\nu_1'\mu'}_{\nu_2'\mu}(\mathbf{k}_2,\mathbf{k}_1|s)\Bigg\}\, {}^{(0)}P^{\mu'\nu_3}_{\mu\nu_4}(\mathbf{k}_1,\mathbf{k}'|s), \end{aligned} \tag{10}$$

$$\begin{aligned} {}^{(2)}P^{\nu_1\nu_3}_{\nu_2\nu_4}(\mathbf{k},\mathbf{k}'|s) = \sum_{\mathbf{k}_1}\sum_{\mu,\mu'}\Bigg\{ & -2\sum_{\nu,\nu'} {}^{(1)}\hat{I}^{\nu'\mu'}_{\nu\mu}(\mathbf{k}_1)\, {}^{(1)}P^{\nu_1\nu'}_{\nu_2\nu}(\mathbf{k},\mathbf{k}_1|s) \\ & + 2\sum_{\mathbf{k}_2}\sum_{\nu_1',\nu_2'} {}^{(1)}P^{\nu_1\nu_1'}_{\nu_2\nu_2'}(\mathbf{k},\mathbf{k}_2|s)\, {}^{(1)}W^{\nu_1'\mu'}_{\nu_2'\mu}(\mathbf{k}_2,\mathbf{k}_1|s) \\ & + \sum_{\mathbf{k}_2}\sum_{\nu_1',\nu_2'} {}^{(0)}P^{\nu_1\nu_1'}_{\nu_2\nu_2'}(\mathbf{k},\mathbf{k}_2|s)\, {}^{(2)}W^{\nu_1'\mu'}_{\nu_2'\mu}(\mathbf{k}_2,\mathbf{k}_1|s) \\ & - \sum_{\nu,\nu'} {}^{(2)}\hat{I}^{\nu'\mu'}_{\nu\mu}(\mathbf{k}_1)\, {}^{(0)}P^{\nu_1\nu'}_{\nu_2\nu}(\mathbf{k},\mathbf{k}_1|s)\Bigg\}\, {}^{(0)}P^{\mu'\nu_3}_{\mu\nu_4}(\mathbf{k}_1,\mathbf{k}'|s), \end{aligned} \tag{11}$$

in which the abbreviations

$${}^{(n)}\hat{I}^{\nu'\mu'}_{\nu\mu}(\mathbf{k}) = \frac{\partial^n}{\partial\kappa_z^n}\hat{I}^{\nu'\mu'}_{\nu\mu}(\mathbf{k},\boldsymbol{\kappa})|_{\kappa=0} \tag{12}$$

are used. In a similar manner, the quantities ${}^{(n)}W$ are defined. Starting from these results, expressions for the drift velocity and the diffusion coefficient are derived using the same computational scheme.

2.1. Drift velocity

In this section, we shall show that, within the one-particle picture of a nondegenerate electron gas, the exact transport theory proposed in [8] is reproduced by our approach. The biased electron ensemble is assumed gradually to approach the steady state, which is reached after sufficiently long time ($t \to \infty$). We shall treat this limit in Laplace space by calculating all quantities in the limit $s \to 0$. The expression for the drift velocity is obtained from equations (3) and (4). First, we note that according to equations (3) and (9), the elements $\omega_{\nu\mu}$ of the matrix, which characterize carrier generation and recombination, satisfy the sum rule $\sum_\mu \omega_{\nu\mu}(s) = 0$. To elucidate the approach, we treat a two-band model, in which the structure of this matrix is identified. From the sum rule, we get

$$\hat{\omega} = \begin{pmatrix} -\omega_1 & \omega_1 \\ \omega_2 & -\omega_2 \end{pmatrix}, \tag{13}$$

which leads to $\det\hat{\omega} = 0$ and $\hat{\omega}^2 = (\omega_1 + \omega_2)\hat{\omega}$. To solve the matrix equation (3), we consider the inverse of the matrix $\hat{\sigma}(s) = s\hat{1} - \hat{\omega}(s)$ in the limit $s \to 0$:

$$\hat{\sigma}^{-1}(s) \overset{s\to 0}{\sim} \frac{1}{s}\frac{1}{\omega_1 + \omega_2}\begin{pmatrix}\omega_2 & \omega_1\\ \omega_2 & \omega_1\end{pmatrix} - \frac{\hat{\omega}}{(\omega_1+\omega_2)^2} = \frac{\hat{n}}{s} - \frac{\hat{\omega}}{(\omega_1+\omega_2)^2}. \tag{14}$$

The elements $n_{\nu\nu'}$ of the (density) matrix $\hat{n}$ introduced in equation (14) do not depend on the first index, and satisfy the sum rule

$$\sum_{\nu'} n_{\nu\nu'}(s) = 1. \tag{15}$$

Taking into account equation (4) in the limit $s \to 0$, the effective drift velocity of the multiband model is introduced by the equation

$$v_{\rm d} \equiv \sum_{\mu,\mu'} n_{\nu\mu}(s) v_{\mu\mu'}(s)|_{s\to 0} = -\mathrm{i}s^2 \sum_{\nu'}\sum_{\mathbf{k},\mathbf{k}'} {}^{(1)}P_{\nu\nu'}(\mathbf{k},\mathbf{k}'|s)|_{s\to 0}. \tag{16}$$

The physical interpretation of this quantity is given in the appendix. Because the right-hand side of equation (16) does not depend on the first index ν, an additional sum $(1/N_{\rm b})\sum_\nu(\cdots)$ can be inserted, with $N_{\rm b}$ being the number of subbands. Let us now express the drift velocity in equation (16) by the formal solution given in equation (10). A convenient physical picture for the drift velocity is obtained by replacing the quantity ${}^{(0)}P$ in equation (10) by the carrier distribution function

$$f_\mu^{\mu'}(\mathbf{k}|s) = s\sum_{\mathbf{k}'}\sum_{\nu} {}^{(0)}P_{\nu\mu}^{\nu\mu'}(\mathbf{k}',\mathbf{k}|s), \tag{17}$$

which according to equation (7) satisfies the kinetic equation

$$\begin{aligned}\left\{s + \frac{e\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}} + \frac{\mathrm{i}}{\hbar}[\varepsilon_{\nu'}(\mathbf{k}) - \varepsilon_\nu(\mathbf{k})]\right\} f_\nu^{\nu'}(\mathbf{k}|s) \\ + \frac{\mathrm{i}}{\hbar}e\mathbf{E}\cdot\sum_\mu[\mathbf{Q}_{\mu\nu}(\mathbf{k}) f_\mu^{\nu'}(\mathbf{k}|s) - \mathbf{Q}_{\nu'\mu}(\mathbf{k}) f_\nu^{\mu}(\mathbf{k}|s)] \\ = s\delta_{\nu\nu'} + \sum_{\mathbf{k}_1}\sum_{\mu,\mu'} f_\mu^{\mu'}(\mathbf{k}_1|s) W_{\mu\nu}^{\mu'\nu'}(\mathbf{k}_1,\mathbf{k}'|s).\end{aligned} \tag{18}$$

In the limit $s \to 0$, the quantum Boltzmann equation is recovered, in which the scattering probabilities $W_{\mu\nu}^{\mu'\nu'}$ depend on the electric field. The final expression for the drift velocity of the multi-subband system has the form

$$v_{\rm d}(s) = \frac{1}{N_{\rm b}}\sum_{\mathbf{k}}\sum_{\nu,\nu'} v_\nu^{\nu'}(\mathbf{k}|s) f_\nu^{\nu'}(\mathbf{k}|s), \tag{19}$$

which collects various intra- and interband contributions given by

$$v_\nu^{\nu'}(\mathbf{k}|s) = v_\nu(\mathbf{k})\delta_{\nu\nu'} - \frac{e\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}} Q_{\nu\nu'}(\mathbf{k}) - \mathrm{i}\sum_{\mathbf{k}'}\sum_\mu {}^{(1)}W_{\nu\mu}^{\nu'\mu}(\mathbf{k},\mathbf{k}'|s). \tag{20}$$

The third term on the right-hand side of equation (20) vanishes when the scattering part of the Hamiltonian $H_{\rm int}$ commutes with the dipole operator. This condition is satisfied when $H_{\rm int}$ does not depend on the velocity operator. Based on an alternative microscopic approach, the same set of equations was derived for the current density in [8].

2.2. Diffusion coefficient

The diffusion coefficient is calculated in the similar way as the drift velocity in the previous section. The definition of the effective longitudinal diffusion coefficient is based on the treatment of the long-wavelength limit as presented in the appendix. From the phenomenological consideration, we obtain

$$D_{zz} = -\frac{s^2}{2}\sum_{\nu'}\sum_{\mathbf{k},\mathbf{k}'} {}^{(2)}P_{\nu\nu'}(\mathbf{k},\mathbf{k}'|s) - \frac{1}{s}v_{\mathrm{d}}^2(s)|_{s\to 0}, \tag{21}$$

which provides the basis for our microscopic description. In this equation for the effective diffusion coefficient, the formal solution of equation (11) is inserted. Similar to the previous section, a specific function is introduced:

$$\varphi_\nu^{\nu'}(\mathbf{k}|s) = -\frac{v_{\mathrm{d}}(s)}{s} f_\nu^{\nu'}(\mathbf{k}|s) - \mathrm{i}s\sum_{\mathbf{k}}\sum_{\mu} {}^{(1)}P_{\mu\nu}^{\mu\nu'}(\mathbf{k},\mathbf{k}'|s), \tag{22}$$

which characterizes diffusion phenomena. From equations (11), (21), and (22), we obtain the general result

$$D_{zz}(s) = \frac{1}{N_{\mathrm{b}}}\sum_{\mathbf{k}}\sum_{\nu,\nu'} v_\nu^{\nu'}(\mathbf{k}|s)\varphi_\nu^{\nu'}(\mathbf{k}|s) - \frac{1}{2N_{\mathrm{b}}}\sum_{\mathbf{k}}\sum_{\nu,\nu'} f_\nu^{\nu'}(\mathbf{k}|s)\sum_{\mathbf{k}'\mu} {}^{(2)}W_{\nu\mu}^{\nu'\mu}(\mathbf{k},\mathbf{k}'|s), \tag{23}$$

in which the first term on the right-hand side has the same form as equation (16). According to equations (7) and (22), the new functions $\varphi_\nu^{\nu'}$ satisfy the quantum kinetic equation

$$\begin{aligned}
&\left\{s + \frac{e\mathbf{E}}{\hbar}\cdot\nabla_{\mathbf{k}} + \frac{\mathrm{i}}{\hbar}[\varepsilon_{\nu'}(\mathbf{k}) - \varepsilon_\nu(\mathbf{k})]\right\}\varphi_\nu^{\nu'}(\mathbf{k}|s)\\
&\qquad + \frac{\mathrm{i}}{\hbar}e\mathbf{E}\cdot\sum_{\mu}[\mathbf{Q}_{\mu\nu}(\mathbf{k})\varphi_\mu^{\nu'}(\mathbf{k}|s) - \mathbf{Q}_{\nu'\mu}(\mathbf{k})\varphi_\nu^{\mu}(\mathbf{k}|s)]\\
&\quad = \sum_{\mathbf{k}_1}\sum_{\mu,\mu'}\varphi_\mu^{\mu'}(\mathbf{k}_1|s)W_{\mu\nu}^{\mu'\nu'}(\mathbf{k}_1,\mathbf{k}'|s)\\
&\qquad + \sum_{\mathbf{k}_1}\sum_{\mu,\mu'} f_\mu^{\mu'}(\mathbf{k}_1|s)v_{\mu\nu}^{\mu'\nu'}(\mathbf{k}_1,\mathbf{k}'|s) - v_{\mathrm{d}}(s)\delta_{\nu\nu'}.
\end{aligned} \tag{24}$$

In contrast to equation (18), additional contributions appear on the right-hand side of equation (24), which are introduced by the velocity matrix

$$\begin{aligned}
v_{\mu\nu}^{\mu'\nu'}(\mathbf{k},\mathbf{k}'|s) &= \tfrac{1}{2}[v_\mu(\mathbf{k}) + v_{\mu'}(\mathbf{k})]\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mu'\nu'}\delta_{\mu\nu}\\
&\quad - \delta_{\mathbf{k}\mathbf{k}'}\frac{e\mathbf{E}}{\hbar}\cdot[\delta_{\mu'\nu'}\nabla_{\mathbf{k}}Q_{\mu\nu}(\mathbf{k}) + \delta_{\mu\nu}\nabla_{\mathbf{k}}Q_{\nu'\mu'}(\mathbf{k})] - \mathrm{i}\,{}^{(1)}W_{\mu\nu}^{\mu'\nu'}(\mathbf{k},\mathbf{k}'|s),
\end{aligned} \tag{25}$$

with

$$\sum_{\mathbf{k}\mu} v_{\nu\mu}^{\nu'\mu}(\mathbf{k}',\mathbf{k}|s) = v_\nu^{\nu'}(\mathbf{k}'|s). \tag{26}$$

The new functions $\varphi_\nu^{\nu'}(\mathbf{k})$ satisfy a completely different sum rule than the carrier distribution functions $f_\nu^{\nu'}(\mathbf{k})$, which are normalized to unity. From equations (16) and (22), we get

$$\sum_{\mathbf{k}}\sum_{\nu}\varphi_\nu^{\nu}(\mathbf{k}|s) = 0, \tag{27}$$

which is in accordance with the result of the one-band model [4, 10].

3. Application: two subbands

The general multi-band approach is now applied to a two-band system. We shall treat semiconductor superlattices (SLs) subject to a dc electric field applied parallel to the SL axis. As the SL period d turns out to be sufficiently large, high-field effects occur already at moderate field strengths. Field-induced intersubband tunnelling is the most interesting quantum effect in multi-subband SLs. These tunnelling transitions lead to an appreciable carrier redistribution and to a resonance peak in the carrier density (Zener resonance). Similar peculiarities due to tunnelling are expected to appear in quantum diffusion. According to our general discussion, we should not be surprised to find peculiarities in quantum diffusion under high-field conditions. It is not clear whether quantum diffusion and quantum transport behave in the same way. To illustrate the main steps of our approach, let us first summarize the calculation of the drift velocity.

3.1. Drift velocity

In this section, the semiclassical intrasubband and quantum-mechanical tunnelling contribution to the drift velocity are calculated for an SL with two subbands. In order to introduce the notation, we present the main steps of previous calculations [11] to keep the paper self-contained. The drift velocity will be calculated for a two-band SL model with constant dipole matrix elements and with an interaction part H_{int} of the Hamiltonian that commutes with the dipole operator. Performing an integration by parts in equation (19), we obtain

$$v_{\text{d}} = -\frac{1}{\hbar N_{\text{b}}} \sum_{\mathbf{k}} \sum_{\nu} \epsilon_{\nu}(k_z) \frac{\partial}{\partial k_z} f_{\nu}^{\nu}(\mathbf{k}) = v_{\text{d}}^{(\text{s})} + v_{\text{d}}^{(\text{t})}, \tag{28}$$

in which $\epsilon_{\nu}(k_z)$ is calculated from the k_z-dependent term of the tight-binding dispersion relation

$$\epsilon_{\nu}(k_z) = \varepsilon_{\nu}(k_z) - \frac{1}{N_{\text{b}}} \sum_{k_z \nu} \varepsilon_{\nu}(k_z). \tag{29}$$

In equation (28), v_{d} is expressed by a semiclassical scattering ($v_{\text{d}}^{(\text{s})}$) and a quantum-mechanical tunnelling ($v_{\text{d}}^{(\text{t})}$) contribution. This decomposition relies on the kinetic equation (18) for the nonequilibrium distribution function, which is used to eliminate the derivative $\partial f_{\nu}^{\nu}(\mathbf{k})/\partial k_z$. For the two contributions to the drift velocity, we obtain

$$v_{\text{d}}^{(\text{s})} = -\frac{1}{eE} \frac{1}{N_{\text{b}}} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\nu,\nu'} \sum_{\mu} \epsilon_{\mu}(k_z) f_{\nu}^{\nu'}(\mathbf{k}') W_{\nu\mu}^{\nu'\mu}(\mathbf{k}', \mathbf{k}), \tag{30}$$

$$v_{\text{d}}^{(\text{t})} = \frac{\text{i}}{\hbar} \frac{1}{N_{\text{b}}} \sum_{\mathbf{k}} \sum_{\nu,\nu'} f_{\nu}^{\nu'}(\mathbf{k}) Q_{\nu\nu'}(\mathbf{k}) [\epsilon_{\nu'}(k_z) - \epsilon_{\nu}(k_z)]. \tag{31}$$

The intrasubband character of $v_{\text{d}}^{(\text{s})}$ results from the dominance of the scattering components $W_{\nu\mu}^{\nu\mu}$ with respect to the coupling constant. In contrast, the tunnelling contribution $v_{\text{d}}^{(\text{t})}$ is calculated from the off-diagonal elements $f_{\nu}^{\nu'}$ ($\nu \neq \nu'$). This fact illustrates its intersubband origin. We are interested in performing analytic calculations as far as possible, permitting us to focus on main physical phenomena. Therefore, we restrict ourselves to applying the relatively crude constant relaxation-time approximation, which inevitably lacks some of the features of a more realistic description of real systems, as, for example, electro-phonon resonances. The simple model has not been chosen to give an accurate representation of real systems. Rather, it is our intent here to use a model simple enough for extensive analytical calculations to demonstrate qualitative features in the quantum transport. In the calculation of $v_d^{(s)}$, the following scattering probabilities are taken into account (see [8]):

$$W_{12}^{12}(\mathbf{k}', \mathbf{k}) = \frac{\delta_{\mathbf{k}',\mathbf{k}}}{\tau_{12}}, \qquad W_{21}^{21}(\mathbf{k}', \mathbf{k}) = \frac{\delta_{\mathbf{k}',\mathbf{k}}}{\tau_{21}},$$
$$W_{11}^{22}(\mathbf{k}', \mathbf{k}) = W_{22}^{11}(\mathbf{k}', \mathbf{k}) = -\frac{\delta_{\mathbf{k}',\mathbf{k}}}{\tau}. \tag{32}$$

The tight-binding dispersion relations of the two-band model are given by

$$\varepsilon_1(\mathbf{k}) = \varepsilon(\mathbf{k}_\perp) + \frac{\Delta_1}{2}(1 - \cos(k_z d)), \tag{33}$$

$$\varepsilon_2(\mathbf{k}) = \varepsilon(\mathbf{k}_\perp) + \varepsilon_g + \Delta_1 + \frac{\Delta_2}{2}(1 + \cos(k_z d)), \tag{34}$$

in which $\varepsilon(\mathbf{k}_\perp)$ refers to the lateral carrier motion in the SL layers. The widths of the minibands and the gap energy are denoted by Δ_i $(i = 1, 2)$ and ε_g, respectively. In our simple model, intersubband tunnelling occurs at the transition energy

$$\hbar\omega_{21} = \varepsilon_g + \frac{\Delta_1 + \Delta_2}{2} + eE(Q_{11} - Q_{22}). \tag{35}$$

We proceed by calculating the nonequilibrium distribution function from the kinetic equation (18). Let us first focus on the equation for the off-diagonal element

$$\left[ie\mathbf{E}\nabla_{\mathbf{k}} + \Delta\varepsilon(k_z) + \hbar\omega_{21} + i\frac{\hbar}{\tau} \right] f_2^1(\mathbf{k}) = e\mathbf{E}\mathbf{Q}_{12}(f_1^1(\mathbf{k}) - f_2^2(\mathbf{k})), \tag{36}$$

within an approximation applicable to high electric fields under the conditions $\Omega\tau_{\mathrm{eff}} > 1$ (with $\Omega = eEd/\hbar$ being the Bloch frequency and τ_{eff} an effective scattering time). The k_z dependence introduced by $\Delta\varepsilon(k_z) = [(\Delta_1 + \Delta_2)] \cos(k_z d)$ is treated in an exact manner by using the transformation

$$f(\mathbf{k}) = f_2^1(\mathbf{k}) \exp\left\{ -\frac{i}{eE} \int_0^{k_z} dk_z' \, \Delta\varepsilon(k_z') \right\} \tag{37}$$

and introducing the k_z-Fourier coefficients of the distribution function

$$f_\nu^{\nu'}(\mathbf{k}) = \sum_{l=-\infty}^{\infty} e^{ilk_z d} f_\nu^{\nu'}(\mathbf{k}_\perp, l). \tag{38}$$

Restricting the sum to the dominating lowest order $l = 0$ term of $f_\nu^\nu(\mathbf{k}_\perp, l)$, we obtain the analytical result

$$f_2^1(\mathbf{k}_\perp, l) = \frac{e}{\hbar}\mathbf{E}\mathbf{Q}_{12} \sum_{l'=-\infty}^{\infty} \frac{(-1)^{l'} J_{l'}(\kappa) J_{l-l'}(\kappa)}{l'\Omega - \omega_{21} - i/\tau} [f_2^2(\mathbf{k}_\perp, 0) - f_1^1(\mathbf{k}_\perp, 0)], \tag{39}$$

in which J_l denote the Bessel functions of order l and $\kappa = (\Delta_1 + \Delta_2)/(2\hbar\Omega)$. The carrier occupation numbers

$$F_\nu = \sum_{\mathbf{k}} f_\nu^\nu(\mathbf{k}) \tag{40}$$

are obtained from the kinetic equation for the diagonal elements of the density matrix, which is expressed by

$$\frac{ieE}{\hbar} Q_{12} \sum_{\mathbf{k}_\perp} [f_2^1(\mathbf{k}_\perp, 0) - f_1^2(\mathbf{k}_\perp, 0)] = -\frac{1}{\tau_{12}} F_1 + \frac{1}{\tau_{21}} F_2. \tag{41}$$

Inserting equation (39) into (41) and considering the principle of detailed balance between carrier generation and recombination [$\tau_{12} = \tau_{21}\exp(\varepsilon_g/k_B T)$], we obtain

$$F_1 - F_2 = \frac{\sinh(\varepsilon_g/(2k_B T))}{\cosh(\varepsilon_g/(2k_B T)) + 2\Omega\tau\Omega\tau_{21}A_0\exp(\varepsilon_g/(2k_B T))}, \tag{42}$$

with

$$A_n = \left(\frac{Q_{12}}{d}\right)^2 \sum_{l=-\infty}^{\infty} l^n \frac{J_l(\kappa)^2}{(l\Omega\tau - \omega_{21}\tau)^2 + 1}. \tag{43}$$

The calculation of the intersubband tunnelling contribution $v_d^{(t)}$ proceeds in a similar way by starting from equation (31). The result

$$v_d^{(t)} = \frac{2d}{N_b\tau}(F_1 - F_2)A_1 \tag{44}$$

describes tunnelling-induced resonant transport, whenever a multiple of the Bloch frequency matches the renormalized energy gap ($l\Omega = \omega_{21}$, with l being an integer).

The quasiclassical scattering-induced drift velocity $v_d^{(s)}$ is assumed to behave regularly. For simplicity, we choose the Esaki–Tsu expression for its description [11]:

$$v_d^{(s)} = \frac{1}{N_b}\sum_{\nu=1,2}\frac{\Delta_\nu d}{2\hbar}\frac{\Omega\tau_\nu}{(\Omega\tau_\nu)^2+1}\frac{I_1(\Delta_\nu/(2k_B T))}{I_0(\Delta_\nu/(2k_B T))}F_\nu. \tag{45}$$

τ_ν denote intrasubband scattering times and I_l the modified Bessel functions. We focus on high electric fields, when Zener tunnelling occurs. In this regime, it is sufficient to exploit the asymptotic relationship between the smooth parts of the drift velocity and the diffusion coefficient given by

$$D_{zz}^{(s)} = \frac{v_d^{(s)} d}{2}\coth\left(\frac{\hbar\Omega}{2k_B T}\right), \tag{46}$$

which is valid in the ultra-quantum limit ($\Omega\tau_{\text{eff}} \gg 1$) [4] and in the ohmic regime ($\hbar\Omega \ll 2k_B T$).

3.2. *Diffusion coefficient*

The diffusion coefficient is calculated in the same way as the drift velocity. For our scattering model, the second term on the right-hand side of equation (23) disappears. Integrating by parts, the remaining expression in this equation is written as

$$D_{zz} = -\frac{1}{\hbar N_b}\sum_{\mathbf{k}}\sum_{\nu}\epsilon_\nu(k_z)\frac{\partial}{\partial k_z}\varphi_\nu^\nu(\mathbf{k}) = D_{zz}^{(s)} + D_{zz}^{(t)}, \tag{47}$$

which according to the kinetic equation (24) decomposes into a tunnelling and a scattering mediated contribution

$$D_{zz}^{(s)} = -\frac{1}{eE}\frac{1}{N_b}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\nu,\nu'}\sum_{\mu}\epsilon_\mu(k_z)\varphi_\nu^{\nu'}(\mathbf{k}')W_{\nu\mu}^{\nu'\mu}(\mathbf{k}',\mathbf{k}) + \frac{1}{2(eE)^2}\frac{1}{N_b}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\nu,\nu'}\sum_{\mu}\epsilon_\mu(k_z)^2 f_\nu^{\nu'}(\mathbf{k}')W_{\nu\mu}^{\nu'\mu}(\mathbf{k}',\mathbf{k}), \tag{48}$$

$$D_{zz}^{(t)} = \frac{\mathrm{i}}{\hbar}\frac{1}{N_b}\sum_{\mathbf{k}}\sum_{\nu,\nu'}\varphi_\nu^{\nu'}(\mathbf{k})Q_{\nu\nu'}(\mathbf{k})[\epsilon_{\nu'}(k_z) - \epsilon_\nu(k_z)] - \frac{\mathrm{i}}{2\hbar eE}\frac{1}{N_b}\sum_{\mathbf{k}}\sum_{\nu,\nu'}f_\nu^{\nu'}(\mathbf{k})Q_{\nu\nu'}(\mathbf{k})[\epsilon_{\nu'}(k_z)^2 - \epsilon_\nu(k_z)^2]. \tag{49}$$

We shall focus on diffusion via tunnelling as described by equation (49). There are two contributions, which are calculated from the off-diagonal elements of the functions $f_\nu^{\nu'}$ and $\varphi_\nu^{\nu'}$. The element $\varphi_2^1(\mathbf{k})$ is straightforwardly obtained by applying the same steps of calculation as outlined in section 3.1. The result

$$\varphi_2^1(\mathbf{k}_\perp, l) = \frac{e}{\hbar}\mathbf{E}\cdot\mathbf{Q}_{12}\sum_{l'=-\infty}^{\infty}\frac{(-1)^{l'}J_{l'}(\kappa)J_{l-l'}(\kappa)}{l'\Omega-\omega_{21}-\mathrm{i}/\tau}[\varphi_2^2(\mathbf{k}_\perp,0)-\varphi_1^1(\mathbf{k}_\perp,0)]$$
$$-\frac{\Delta_1-\Delta_2}{8\hbar}\Omega Q_{12}\sum_{l'=-\infty}^{\infty}\frac{J_{l-l'}(\kappa)}{l'\Omega-\omega_{21}-\mathrm{i}/\tau}[f_2^2(\mathbf{k}_\perp,0)-f_1^1(\mathbf{k}_\perp,0)]$$
$$\times\left[\frac{(-1)^{l'-1}J_{l'-1}(\kappa)}{(l'-1)\Omega-\omega_{21}-\mathrm{i}/\tau}-\frac{(-1)^{l'+1}J_{l'+1}(\kappa)}{(l'+1)\Omega-\omega_{21}-\mathrm{i}/\tau}\right] \tag{50}$$

consists of two quite different contributions. The structure of the first term corresponds to the same one as in equation (39), whereas the unwieldy second term on the right-hand side of equation (50) fortunately disappears in equation (49). In the final result for the tunnelling part of the diffusion coefficient

$$D_{zz}^{(\mathrm{t})} = \frac{1}{N_\mathrm{b}}\frac{d^2}{\tau}(\Omega\tau)^2\left[\frac{\Delta_1-\Delta_2}{\Delta_1+\Delta_2}(F_2-F_1)A_2+2\frac{P_1-P_2}{d}A_1\right], \tag{51}$$

there remain two quite different contributions. One of them exhibits a Zener resonance and is proportional to the field-induced change of occupation numbers. This term is always positive because (i) there is no population inversion ($F_2 < F_1$) in a two-band system [11], and (ii) the width Δ_1 of the lowest subband is always smaller than the width Δ_2 of the upper subband. The second contribution in equation (51), which is calculated from the quantities

$$P_\nu = \sum_{\mathbf{k}}\varphi_\nu^\nu(\mathbf{k}), \qquad P_1+P_2=0, \tag{52}$$

behaves quite differently. Obviously, the carrier occupation numbers do not enter this expression. To elucidate the nature of this tunnelling-induced diffusivity, let us calculate the quantities P_ν. Similarly to the previous section, we obtain from equation (24)

$$\frac{\mathrm{i}eE}{\hbar}Q_{12}\sum_{\mathbf{k}_\perp}[\varphi_2^1(\mathbf{k}_\perp,0)-\varphi_1^2(\mathbf{k}_\perp,0)] = -\frac{1}{\tau_{12}}P_1+\frac{1}{\tau_{21}}P_2+v_{\mathrm{d}_1}-v_\mathrm{d}, \tag{53}$$

which together with equation (50) is easily solved. From the solution

$$P_1-P_2 = \frac{v_{\mathrm{d}_1}-v_{\mathrm{d}_2}}{2}\frac{\tau_{21}\exp(\varepsilon_\mathrm{g}/(2k_\mathrm{B}T))}{\cosh(\varepsilon_\mathrm{g}/(2k_\mathrm{B}T))+2\Omega\tau\Omega\tau_{21}A_0\exp(\varepsilon_\mathrm{g}/(2k_\mathrm{B}T))}, \tag{54}$$

with

$$v_{\mathrm{d}_\nu} = \sum_{\mathbf{k}}v_\nu(k_z)f_\nu^\nu(\mathbf{k}), \tag{55}$$

we can see that $P_1 - P_2$ is proportional to the difference of the subband velocities $v_{\mathrm{d}_1} - v_{\mathrm{d}_2}$. This contribution physically describes field-induced diffusion, when the drift velocities of the carrier subsystems deviate from each other. In contrast to the difference of occupation numbers $F_1 - F_2$, which, for a two-band model, cannot change its sign as a function of the electric field, the difference of velocities $v_{\mathrm{d}_1} - v_{\mathrm{d}_2}$ may become positive or negative depending on the electric field strength and the SL parameters. Negative values of $v_{\mathrm{d}_1} - v_{\mathrm{d}_2}$ are expected to occur in the vicinity of an intersubband tunnelling resonance characterized by $F_1 \approx F_2$. In this case, the tunnelling contribution to the diffusion coefficient leads to a Zener antiresonance. When intersubband tunnelling becomes most effective ($F_1 = F_2$), the tunnelling contribution to the drift velocity disappears ($v_\mathrm{d}^{(\mathrm{t})} = 0$), but there remains a contribution to quantum diffusion that exhibits a tunnelling resonance or antiresonance, depending on whether the subband velocity v_{d_1} is larger or smaller than v_{d_2}.

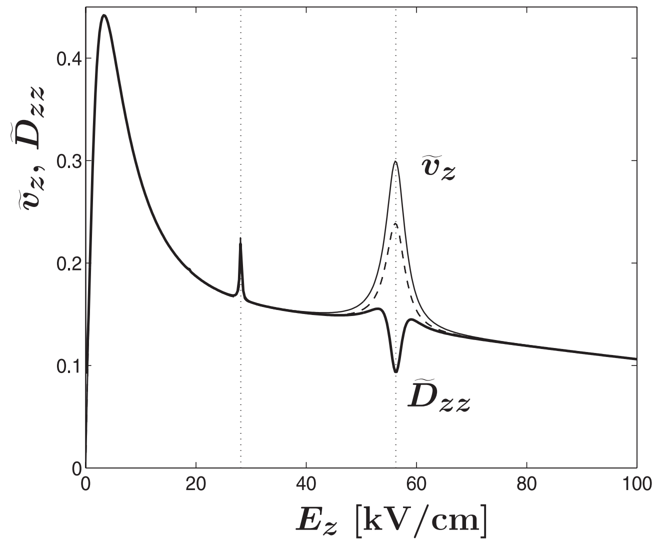

Figure 1. The dimensionless drift velocity $\tilde{v}_z = v_z/(2d/\tau)$ (thin solid curve) and longitudinal diffusion coefficient $\tilde{D}_{zz} = D_{zz}/(d^2/\tau)$ (thick solid curve) as a function of the electric field E_z. The dashed curve shows the scattering-induced contributions $\tilde{v}_z^{(s)}$ and $\tilde{D}_{zz}^{(s)}$, which according to equation (46) coalesce. The positions of Zener resonances are indicated by vertical dotted lines. The parameters used in the calculation are $d = 20$ nm, $\varepsilon_g = 100$ meV, $\Delta_1 = 5$ meV, $\Delta_2 = 20$ meV, $(Q_{12}/d)^2 = 0.1$, $\tau_1 = 0.1$ ps, $\tau_2 = 0.05$ ps, $\tau_{21} = 2$ ps, $\tau = 1$ ps and $T = 4$ K.

3.3. Numerical results

In the numerical analysis of the electric-field-dependent diffusion coefficient, we concentrate on the tunnelling contribution given by equation (51). For simplicity, the scattering-mediated diffusivity is calculated from the asymptotic expression in equation (46) (valid in the ultra-quantum limit ($\Omega\tau_{\mathrm{eff}} \gg 1$) and in the ohmic regime ($\hbar\Omega \ll 2k_B T$)) together with the Esaki–Tsu result in equation (45). The dimensionless drift velocity $v_z/(2d/\tau)$ and longitudinal diffusion coefficient $D_{zz}/(d^2/\tau)$ are shown in figures 1 and 2 as a function of the electric field strength for different scattering parameters and temperatures. In both figures, the drift velocity (thin solid curve) exhibits at low electric fields an ohmic behaviour, which, with increasing field strength, is followed by a region of negative differential conductivity and the appearance of a strong Zener resonance (marked by a dotted vertical line). The scattering-induced contribution $v_d^{(s)}/(2d/\tau)$ (which coalesces with the dimensionless diffusion coefficient) is shown by the dashed line. In addition to the main Zener resonance, a satellite structure is resolved. In the vicinity of the intersubband tunnelling resonance, the field dependence of the diffusion coefficient deviates remarkably from the behaviour of the drift velocity and exhibits a Zener antiresonance. This antiresonance, which is due to the tunnelling contribution $D_{zz}^{(t)}$ to the diffusion coefficient, occurs under the conditions $F_1 \approx F_2$ and $\tau_2 < \tau_1$.

The experimental observation of this antiresonance requires the suppression of domain formation in a suitably designed strongly coupled SL. Moreover, it is necessary to figure out an appropriate experimental setup to identify the Zener antiresonance in quantum diffusion. Whereas the physical meaning of the longitudinal diffusion coefficient D_{zz} becomes obvious in the ohmic regime due to the Einstein relation, its understanding becomes more difficult for the considered two-band model in the region of quantizing electric fields. Therefore, we believe that the experimental verification of the predicted Zener antiresonance in quantum diffusion is a challenge that deserves further investigation.

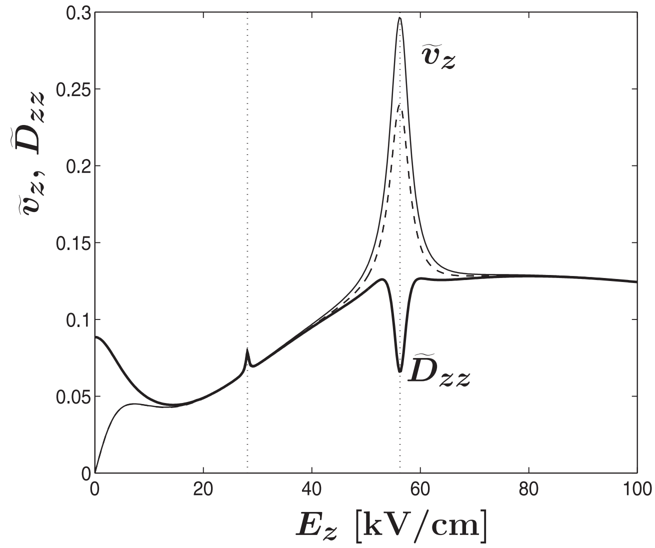

Figure 2. $\tilde{v}_z$ (thin solid curve) and $\tilde{D}_{zz}$ (thick solid curve) versus E_z for $T = 77$ K and the following set of scattering parameters: $\tau_1 = 0.05$ ps, $\tau_2 = 0.01$ ps, $\tau_{21} = 1$ ps, and $\tau = 0.5$ ps. The dashed curve shows the scattering-induced contributions $\tilde{v}_z^{(s)}$ and $\tilde{D}_{zz}^{(s)}$.

4. Summary

We have developed a microscopic quantum theory for the carrier diffusion in multi-band semiconductors and semiconductor SLs, at which an electric field of arbitrary strength is applied. It was demonstrated that diffusion in biased semiconductors is governed by a quantity $\varphi_\nu^{\nu'}(\mathbf{k})$ that refers to an initial inhomogeneity of the carrier system and that differs from the nonequilibrium distribution function $f_\nu^{\nu'}(\mathbf{k})$, from which the drift velocity is calculated. For this new quantity, a kinetic equation was derived, which replaces the Boltzmann equation (or its quantum-mechanical extension). This general theory of quantum diffusion within the one-particle picture is completely exact. Results were obtained for an SL with two subbands. We focused on the electric-field regime, in which intersubband tunnelling is expected to occur. It was shown that both the drift velocity and the longitudinal diffusion coefficient decompose into a scattering- and tunnelling-induced contribution. Depending on the SL parameters (such as, for example, the barrier width, the scattering times, and the miniband widths), the longitudinal diffusion coefficient exhibits a Zener resonance or antiresonance. This result has to be contrasted with the drift velocity, in which always a Zener resonance, but never an antiresonance, occurs. This discrepancy underlines the fact that both quantities have a different physical origin and, therefore, may behave quite differently at high electric-field strengths. We conclude that the Einstein relation between the drift velocity and the diffusion coefficient is not valid at high electric fields. This observation is in line with results derived by applying the Chapman–Enskog approximation to the Boltzmann–Poisson equations [14, 15]. In this paper, we have identified peculiarities in quantum diffusion at the Zener tunnelling resonance, which cannot be described by the Einstein relation.

Our numerical results were derived in the simple relaxation-time approximation, which was used to demonstrate qualitative features of intersubband tunnelling, but was not chosen to give an accurate representation of real systems. Further progress is related to studying realistic models for elastic and inelastic scattering. Several applications of our theory are conceivable. Taking into account the electric-field dependence of scattering, it is expected that combined Zener-phonon resonances [12] can be observed in quantum diffusion. Another application of our general approach could be the treatment of quantum diffusion associated with the real-space transfer of carriers [13] during the parallel transport in SLs.

Acknowledgment

Partial support by the Deutsches Zentrum für Luft- und Raumfahrt is gratefully acknowledged.

Appendix. Phenomenological consideration

In this appendix, we present a phenomenological analysis of the long-wavelength behaviour of the Fourier transformed propagator $P_{\nu\nu'}(q,s)$. We restrict the discussion to a two-band model and solve the set of linear equations

$$sP_{\nu\nu'} = \delta_{\nu\nu'} + \mathrm{i}q\sum_{\mu} P_{\nu\mu}v_{\mu\nu'} - q^2\sum_{\mu} P_{\nu\mu}D_{\mu\nu'} + \sum_{\mu} P_{\nu\mu}\omega_{\mu\nu'}, \tag{A.1}$$

which are obtained by Fourier transforming equation (1). The analytic solution is treated in the limit $s \to 0$ and $q \to 0$. Taking into account equation (13), we obtain the following propagator for an effective drift-diffusion equation:

$$P_{\nu\nu'}(q,s) = \frac{n_{\nu'}}{s - \mathrm{i}qv_{\mathrm{eff}} + q^2 D_{\mathrm{eff}}}, \tag{A.2}$$

with the drift velocity

$$v_{\mathrm{eff}} = \sum_{\mu\mu'} n_\mu v_{\mu\mu'} \equiv v_{\mathrm{d}}, \tag{A.3}$$

and the diffusion coefficient

$$D_{\mathrm{eff}} = D_{\mathrm{d}} + \frac{1}{\omega_1+\omega_2}\left[v_{\mathrm{d}}(v_{11}+v_{22}) + v_{12}v_{21} - v_{11}v_{22} - v_{\mathrm{d}}^2\right] \tag{A.4}$$

of the two-band model. In equation (A.2), we used the abbreviations

$$D_{\mathrm{d}} = \sum_{\mu\mu'} n_\mu D_{\mu\mu'}, \tag{A.5}$$

$$n_1 = \frac{\omega_2}{\omega_1+\omega_2}, \qquad n_2 = \frac{\omega_1}{\omega_1+\omega_2}. \tag{A.6}$$

In contrast to v_{eff}, the effective diffusion coefficient D_{eff} is not equal to D_{d}. There is an additional contribution to the diffusion coefficient, which exists also under the condition $D_{\nu\nu'} = 0$. The physical origin of this additional term is elucidated by the equivalent form

$$D_{\mathrm{eff}} = D_{\mathrm{d}} + \frac{v_{+-}}{\omega_1+\omega_2}[v_{-+} - v_{+-}(n_1-n_2)^2 + (v_{++} - v_{--})(n_2-n_1)], \tag{A.7}$$

with

$$v_{++} = \tfrac{1}{2}(v_{11}+v_{12}+v_{21}+v_{22}), \qquad v_{+-} = \tfrac{1}{2}(v_{11}-v_{12}+v_{21}-v_{22}),$$
$$v_{-+} = \tfrac{1}{2}(v_{11}-v_{12}-v_{21}+v_{22}), \qquad v_{--} = \tfrac{1}{2}(v_{11}+v_{12}-v_{21}-v_{22}).$$

The second term on the right-hand side of equation (A.7) is proportional to v_{+-}. This term leads to a spreading of an initial charge carrier inhomogeneity even when $D_{\mathrm{d}} = 0$. Under the condition $v_{12} = v_{21} = 0$ and $v_{11} \neq v_{22}$, the carriers in the two subbands move with different velocities so that an initial δ-like package is smeared out after a given time t between the space coordinates $v_{11}t$ and $v_{22}t$. We conclude that there is a contribution to the effective diffusion coefficient, which is proportional to $|v_{11} - v_{22}|$. This observation enables us to understand the physical origin of the Zener antiresonance. At the intersubband tunnelling transition, there is strong mixing of states so that the subbands lose their single character. Consequently, only a common occupation number and a common drift velocity appear so that the additional contribution in equation (A.7) disappears, giving rise to a minimum of the diffusion coefficient ($D_{\text{eff}} \approx D_{\text{d}}$) at the tunnelling resonance.

From equation (A.2) it is easily seen how the effective drift velocity and the effective diffusion coefficient are expressed by the moments of the propagator $P_{\nu\nu'}(q, s)$. We obtain

$$v_{\text{eff}} = -\mathrm{i}s^2 \sum_{\nu'} {}^{(1)}P_{\nu\nu'}(s)|_{s\to 0}, \tag{A.8}$$

$$D_{\text{eff}} = -\frac{s^2}{2} \sum_{\nu'} {}^{(2)}P_{\nu\nu'}(s) - \frac{v_{\text{d}}^2(s)}{s}\Big|_{s\to 0}, \tag{A.9}$$

which was used in equations (16) and (21) to define the drift velocity and the diffusion coefficient, respectively.

References

[1] Kazarinov R F and Suris R A 1971 *Fiz. Tekh. Poluprov.* **5** 797
Kazarinov R F and Suris R A 1971 *Sov. Phys.—Semicond.* **5** 207 (Engl. Transl.)
[2] Gmachl C, Capasso F, Sivco D L and Cho A Y 2001 *Rep. Prog. Phys.* **64** 1533
[3] Thobel J L, Sleiman A and Fauquembergue R 1997 *J. Appl. Phys.* **82** 1220
[4] Bryksin V V and Kleinert P 2003 *J. Phys.: Condens. Matter* **15** 1415
[5] Matulionis A, Raguotis R and Katilius R 1997 *Phys. Rev.* B **56** 2052
[6] Reggiani L, Starikov E, Gruzinskis V and Varani L 1997 *Semicond. Sci. Technol.* **12** 141
[7] Katilius R, Liberis J, Matulionis A, Raguotis R, Sakalas P, Nougier J P, Vaissiere J C, Varani L and Rota L 1999 *Phys. Rev.* B **60** 11487
[8] Bryksin V V, Woloschin V C and Rajtzev A W 1980 *Fiz. Tverd. Tela* **22** 3076
Bryksin V V, Woloschin V C and Rajtzev A W 1980 *Sov. Phys.—Solid State* **22** 1796 (Engl. Transl.)
[9] Kudinov E K and Firsov Y A 1965 *Zh. Eksp. Teor. Fiz.* **49** 867
Kudinov E K and Firsov Y A 1966 *Sov. Phys.—JETP* **22** 603 (Engl. Transl.)
[10] Dedulevich S, Kantsleris Z and Matulis A 1989 *Zh. Eksp. Teor. Fiz.* **95** 1701
[11] Kleinert P and Bryksin V V 2001 *Physica* B **304** 60
[12] Kleinert P 2000 *J. Phys.: Condens. Matter* **12** 8467
[13] Bryksin V V and Kleinert P 1997 *J. Phys.: Condens. Matter* **9** 7391
[14] Liotta S F and Majorana A 2002 *Int. J. Comput. Math. Electr. Electron. Eng.* **21** 31
[15] Bonilla L L, Escobedo R and Perales A 2003 *Phys. Rev.* B **68** 241304(R)