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Balance equations for electron transport in a general energy band

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Abstract. The conventional way of developing a momentum balance equation by generating the first-order moment (with the momentum k as the moment operator) from the Boltzmann transport equation relies on the fact that the distribution function $f(k)$ approaches zero rapidly enough that the integral $\int \nabla(k) f(k)\, d^3k$ is negligible. This is not valid for an energy band (e.g. a superlattice miniband) whose width (in at least one direction of the k-space) is comparable with $k_B T_e$ (T_e is the electron temperature). It is demonstrated that by choosing the moment operator to be the velocity function $v(k) \equiv \nabla\varepsilon(k)$ a compact moment equation, which is valid for a general energy band and represents an effective momentum balance of the carrier system, can be derived for the distribution function $f(k)$ which is a continuous function of k in the periodic zone scheme. The effective momentum balance equation and the energy balance equation thus obtained share the same formal expressions as the acceleration and energy-balance equations in Lei's non-parabolic method. These equations, with the distribution function suggested by Huang and Wu, are applied to the discussion of high electric field transport of electrons in non-parabolic Kane bands and superlattice minibands. The results are compared with the predictions from Lei's non-parabolic method and from a carrier temperature model.

1. Introduction

The Lei–Ting [1] balance-equation approach to hot-electron transport in semiconductors, which was proposed 10 years ago, has been successfully applied to a variety of transport problems in different types of system. This theory is based on the separation of the centre of mass of the system from the relative motion of electrons in the presence of the electric field. Such a separation is valid only for electrons moving in a parabolic band or for systems which can be described by a constant effective mass. Recent interest in a semi-analytical and realistic theory capable of dealing with superlattice miniband transport [2] has stimulated many investigations on extending the Lei–Ting balance-equation method to general energy band structures. Several extensions have been proposed recently with different results.

Magnus *et al* [3] suggested that the exact set of the original Lei–Ting balance equations as given in [1] can still be used to describe transport in a general energy band as long as the true (rather than the parabolic) energy dispersion relation is taken into account in the electron density–density correlation function. They have applied these equations to the investigation of the electron transport in GaAs/AlGaAs heterojunctions with non-parabolicity (Kane type) included [4].

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The present author [5] extended the Lei–Ting theory to an arbitrary energy band. His non-parabolic method describes the drifting Bloch electrons under the influence of a uniform electric field by the use of two parameters: the centre-of-mass momentum and the electron temperature. The balance equations comprise an equation of motion of the centre of mass, a mass-variable single particle under the influence of the electric field, and an equation of energy balance between the power supplied by the electric field and energy loss rate of the electron system. These equations have been applied to superlattice miniband transport [6], yielding an Esaki–Tsu negative differential conductivity (NDC), reproducing the experimental peak drift velocity v_p and the threshold electric field as functions of the miniband width [7], and accounting for the low-temperature saturation of v_p [8]. The predictions of this non-parabolic method have also been confirmed by a recent calculation based on the three-dimensional Boltzmann equation [9].

Recently, Huang and Wu (HW) [10] proposed a set of balance equations for electron transport in a general energy band under the influence of an electric field, in which the momentum and energy losses are to be evaluated with a distribution function which is obtained by maximizing the system entropy, subject to a given total number of electrons and a given total energy and, in addition, subject to a restricted condition that the average drift velocity is also prescribed. Although these equations are not capable of reproducing the well established Esaki–Tsu negative differential mobility for superlattice miniband transport [11], the distribution function produced by HW is very attractive and plausible.

In this paper we point out that, from the viewpoint of the Boltzmann equation, the original Lei–Ting momentum balance equation (i.e. the momentum balance suggested by Magnus *et al* [3]) and the momentum balance equation suggested by HW [10] are generally not valid for narrow energy bands. A balance equation, which is valid for a general energy band and represents an effective momentum balance, can be derived by taking an appropriate 'moment' from the Boltzmann equation with a prescribed distribution function. The effective momentum and energy balance equations thus obtained share the same formal expressions as the acceleration and energy balance equations in Lei's non-parabolic method, but with the original 'distribution function' replaced by the prescribed distribution function. The derived equations with the distribution function suggested by HW [10] are applied to the discussion of hot-carrier transport in non-parabolic Kane bands and in superlattice minibands. The results are compared with those from Lei's non-parabolic method and from a carrier temperature model.

This paper is organized as follows. For the readers' convenience and to facilitate comparison we rewrite the major equations and formulae from Lei's non-parabolic method and from the paper of HW in sections 2 and 3 respectively. In section 4 we discuss in detail the derivation of balance equations from the Boltzmann equation for a general energy band. In section 5 we propose an electron temperature (ET) model for a general energy band system. These balance equation theories and models are applied to non-parabolic Kane bands in section 6, and to superlattice minibands in section 7, before we conclude in section 8.

2. Lei's non-parabolic method

Lei's non-parabolic method deals with many interacting Bloch electrons which are drifting under the influence of a uniform electric field. It assumes that strong intercarrier couplings promote rapid thermalization of electrons in a reference frame in which the total momentum of carriers vanishes. This enables us to describe these drifting Bloch electrons under the

influence of a uniform electric field E by the use of two parameters, namely the centre-of-mass momentum $P_d \equiv Np_d$ (N is the total number of the electrons) and the ET T_e. They are included in the initial density matrix, which represents a thermoequilibrium-type state and is thought to be close to the final transport state that we are trying to find. Balance equations are derived by evaluating the statistical averages of the rates of changes in the centre-of-mass velocity and the electron energy operators. To leading order of the scattering potentials this yields the following acceleration and energy balance equations for the steady transport state:

$$eE \cdot \mathcal{K} + A = 0 \tag{1}$$

$$eE \cdot v_d - W = 0. \tag{2}$$

Here $A = A_i + A_p$ is the frictional acceleration due to impurities (A_i) and phonon-s (A_p), and W is the electron energy loss rate (per carrier) due to phonon-s. The centre-of-mass velocity or the average drift velocity v_d of the carriers, is given by

$$v_d = \frac{2}{N}\sum_k v(k) f(\varepsilon(k - p_d)) \tag{3}$$

where $v(k) \equiv \nabla\varepsilon(k)$ is the velocity function, and $f(\varepsilon) \equiv 1/[\exp(\varepsilon - \mu)/T_e + 1]$ stands for the Fermi function at the temperature T_e with μ the chemical potential to be determined by the total number of carriers: $N = 2\sum_k f(\varepsilon(k))$. Equation (1) is the equation of motion of the centre of mass, which is a mass-variable single particle with an inverse effective mass tensor $\mathcal{K}/N$, given by

$$\mathcal{K} = \frac{2}{N}\sum_k \nabla\nabla\varepsilon(k) f(\varepsilon(k - p_d)). \tag{4}$$

The impurity-induced frictional acceleration A_i, the phonon–induced frictional acceleration A_p, and the energy transfer rate W from the electron system to the phonon system have the following form [5]:

$$A_i = \frac{2\pi n_i}{N}\sum_{k,q} |\bar{u}(q)|^2 |g(k,q)|^2 [v(k+q) - v(k)]\delta[\varepsilon(k+q) - \varepsilon(k)][f(\varepsilon(k - p_d)) - f(\varepsilon(k + q - p_d))] \tag{5}$$

$$A_p = \frac{4\pi}{N}\sum_{k,q,\lambda} |\tilde{M}(q,\lambda)|^2 |g(k,q)|^2 [v(k+q) - v(k)]\delta[\varepsilon(k+q) - \varepsilon(k) + \Omega_{q\lambda}] \times \{n(\Omega_{q\lambda}/T)[f(\varepsilon(k - p_d)) - f(\varepsilon(k + q - p_d))] - f(\varepsilon(k - p_d))[1 - f(\varepsilon(k + q - p_d))]\} \tag{6}$$

$$W = \frac{4\pi}{N}\sum_{k,q,\lambda} |M(q,\lambda)|^2 |g(k,q)|^2 \Omega_{q\lambda}\delta[\varepsilon(k+q) - \varepsilon(k) + \Omega_{q\lambda}]\{n(\Omega_{q\lambda}/T) \times [f(\varepsilon(k - p_d)) - f(\varepsilon(k + q - p_d))] - f(\varepsilon(k - p_d))[1 - f(\varepsilon(k + q - p_d))]\}. \tag{7}$$

Here

$$\bar{u}(q) = u(q)/\epsilon(q, \varepsilon(k - p_d) - \varepsilon(k + q - p_d)) \tag{8}$$

and

$$\bar{M}(q,\lambda) = M(q,\lambda)/\epsilon(q, \varepsilon(k-p_d) - \varepsilon(k+q-p_d)) \tag{9}$$

are the dynamically screened impurity scattering potential and the dynamically screened electron–phonon matrix element, $u(q)$ is the bare impurity potential and $M(q,\lambda)$ is the (unscreened) coupling matrix element between the electron and λth branch phonon in the plane-wave representation. $\epsilon(q,\omega)$ is the RPA dielectric function of the electron system. So far, in most numerical investigations, only the static screening approximation has been used: $\bar{u}(q) \sim u(q)/\epsilon(q,0)$ and $\bar{M}(q,\lambda) \sim M(q,\lambda)/\epsilon(q,0)$.

The acceleration balance equation (1) and the energy balance equation (2) constitute the basis of the method for steady-state transport. These equations reduce to the original Lei–Ting balance equations in the parabolic limit.

3. Huang–Wu distribution function

Recently, HW [10] proposed a set of balance equations for electron transport in a general energy band under the influence of an electric field. It takes the following form in the stationary conduction:

$$NeE = \text{momentum loss by scattering (with phonon-s and impurities)} \tag{10}$$

$$NeE \cdot v_d = \text{energy loss by scattering (with phonon-s).} \tag{11}$$

Here the momentum loss and energy loss are calculated with a distribution function

$$f_v(k) = 1/[[\exp\{\beta[\varepsilon(k) - p_v \cdot \nabla\varepsilon(k) - \mu]z\} + 1]] \tag{12}$$

which is obtained by HW [10] as a distribution function of the electron gas by maximizing its entropy, subject to a given total number of electrons and a given total energy and, in addition, subject to the restricted condition that the average drift velocity is also prescribed. The drift velocity v_d is given by

$$v_d = \frac{2}{N}\sum_k v(k) f_v(k) \tag{13}$$

and the parameters β, μ and p_v are determined by the total number of carriers given by

$$N = 2\sum_k f_v(k) \tag{14}$$

together with the momentum and energy balance equations (10) and (11). I shall refer to the function $f_v(k)$ (equation (12)) as the HW distribution function.

As has been pointed out by the present author [11], the distribution function obtained in this way apparently depends on the prescribed condition that one chooses. So far we have no specific reason why one should maximize the entropy within the constant-velocity surface of the phase space. For instance, one can maximize the entropy subject to a prescribed average momentum instead of average velocity. This gives a distribution function of the form

$$f_p(k) = 1/[[\exp\{\beta[\varepsilon(k) - v_k \cdot p(k) - \mu]\} + 1]] \tag{15}$$

where β, μ and v_κ are parameters, and $p(k)$ stands for the momentum of an electron in the k-state, which is a periodic function of k and equals k within the Brillouin zone (BZ). We can also express the momentum and energy balance equations (10) and (11) and equations (13) and (14) in terms of the distribution function $f_p(k)$. The resultant set of balance equations is in fact somewhat similar to those suggested by Magnus *et al* [3]. The main difference is that in the latter case v_d is taken to be equal to v_κ rather than related to v_κ by equation (13).

Although equations (10) and (11) themselves leave some ambiguity on how to evaluate the the 'momentum loss by scattering', the reasonable way of calculating this quantity should be by means of the Fermi golden rule together with the electron distribution or, equivalently, the collision integral term of the Boltzmann equation. In this way the 'momentum loss by scattering' turns out to be $-Nf$ *given by* equation (21) of the next section. Unfortunately, equations thus obtained are unable to reproduce the well established Esaki–Tsu negative differential mobility for superlattice miniband transport [11], irrespective of which of the functions $f_v(k)$ or $f_p(k)$ is used in calculating the momentum and energy losses. Therefore, these equations cannot be a good description for high-field transport at least for this type of strongly non-parabolic band. It should be noted, however, that this conclusion is not related to the form of the distribution function used.

In order to see what is missed in these equations we shall, in the next section, investigate the moment equations from the Boltzmann transport equation for a general energy band.

4. Moment equations of the Boltzmann equation for a general energy band

Consider electrons moving within a single energy band. The electron Bloch state can be described by the lattice wavevector k within a Brillouin zone BZ. In the periodic zone scheme, k and $k+G$ (G is a reciprocal-lattice vector) represent the same electron state and the energy dispersion $\varepsilon(k)$ is a periodic function:

$$\varepsilon(k) = \varepsilon(k+G). \tag{16}$$

The steady-state Boltzmann equation for a spatially homogeneous system under the influence of a uniform electric field is written as

$$eE \cdot \nabla f(k) = \left(\frac{\partial f}{\partial t}\right)_c. \tag{17}$$

Here $f(k)$ is the distribution function and $(\partial f/\partial t)_c$ stands for the collision term.

A general moment equation is obtained by multiplying equation (17) by an arbitrary scalar or vector function $g(k)$ (moment operator) and summing over all the electron states or integrating over k in a BZ to give

$$eE \cdot \int_{BZ} \nabla g(k) f(k) \frac{d^3k}{4\pi^3} - \frac{eE}{4\pi^3} \cdot \oint_{S_{BZ}} ds\, g(k) f(k) = -\int_{BZ} \left(\frac{\partial f}{\partial t}\right)_c g(k) \frac{d^3k}{4\pi^3} \tag{18}$$

The second term on the left-hand side is a closed area integration over the boundary surface S_{BZ} of the BZ.

Taking $g(k) = k$, we have

$$eE \int_{BZ} f(k) \frac{d^3k}{4\pi^3} - \frac{eE}{4\pi^3} \cdot \oint_{S_{BZ}} ds\, k f(k) = -\int_{BZ} \left(\frac{\partial f}{\partial t}\right)_c k \frac{d^3k}{4\pi^3}. \tag{19}$$

The first term on the left-hand side gives

$$eE\int_{\mathrm{BZ}} f(k)\frac{\mathrm{d}^3k}{4\pi^3} = NeE. \tag{20}$$

The right-hand side is exactly the momentum loss rate of the electron system due to impurity and phonon scatterings, $-F \equiv -Nf$, which can be written in the form

$$\begin{aligned} f = {} & \frac{2\pi n_{\mathrm{i}}}{N}\sum_{k,q}|u(q)|^2|g(k,q)|^2[p(k+q)-p(k)]\delta(\varepsilon(k+q)-\varepsilon(k))[f(k)-f(k+q)] \\ & + \frac{4\pi}{N}\sum_{k,q,\lambda}|M(q,\lambda)|^2|g(k,q)|^2[p(k+q)-p(k)]\delta[\varepsilon(k+q)-\varepsilon(k)+\Omega_{q\lambda}] \\ & \times\{n(\Omega_{q\lambda}/T)[f(k)-f(k+q)]-f(k)[1-f(k+q)]\}. \end{aligned} \tag{21}$$

In the case of a parabolic band for which $\varepsilon(k) = k^2/2m$ and the BZ boundary is thought to be at $|k| \to \infty$, the second term on the left-hand-side of equation (19) vanishes owing to the exponential decay of the Fermi function at large $|k|$. Equation (19) reduces to $NeE = -F$, i.e. the momentum balance equation suggested by HW if the distribution function $f_{\mathrm{v}}(k)$ (equation (12)) is used for $f(k)$. For a realistic wide-band system such a conclusion may still be approximately true if the effective band width is much larger than the effective temperature parameter in the distribution function. Even in this case, however, one has to exercise caution in high-field transport, since the electron temperature can be very high at high electric fields such that the the second term on the left-hand side of equation (19) may not be negligible.

For a narrow band or an energy band which is narrow in one or two directions in the k-space, the second term on the left-hand side of equation (19) can be as large as the first term. Consider, for example, a superlattice miniband given by $\varepsilon(k) = (k_x^2 + k_y^2)/2m + (\Delta/2)[1 - \cos(k_z d)]$ (d is the superlattice period and Δ is the miniband width) with an electric field applied along the superlattice growth axis (z direction). In the case of a Maxwell–Boltzmann distribution function $f(k) \sim \exp[-\varepsilon(k)/T]$, the ratio of the second term to the first term of the z component of equation (19) can be shown to be ($I_0(x)$ is the zeroth-order Bessel function)

$$\frac{\exp(-\Delta/2T)}{I_0(\Delta/2T)} \sim 1 \quad \text{for small } \frac{\Delta}{2T}$$

and thus the second term on the left-hand-side of equation (19) is not negligible. Therefore, from the viewpoint of the moment equation of the Boltzmann equation, the original Lei–Ting momentum balance equation (i.e. the momentum balance equation suggested by Magnus *et al* [3] and the momentum balance equation suggested by HW [10], are generally not effective for narrow-band systems, since the above surface integration term has been neglected in these equations.

To obtain, from the Boltzmann equation, a compact moment equation corresponding to a momentum balance, we choose the moment operator to be the velocity function: $g(k) = v(k) \equiv \nabla\varepsilon(k)$. In the periodic zone scheme, the velocity function, as the energy function $\varepsilon(k)$, is a periodic and continuous function of k. Thus, if the distribution function $f(k)$ is also a periodic and continuous function of k, $v(k)f(k)$ takes the same value at

two points separated by a reciprocal-lattice vector on opposite sides of the BZ boundary and the closed area integration over the BZ surface in equation (18) vanishes:

$$\oint_{S_{BZ}} ds\ v(k) f(k) = 0. \tag{22}$$

The moment equation (18) then reduces to

$$eE \cdot \mathcal{K} = -A \tag{23}$$

with

$$\mathcal{K} = \frac{2}{N} \sum_k \nabla\nabla\varepsilon(k) f(k) \tag{24}$$

and

$$A = \frac{2}{N} \sum_k \left(\frac{\partial f}{\partial t}\right)_c v(k). \tag{25}$$

This is exactly the acceleration balance equation (1) in Lei's non-parabolic method. In fact, in the presence of impurity and phonon- scatterings the frictional acceleration A is given by the sum of A_i and A_p, having the same expressions as equations (5) and (6) (with static screened $\bar{u}(q)$ and $M(q, \lambda)$, except that function $f(\varepsilon(k - p_d))$ there is replaced by a general distribution function $f(k)$ satisfying the above mentioned condition; it changes continuously with changing k in the periodic zone scheme.

The requirement that the distribution function must be a continuous function of k excludes the possibility of using $f_p(k)$ (equation (15)) as a prescribed distribution function in obtaining such a moment equation, since the momentum function $p(k)$ is not continuous at the BZ boundary. However, both the function $f(\varepsilon(k - p_d))$ and the Huang–Wu distribution function $f_v(k)$ are such functions and can be used in this acceleration balance equation.

In the limit of a parabolic band both Lei's non-parabolic equations (1) and (2) and the balance equations (1) and (2) with the HW distribution function $f_v(k)$ reduce to the original Lei–Ting balance equations [5]. On the other hand, comparing function $f(\varepsilon(k - p_d))$ with the function $f_v(k)$ (equation (12)), we can see that they are equivalent at small p_d (small p_v). Therefore, the balance equations (1) and (2) with the HW distribution function yield exactly the same predictions as those of Lei's non-parabolic methods for arbitrary energy bands in the case of weak electric field transport. Different results from these two sets of balance equations show up only for strong electric field transport in strongly non-parabolic bands.

In investigating the streaming terms of a hydrodynamic transport model, Woolard *et al* [12] pointed out that the use of the velocity function $g(k) = v(k)$ for the moment operator leads to a significant improvement over the use of the momentum function $g(k) = k$ in the case of a non-parabolic Kane band. They arrived at this conclusion primarily on the basis of the fact that the resultant equation with $v(k)$ can be manipulated more easily and a simplifying approximation can be seen more clearly. The present analysis shows that the more fundamental reason for this is the non-zero surface integration term inherent in the k-induced equation (19) for a realistic energy band of finite width, which is always the case.

The ambiguity left by the form of equation (10) may allow one to explain that 'the momentum loss by scattering' is obtained by calculating the acceleration A and multiplying the average effective mass $(\mathcal{K}/N)^{-1}$, as defined by equations (24) and (25). Then, equation (10) is simply identical with equation (2).

5. Electron temperature model

The ET model [13–15] has been a simple method for investigating hot-carrier transport in the literature, which is especially popular in the qualitative analysis of the experimental data. Basically the ET model assumes that the only effect of a strong electric field is to raise the ET T_e. If the weak-electric-field mobility of the electron system at the lattice temperature T is $\mu_0(T)$, the electron mobility in a strong electric field E is given by $\mu_0(T_e)$, where the ET T_e is determined by an energy balance such that the energy supplied per unit time by the electric field equals the electron energy loss W and the latter is to be calculated using a weak-field distribution function but replacing the lattice temperature T by T_e.

This ET model can be easily extended to a general energy band, as long as equation (1) is used to calculate the weak-field mobility $\mu_0(T)$. Note that for this purpose we need only a small p_d limit for function $f(k - p_d)$ or small p_v limit for function $f_v(k)$; thus there is no difference using Lei's balance equations (1) and (2), or using equations (1) and (2) with the HW distribution function. The energy balance equation for determining T_e is

$$e\mu_0(T_e)E^2 - W(T_e) = 0. \tag{26}$$

Here the drift velocity is assumed to be in the same direction as the electric field such that $v_d = \mu_0(T_e)E$.

6. Application to Kane bands

To see the difference between Lei's non-parabolic equations (1) and (2) and the balance equations (1) and (2) with the HW distribution function, we first applied them to analyse electron transport in a non-parabolic Kane band with the energy dispersion $\varepsilon(k)$ given by

$$\varepsilon(1 + \alpha\varepsilon) = \frac{k^2}{2m}. \tag{27}$$

This Kane $k \cdot p$ model is widely used in the literature to describe the non-parabolicity of the electron energy dispersion of the Γ valley in narrow gap compound semiconductors. Here m is the electron effective mass at the band bottom, and $\alpha \sim 1/E_g$ is the non-parabolic coefficient, E_g being the band gap between the conduction and the valence bands.

Figure 1 shows the calculated drift velocity as a function of the electric field for n-doped GaAs ($\alpha = 0.613$ eV, $m = 0.067m_e$ (m_e is the free electron mass) and the impurity density n_i = electron density $n = 1.0 \times 10^{18}$ cm^3) at the lattice temperature $T = 77$ K. The chain line is obtained from Lei's non-parabolic method (equations (1) and (2)), and the solid line from balance equations (1) and (2) with the HW distribution function. The parameters used in the calculations are typical values for GaAs. Scatterings due to charged impurities, acoustic phonon-s and polar optic phonon-s are included in the calculation. As expected, for this weak non-parabolic system ($\alpha = 0.613$ eV), predictions by these two methods are essentially the same except at the highest-electric-field region plotted in the figure.

Different predictions by Lei's non-parabolic method and by balance equations (1) and (2) with HW distribution function show up when the electric field $E > 1$ kV cm^{-1} for stronger non-parabolic Kane band ($\alpha = 2.73$ eV), as is shown in figure 2, where we plot the calculated drift velocity versus the electric field for an n-type InAs system ($m = 0.022m_e$) with electron density $n = 1.0 \times 10^{18}$ cm^{-3} at lattice temperature $T = 300$ K, using Lei's non-parabolic method (chain lines) and using balance equations with the HW distribution

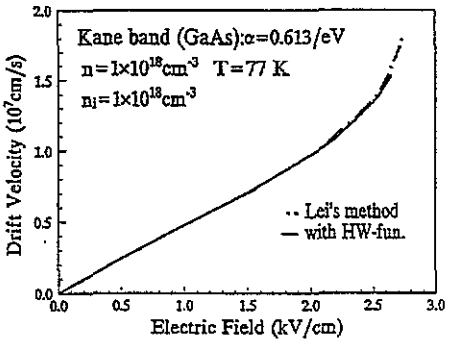

Figure 1. Drift velocity v_d against electric field E, calculated from Lei's non-parabolic method (— · —) and from the balance equations (1) and (2) with the HW distribution function (——) for an n-doped GaAs system (Kane band: $\alpha = 0.613$; $m = 0.067m_e$) with the impurity density n_i = electron density $n = 1.0 \times 10^{18}$ cm^{-3} at lattice temperature $T = 77$ K.

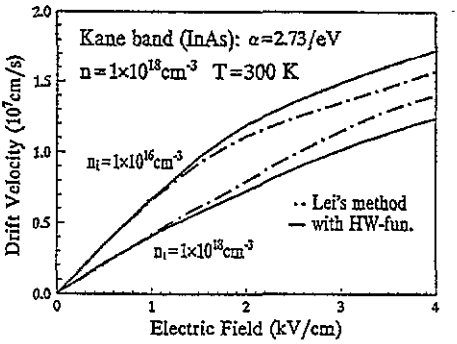

Figure 2. Drift velocity v_d against electric field E, calculated from Lei's non-parabolic method (— · —) and from the balance equations (1) and (2) with the HW distribution function (——) for n-type InAs (Kane band: $\alpha = 2.73$; $m = 0.022m_e$) with the electron density $n = 1.0 \times 10^{18}$/cm^3 at a lattice temperature $T = 77$ K, assuming two different impurity densities.

function (solid lines). In the lower set of curves, which corresponds to an impurity density $n_i = 1.0 \times 10^{18}$ cm^{-3} and impurity scattering dominates the momentum relaxation process, the HW function yields a lower drift velocity than predicted by Lei's non-parabolic method. This situation is changed when the impurity scattering is weakened and polar optic phonon scattering dominates the momentum relaxation. To see this we deliberately assume a much smaller impurity density ($n_i = 1.0 \times 10^{16}$ cm^{-3}) and keep the electron density unchanged, such that at $T = 300$ K the phonon scattering is stronger than the impurity scattering. The calculated result is plotted as the upper set of the curves in figure 2, showing that the HW distribution function yields a higher drift velocity than that of Lei's non-parabolic method when $E > 1$ kV cm^{-1}.

7. Application to superlattice miniband transport

In this section we apply the above balance equations to discuss the miniband transport of a superlattice with an electric field applied along its growth axis (z direction).

For the lowest miniband of the superlattice the electron energy spectrum can be written

$$\varepsilon(k) = \frac{k_x^2 + k_y^2}{2m} + \frac{\Delta}{2}[1 - \cos(k_z d)] \tag{28}$$

where m is the band effective mass, d is the superlattice period and Δ is the (lowest) miniband width. We consider a family of n-type GaAs-based quantum well superlattices having the same period $d = 4.5$ nm and well width $a = 3.5$ nm, but different miniband widths ranging from 200 to 900 K. Scatterings due to charged impurities, bulk polar optic phonon-s (Fröhlich coupling with electrons) and acoustic phonon-s (deformation potential and piezoelectric couplings with electrons) are taken into account (including static screening). The elastic scattering strength is characterized by the magnitude of the low-temperature (4.2 K) linear mobility $\mu(0)$ in each case. The electron band effective mass and

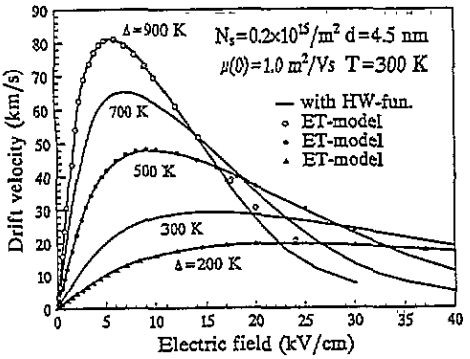

Figure 3. Drift velocity v_d against electric field E in superlattice vertical transport at a lattice temperature $T = 300$ K, calculated from the balance equations (1) and (2) with the HW distribution function (12) (——), for a family of GaAs-based quantum well superlattices of different miniband widths Δ ranging from 200–900 K, but with same period $d = 4.5$ nm, well width $a = 3.5$ nm, carrier sheet density $N_s = 0.2 \times 10^{15}$ m^{-2} and low-temperature (4.2 K) linear mobility $\mu(0) = 1.0$ m^2 V^{-1} s^{-1}: ○, ● and △ indicate the calculated results from the ET model for $\Delta = 900$ K, 500 K and 200 K systems, respectively, of the family.

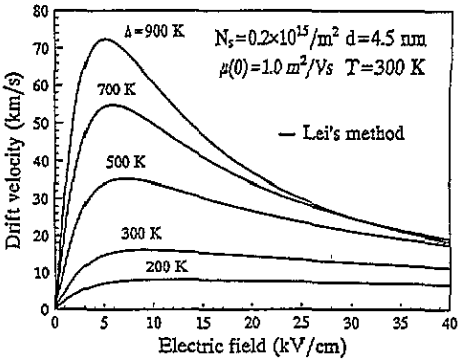

Figure 4. Drift velocity v_d against electric field E in superlattice vertical transport at a lattice temperature $T = 300$ K, calculated from Lei's non-parabolic method, for the same family of GaAs-based quantum well superlattices as described in figure 3.

all the other material parameters are taken to be typical values of GaAs, e.g. $m = 0.07m_e$ (m_e being the free electron mass).

In figure 3 we plot the drift velocity v_d as a function of the electric field E at the lattice temperature $T = 300$ K for this family of GaAs-based superlattices assuming a carrier sheet density $N_s = 0.2 \times 10^{15}$ m^{-2} and a low-temperature (4.2 K) linear mobility $\mu(0) = 1.0$ m^2 V^{-1} s^{-1}. The solid curves are calculated from balance equations (1) and (2) with the HW distribution function. Marked NDC is exhibited in all the systems (different miniband widths) investigated. For comparison we plot in figure 4 the drift velocity versus electric field, calculated from Lei's non-parabolic equations (1) and (2) for the same family of superlattices. Also, we plot in figure 3 the calculated results ET model (section 5) for selected systems as open circles, full circles and full triangles. Strangely enough, up to an electric field already very deep in the negative-differential-mobility regime the predictions of the ET model are almost identical with those obtained from balance equations (1) and (2) with the HW function. Compared with the predictions of Lei's non-parabolic method, equations (1) and (2) with the HW function yield a higher peak drift velocity and a much steeper v_d decrease at the NDC regime. This latter behaviour can be seen more clearly from figure 5, where we plot the drift velocity v_d normalized by its peak value v_p as a function of the dimensionless electric field E/E_c (E_c is the electric field at which the drift velocity peaks). For comparison the Esaki–Tsu result [2, 18]

$$\frac{v_d}{v_p} = \frac{2E/E_c}{1 + (E/E_c)^2} \tag{29}$$

is also shown as open circles in this figure. The v_d/v_p versus E/E_c behaviour predicted by Lei's non-parabolic method is somewhat similar to or less steep than that of equation (29). At a given lattice temperature, the larger the miniband width, the steeper is the v_d/v_p versus

E/E_c curve [18]. These predictions are in qualitative agreement with experiments [16, 17], and have also been confirmed by a recent theoretical analysis based on three-dimensional Boltzmann equation [9]. Up to now, a v_d/v_p versus E/E_c behaviour descending at high E/E_c much more steeply than that of equation (2), as predicted by the balance equations with the HW distribution function, has not yet been observed experimentally nor yet been obtained by other theories. Whether it will or not remains to be seen.

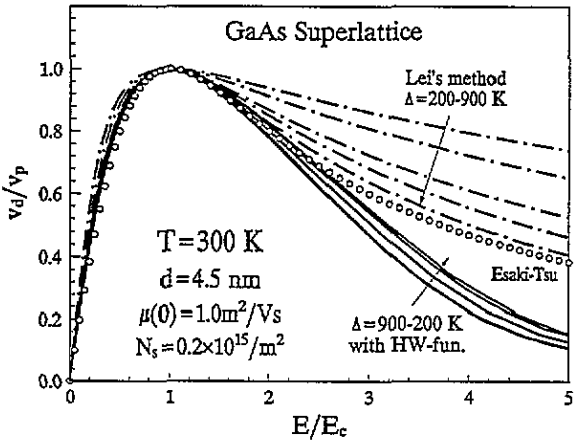

Figure 5. Drift velocity v_d normalized by its peak value v_p shown as a function of the dimensionless electric field E/E_c (E_c is the electric field at which the drift velocity peaks) for the same family of GaAs-based quantum well superlattices as described in figure 3. ——, predictions of balance equations (1) and (2) with the HW distribution function (12); — · —, predictions from Lei's non-parabolic method; O, results of the Esaki–Tsu theory, equation (27).

8. Conclusion

From the analysis based on the Boltzmann transport equation, we have demonstrated that the conventional form of momentum balance equation (10) is generally not a valid equation for an energy band (e.g. a superlattice miniband) whose width (in at least one direction of k-space) is comparable with the ET T_e. A compact moment equation, which is valid for a general energy band and represents an effective momentum balance of the carrier system, can be derived as the moment equation of the Boltzmann equation by choosing the moment operator to be the velocity function $v(k) \equiv \nabla\varepsilon(k)$. This equation turns out to be of the same form as the acceleration balance equation (1) in Lei's non-parabolic method with the original 'distribution function' $f(\varepsilon(k - p_d))$ replaced by a general prescribed distribution function $f(k)$ which is a continuous function of k in the periodic zone scheme. Specifically, putting the HW distribution function $f_v(k)$ into the balance equations (1) and (2), we have another balance equation theory, which, although being equivalent to Lei's non-parabolic method at low fields, represents a different method. On applying these two balance equation theories to non-parabolic Kane bands and superlattice minibands we find that the significant difference between Lei's non-parabolic method and the balance equations (1) and (2) with the HW distribution function is that the latter predicts a normalized v_d/v_p versus E/E_c curve falling down at high E/E_c much more steeply than predicted by the former. So far the available experimental and theoretical results seem to favour the former. Nevertheless, more accurate data are desirable for a definite judgment.

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