Generalized drift-diffusion model for miniband superlattices

L. L. Bonilla, R. Escobedo
Departamento de Matemáticas, Escuela Politécnica Superior,
Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Spain

Álvaro Perales
Departamento de Automática, Escuela Politécnica,
Universidad de Alcalá, 28871 Alcalá de Henares, Spain

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A drift-diffusion model of miniband transport in strongly coupled superlattices is derived from the single-miniband Boltzmann-Poisson transport equation with a BGK (Bhatnagar-Gross-Krook) collision term. We use a consistent Chapman-Enskog method to analyze the hyperbolic limit, at which collision and electric field terms dominate the other terms in the Boltzmann equation. The reduced equation is of the drift-diffusion type, but it includes additional terms, and diffusion and drift do not obey the Einstein relation except in the limit of high temperatures.

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In recent years, nonlinear charge transport in semiconductor superlattices (SLs) has blossomed as a field, driven by the availability of many experimental results and by theoretical analyses and simulations of rate equation models. As it often happens, these models have not been derived from more fundamental “first principles formulizations” such as kinetic theory. The situation is different depending on whether the SLs are weakly or strongly coupled. In weakly coupled SLs, neighboring quantum wells are separated by “thick” barriers and vertical transport occurs via sequential resonant tunneling through them. Provided intersubband scattering is much faster than escape times from a quantum well and the latter are much smaller than dielectric relaxation times, electrons are at local equilibrium in the subband of lowest energy. Then the tunneling current density across a barrier under stationary conditions can be calculated from “first principles” using the Transfer Hamiltonian method. Green functions for a SL under a constant external field, etc. This tunneling current (that depends on the electron density in the two quantum wells separated by the barrier and on the local value of the electric field) is then inserted in a discrete rate equation model including charge continuity and a discrete Poisson equation. No derivation of this very reasonable model seems to be known to this date, although its validity has been corroborated by numerous experiments.

In strongly coupled SLs, barriers are “thin”, minibands are wide, and quantum wells cannot be considered as separate entities. Practical models to analyze nonlinear transport are of the drift-diffusion type or hydrodynamic models. Drift-diffusion equation (DDE) models typically use a drift velocity obtained from a simplified kinetic equation and a diffusion coefficient that obeys the Einstein relation. The resulting model is a variant of the well-known Kroemer DDE for the Gunn effect in bulk n-GaAs. For the large fields involved and for the non-parabolic SL miniband energy, using an Einstein relation to figure out the diffusion coefficient is questionable and, in fact, incorrect except in a particular limit. Hydrodynamic models are considerably more complicated and have been solved numerically, but not many analyses of them have been carried out. The same applies to quantum diffusion theories. “First-principles derivations” typically solve a kinetic equation numerically or approximately assuming a constant applied electric field and ignoring space and time dependence. Then a current density across the SL is calculated for different values of the field, and a drift velocity and a diffusion coefficient are figured out. These functions are then inserted in a DDE. Results that are “valid for any type of SL” typically mean that stationary, space-independent solutions of a sufficiently general kinetic equation have been found numerically. Again the crucial derivation of a rate equation model from a kinetic equation is missing. In this paper, we provide such a derivation starting from a simple Boltzmann-Poisson system that describes one-dimensional (1D) electron transport in the lowest miniband of a strongly coupled SL:

\[
\frac{\partial f}{\partial t} + v(x)\frac{\partial f}{\partial x} + \frac{eF}{\hbar} \frac{\partial f}{\partial k} = -\nu_e (f - f^{FD})
\]

\[
-\nu_i \frac{f(x, k, t) - f(x, -k, t)}{2},
\]

\[
\varepsilon \frac{\partial F}{\partial x} = \frac{e}{l} (n - N_D),
\]

\[
n = \frac{1}{2\pi} \int_{-\pi/l}^{\pi/l} f(x, k, t) dk = \frac{1}{2\pi} \int_{-\pi/l}^{\pi/l} f^{FD}(k; n) dk,
\]

\[
f^{FD}(k; n) = \frac{m* k_B T}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{\mu - E(k)}{k_B T} \right) \right].
\]

Here \(l, \varepsilon, f, n, N_D, k_B, T, F, m^*\) and \(e > 0\) are the SL period, the dielectric constant, the one-particle distribution function, the 2D electron density, the 2D doping density, the Boltzmann constant, the lattice temperature, minus the electric field, the effective mass of the electron, and minus the electron charge, respectively. The first collision term represents energy relaxation to-
We therefore define straightforwardly calculated in terms of its Fourier coefficients as

\[ f^{(0)}(k; n) = \sum_{j=-\infty}^{\infty} f_{j}^{(0)} e^{ijkl}, \]

with \( f_{j}^{(0)} = (1 - i j \mathcal{F}/\tau_e) f_{j}^{FD}/(1 + j^2 \mathcal{F}^2) \), in which \( \mathcal{F} = F/F_M \), \( F_M = \hbar \sqrt{\nu_e (\nu_e + \nu_i)/\epsilon_c} \), and \( \tau_e = \sqrt{\nu_e (\nu_e + \nu_i)/\nu_e} \).

Since \( f_{j}^{FD} \) is an even function of \( k \), its Fourier coefficient \( f_{j}^{FD} \) is real. Note that Eq. (3) implies \( f_{0}^{(0)} = f_{0}^{FD} = n \).

We shall derive a reduced balance equation for the electron density by using the Chapman-Enskog ansatz in Eq. (5):

\[ f(x, k; t) = f^{(0)}(k; n) + \sum_{m=1}^{\infty} \frac{f^{(m)}(k; n)}{m} e^{m}, \]  

\[ \frac{\partial n}{\partial t} = \sum_{m=0}^{\infty} N^{(m)}(n) e^{m}. \]

The coefficients \( f^{(m)}(k; n) \) depend on the ‘slow variables’ \( x \) and \( t \) only through their dependence on the electron density and the electric field (which is itself a functional of \( n \)). The electron density obeys a reduced evolution equation in which the functionals \( N^{(m)}(n) \) are chosen so that the \( f^{(m)}(k; n) \) are bounded and \( 2\pi l \)-periodic in \( k \). Moreover the condition, \( \int_{-\pi/l}^{\pi/l} f^{(m)}(k; n) dk = 2\pi f_{0}^{(m)}/l = 0, \ m \geq 1 \), ensures that \( f^{(m)} \), \( m \geq 1 \), do not contain contributions proportional to the zero-order term \( f^{(0)} \). \( N^{(m)}(n) \) can be found by integrating over \( k \), using, and inserting in the result:

\[ N^{(m)}(n) = \int_{0}^{\pi/l} v(k) f^{(m)}(k; n) dk/(2\pi). \]

Then, integration of Eq. (2) over \( x \) yields

\[ \frac{\varepsilon}{2\pi} \nabla F + \frac{e}{2\pi} \sum_{m=0}^{\infty} \int_{-\pi/l}^{\pi/l} v(k) f^{(m)}(k; n) dk = J(t), \]

where \( J(t) \) is the total current density. To find the equations for \( f^{(m)} \), we insert and into, and equate like powers of \( \varepsilon \):

\[ \mathcal{L} f^{(1)} = - \left( \frac{\partial}{\partial t} + v(k) \frac{\partial}{\partial x} \right) f^{(0)} \bigg|_{0}^{1}, \]  

\[ \mathcal{L} f^{(2)} = - \left( \frac{\partial}{\partial t} + v(k) \frac{\partial}{\partial x} \right) f^{(1)} \bigg|_{0}^{1}, \]

and so on. We have defined \( \mathcal{L} u(k) = e\hbar^{-1} du(k)/dk + (\nu_e + \nu_i/2) u(k) + \nu_i u(-k)/2 \), and the subscripts 0 and 1 mean that \( \partial n/\partial t \) is replaced by \( N^{(0)}(n) \) and by \( N^{(1)}(n) \), respectively.

The linear equation \( \mathcal{L} u = S \) has a bounded \( 2\pi l \)-periodic solution provided \( \int_{-\pi/l}^{\pi/l} S dk = 0 \). This solvability condition together with Eqs. (5), (9), etc. also yield the previously found \( N^{(m)} \) and the reduced equation for \( \mathcal{M} \).

Keeping only the leading order terms in \( \mathcal{M} \), we obtain

\[ \varepsilon \frac{\partial F}{\partial t} + e n \mathcal{M} \left( \frac{n}{N_D} \right) v_M V(\mathcal{F}) = J(t), \]

\[ V(\mathcal{F}) = \frac{2F}{1 + F^2}, \quad v_M = \frac{\Delta l \mathcal{I}_1(M)}{4\hbar \nu_e \mathcal{I}_0(M)}, \]

\[ \mathcal{I}_m(s) = \int_{-\pi}^{\pi} \cos(mk) \ln \left( 1 + e^{-\delta+\delta \cos k} \right) dk. \]
provided $\mathcal{M}(n/N_D) = I_2(\mu) I_0(M)/[I_1(M) I_0(\mu)], \mu \equiv \mu/(k_B T)$, and $\delta = \Delta/(2k_B T)$. Using Eq. (3), the dimensionless chemical potential $\tilde{\mu} = \mu/(n/N_D)$ is calculated graphically in Fig. 1 as a function of $n/N_D$, with $\tilde{\mu}(1) = M$. Then we have $M(1) = 1$. In the Boltzmann limit, $M = 1$ for any $n$, and the electron current density in (10) has the usual drift form. Thus $\mathcal{M}$ is a low-temperature, density-dependent correction to the usual drift current density. The drift velocity, $v_M V(f)$, has the Esaki-Tsu form with a maximum that becomes

$$v_M \approx \Delta I_1(\delta) \sqrt{\pi e}/[4h I_0(\delta) \sqrt{\pi e} + v_i]$$

in the Boltzmann limit (i.e., $I_0(\delta)$ is the modified Bessel function of the first order).

The first-order correction in (1) is found by first solving (8). After straightforward but lengthy calculations and setting $\epsilon = 1$, we obtain (here $g'$ means $dg/dn$):

$$\frac{\partial F}{\partial t} + \mathcal{V}(M) \frac{\partial F}{\partial x} = \frac{eN_D}{I} \left(1 + \frac{\epsilon l}{eN_D} \frac{\partial F}{\partial x}\right)$$

$$= D \left( \frac{\partial F}{\partial x} \right)^2 + A \left( \frac{\partial F}{\partial x} \right) J(t),$$

$$A = 1 + \frac{2ev_M^2 F_M^3}{\epsilon L(v_e + v_i)(F_M^2 + F_e^2)} n_M,$n_M,

$$\mathcal{V} = v_M V(M) \left( A - \frac{\Delta E}{2} \frac{\partial F}{\partial x} \right),$$

$$D = \frac{\Delta \xi F_M}{8\hbar e \tau_e (F_M^2 + F_e^2)} \left(1 - \frac{4\hbar v_M C}{\Delta l}\right),$$

$$B = \frac{(5F_M^2 - 4F_e^2)M_2}{(F_M^2 + 4F_e^2)^2} \frac{4\hbar v_M F_M^2 (F_M^2 - F_e^2)(\tau_e + \tau_e') (nM)'}{\Delta l (F_M^2 + F_e^2)^3},$$

$$C = \frac{\tau_e (F_e^2 - 2F_M^2)(nM_2)'}{F_M^2 + 4F_e^2} + 8\hbar v_M [F_M (nM')]^2 \frac{\Delta l (F_M^2 + F_e^2)^2}{\Delta l (F_M^2 + F_e^2)^3}.$$ (13)

(14)

(15)

(16)

(17)

(18)

Here the density-dependent function $\mathcal{M}_2(n/N_D) = I_3(\mu) I_0(M)/[I_2(M) I_0(\mu)]$ becomes simply the constant $I_2(\delta)/I_1(\delta)$ in the Boltzmann limit. Despite its formidable appearance, the generalized drift-diffusion equation (GDDE) (13) is (in dimensionless units) a small perturbation of the drift equation (12), analyzed in studies of the Gunn effect a long time ago. Table I shows that the solution of the GDDE and (12) yield self-oscillations of the current with frequencies that agree with those measured by Schomburg et al. (14).

An often used DDE consists of Eq. (12) (with $\mathcal{M} \equiv 1$) plus a diffusion term obeying the Einstein relation $\partial F/\partial x$.

$$\frac{\partial F}{\partial t} + \epsilon v_M n \frac{I}{I} V(f) = J(t) + \frac{k_B T e v_M}{F} \frac{\partial n}{\partial x}.$$ (19)

The difference between the predictions of Table I: Numerical values of the oscillation frequencies $v_{\text{num}}$, compared with the experimental value $v_{\text{exp}}$ for five of the SLs of Ref. 13, together with the corresponding applied voltage $\Phi$. $d_w$ and $d_B$ are well and barrier widths, respectively.

| $d_w$ (Å) | $d_B$ (Å) | $N_D/l$ (cm$^{-3}$) | $v_{\text{exp}}$ (GHz) | $v_{\text{num}}$ (GHz) | $\Phi$ (V) |
|-----------|-----------|---------------------|------------------------|------------------------|-----------|
| 51.3      | 8.7       | 1.4 × 10$^{17}$     | 19.44                  | 19.5                   | 0.95      |
| 48        | 9         | 8 × 10$^{16}$       | 29.12                  | 29.1                   | 1.07      |
| 40        | 10        | 8 × 10$^{16}$       | 46.35                  | 46.5                   | 1.2       |
| 36.4      | 9.3       | 10$^{17}$           | 52.79                  | 52.8                   | 1.24      |
| 35.4      | 9.6       | 9 × 10$^{16}$       | 65                     | 65                     | 1.73      |

$N_D = 0.84 \times 10^{11}$ cm$^{-2}$, $\Delta = 43$ meV, $v_e = v_i = 10^{13}$ Hz, $x_0/l = 0.75$. We have selected bias and boundary conditions so that dipole mediated current self-oscillations occur in this SL: voltage bias divided by SL length equals 1.2 $F_M$, and $F = 2J_0/(eN_D V_M)$ at both SL ends. The difference in oscillation frequency and wave shape can be explained by taking into account the equal-area rule as in the theory of the Gunn effect. The taller wave of the GDDE moves at a slower average speed than the wave of (12).

FIG. 2: (a) Current ($J_0 = \epsilon v_M N_D/l$) vs. time during self-oscillations for a 100-period SL at 300K, as described by the GDDE in the Boltzmann limit (solid line) and by the DDE (dashed line). (b) Comparison between the dipole wave for the DDE, (1), and the dipole wave for the GDDE, (2).

For SLs with a smaller value of $\epsilon$, the difference between the predictions of the GDDE and the DDE (12) is smaller. Is there a limit in which these equations agree? To explore this, we calculate the deviation of drift velocity and diffusion coefficient in the GDDE from the Einstein relation (setting $n = N_D$ and $\tilde{\mu} = M$):

$$R(F) = \frac{e F D(F,0)}{k_B T V(F,0)} = \frac{\Delta I_0}{4k_B T l l}$$

\[\text{TABLE I: Numerical values of the oscillation frequencies}\]
FIG. 3: Ratio $R(F)$ at: (a) 10 K, and (b) 300 K. (c) Relative error of the Boltzmann limit result with respect to using the Fermi-Dirac distribution.

For $\epsilon \ll 1$, $R(F) \sim 1 + \frac{\Delta^2}{8k_B T^2} \left[ \frac{3F^2}{2(F_M^2 + 4F^2)} - \frac{F_M^2/(F_M^2 + F^2)}{\epsilon l/F_M^2 + F^2} \right]$. \hfill (21)

Ignoring correcting terms, in this limit the right hand side of Eqs. (21) becomes 1 and the Einstein relation holds. Fig. 3 shows the deviation from the Einstein relation at different temperatures, either using the Fermi-Dirac distribution in Eq. (21), using its Boltzmann limit, or the two-term approximation \hfill (21). Deviations are more appreciable at low temperatures. In the limit $k_B T \gg \max(\Delta, \pi \hbar^2 N_D/m^*)$, the GDDE \hfill (19) becomes the DDE \hfill (19) up to terms of order $\epsilon \delta$ if we set $A = 1 + O(\epsilon) \sim 1$.

In conclusion, we have derived a generalized drift-diffusion model for charge transport in miniband superlattices by means of a consistent Chapman-Enskog method. At all temperatures, its predictions deviate appreciably from those of the usual DDE with the Esaki-Tsu drift velocity and diffusion obeying the Einstein relation. The DDE holds in the limit $\epsilon \ll 1$, $k_B T \gg \max(\Delta, \pi \hbar^2 N_D/m^*)$, which is not very realistic for many strongly coupled SLs, even at room temperature. Detailed analyses and comparison between the predictions of the two DD models and those of the original kinetic equation will be considered in future works.

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1. E-address bonilla@ing.uc3m.es.
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15. This trick avoids using nondimensional equations, thereby enlarging greatly the paper. Our criterion yields $\epsilon = 0.7$ for the SL in Ref. 3 at 300K, overestimating the ratio of the drift term $\nu(k)$$/\partial x$ to the term $(\epsilon F/h)\partial f/\partial k$, or to the collision terms. The asymptotic description of the Gunn effect in F. J. Higueras and L. L. Bonilla, Physica D 57, 161 (1992) shows that, during self-sustained or driven current oscillations, the field variation is larger than $N_M$ and the average drift velocity is smaller than $V_M$. A more realistic estimation yields a 20 times smaller $\epsilon$.

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