In recent years, nonlinear charge transport in semiconductor superlattices (SL's) 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 formulations” such as kinetic theory. The situation is different depending on whether the SL’s are weakly or strongly coupled. In weakly coupled SL’s, 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 (which 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 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:

$$\frac{\partial f}{\partial t} + v(k) \frac{\partial f}{\partial x} + \frac{eF}{\hbar} \frac{\partial f}{\partial k} = -v(k)(f - f^{PD}) - v_i \frac{f(x,k,t) - f(x,-k,t)}{2},$$ (1)

$$\frac{\partial F}{\partial x} = e\frac{\partial}{\partial x} \frac{\partial E}{\partial x} = e \left( n - N_D \right),$$ (2)

$$n = \frac{l}{2\pi} \int_{-\pi/l}^{\pi/l} f(x,k,t) dk = \frac{l}{2\pi} \int_{-\pi/l}^{\pi/l} f^{PD}(k;n) dk,$$ (3)

$$f^{PD}(k;n) = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{\mu - E(k)}{k_B T} \right) \right].$$ (4)

Here l, e, 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 towards a 1D effective Fermi-Dirac distribution \( f^{PD}(k;n) \) (local equilibrium) with collision fre-
frequency \( \nu_e \). The second collision term accounts for impurity elastic collisions: 
\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_0(x,k,k') \delta(E(k) - E(k')) |f(k') - f(k)| d^2k' = 2 \phi_0(x,k,-k)|f(-k) - f(k)|(\Delta l \sin kl) = \nu_l|f(-k) - f(k)|/2,
\]
provided we use the tight-binding miniband dispersion relation, \( E(k) = (\Delta/2)(1 - \cos kl) \) (\( \Delta \) is the miniband width), and ignore transversal degrees of freedom.\(^\text{11}\) For simplicity, \( \nu_e \) and \( \nu_l \) will be fixed constants.

Exact and Fermi-Dirac distribution functions have the same electron density, thereby preserving charge continuity as in the BGK (Bhatnagar-Gross-Krook) models of collision processes.\(^\text{12}\) Then the chemical potential \( \mu \) depends on \( n \) and is found by inverting the exact relation (3); cf. Fig. 1. BGK collision terms with a Boltzmann distribution function, the Boltzmann limit of Eq. (4), were introduced by Ignatov \textit{et al.},\(^\text{13}\) who adapted collision models by Kiticr,ov \textit{et al.} containing inelastic energy relaxation and elastic impurity momentum relaxation terms.\(^\text{14}\)

To derive a reduced balance equation for \( n \), we shall assume that the electric-field contribution in Eq. (1) is comparable to the collision terms and that these terms dominate the other two. This is the so-called hyperbolic limit, in which the ratio of \( \partial f/\partial t \) or \( v(k) \partial f/\partial x \) to \( (eF/\hbar)\partial f/\partial k \) is of order \( \epsilon \ll 1 \). Let \( v_M \), and \( F_M \) be electron velocity and field scales typical of the macroscopic phenomena described by the sought balance equation; for example, let them be the positive values at which the (zeroth order) drift velocity reaches its maximum. In the hyperbolic limit, the time \( t_0 \) it takes an electron with speed \( v_M \) to traverse a distance \( x_0 = eF_M t_0/(\hbar n_{D}) \), over which the field variation is of order \( F_M \), is much longer than the mean free time between collisions, \( \tau_\epsilon^{-1} \approx \tau_t \). We therefore define \( \epsilon = t_1 t_0 = \hbar v_M n_{D}/(eF_M^2) \) and formally multiply the two first terms on the left side of (1) by \( \epsilon \).\(^\text{15}\) After obtaining the number of desired terms, we set \( \epsilon = 1 \). The solution of Eq. (1) for \( \epsilon = 0 \) is straightforwardly calculated in terms of its Fourier coefficients as 
\[
\hat{f}^{(0)}(k;n) = \sum_{\pm} \int_{-\infty}^{\infty} \hat{f}^{(0)}(k,n) e^{i\pm kx} dx,
\]
With \( \hat{f}^{(0)}(1) = (1 - ij \mathcal{F} \tau_\epsilon) \hat{f}^{FD}(1 + j2\mathcal{F}) \), in which \( \mathcal{F} = F/F_M \), \( F_M = \hbar (v_c + v_f)/e \), and \( \tau_\epsilon = (v_c + v_f)/v_e \). Since \( \hat{f}^{FD}(1) \) is an even function of \( k \), its Fourier coefficient \( f^{FD}_j \) is real. Note that Eq. (3) implies \( f^{(0)}_J = f^{FD}_0 = n \).

We shall derive a reduced balance equation for the electron density by using the Chapman-Enskog ansatz,\(^\text{16}\)
\[
f(x,k,t;\epsilon) = f^{(0)}(k;n) + \sum_{m=1}^{\infty} f^{(m)}(k;n) \epsilon^m, \tag{5}
\]
\[
\frac{\partial n}{\partial t} = \sum_{m=1}^{\infty} N^{(m)}(n) \epsilon^m. \tag{6}
\]
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 (6) in which the functionals \( N^{(m)}(n) \) are chosen so that the \( f^{(m)}(k;n) \) are bounded and 2\( \pi \) periodic in \( k \). Moreover, the condition \( \int_{-\pi}^{\pi} f^{(m)}(k;n) dk = 2\pi f^{(m)}_0/1 = m, m \geq 1 \), 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 Eq. (1) over \( k \), using Eq. (3), and inserting Eq. (5) in the result: 
\[
N^{(m)}(n) = -i [\partial f^{(0)}/\partial x] f^{(m)}(k;n) dk/2 \pi. \tag{7}
\]
Then, integration of Eq. (2) over \( x \) yields
\[
\frac{dF}{dt} + \frac{e}{2\pi} \sum_{m=0}^{\infty} \epsilon^m \int_{-\pi}^{\pi} v(k) f^{(m)}(k;n) dk = J(t), \tag{8}
\]
where \( J(t) \) is the total current density. To find the equations for \( f^{(m)} \), we insert Eq. (5) and (6) in Eq. (1), and equate like powers of \( \epsilon \):
\[
\mathcal{L}_f^{(1)} = -\left( \frac{\partial}{\partial t} + v(k) \frac{\partial}{\partial x} \right) f^{(0)}|_0, \tag{9}
\]
and so on. We have defined \( \mathcal{L} u(k) = eF \hbar^{-1} d\mu(k)/dk + (\nu_e + \nu_f/2) u(k) + \nu_e u_- (k)/2 \), and the subscript 0 and 1 mean that \( \partial n/\partial t \) is replaced by \( \nu^{(0)}(n) \) and by \( \nu^{(1)}(n) \), respectively.

The linear equation \( \mathcal{L} u = -S \) has a bounded 2\( \pi \)-periodic solution provided \( \int_{-\pi}^{\pi} S dk = 0 \). This solvability condition together with Eqs. (8), (9), etc., also yield the previously found \( N^{(m)} \) and the reduced equation (7). Keeping only the leading order terms in Eq. (7), we obtain
\[
\frac{dF}{dt} + \frac{n}{1 + F^2} \mathcal{M} \frac{n}{N_D} v_M V(\mathcal{F}) = J(t), \tag{10}
\]
\[
V(\mathcal{F}) = \frac{2 \mathcal{F}}{1 + \mathcal{F}^2}, \quad v_M = \frac{\Delta l T(M)}{4 h \tau_\epsilon l_0(M)}, \tag{11}
\]
\[
\mathcal{I}_m(s) = \int_{-\pi}^{\pi} \cos (ms) \ln (1 + e^{-\delta + \delta \cos k}) dk, \tag{12}
\]
provided \( \mathcal{M}(n/N_D) = \mathcal{I}_1(\mu) I_0(M)/[\mathcal{I}_1(M) I_0(\mu) \mu = \mu I(k_B T), \text{ and } \delta = \Delta l(2k_B T). \) Using Eq. (3), the dimensionless chemical potential \( \mu = \mu (n/N_D) \) is calculated.
Here the density-dependent function $M$ of the generalized drift-diffusion equation has the Esaki-Tsu form with a maximum that becomes $v_M = \Delta I(\delta) \sqrt{v_e / [4hI_0(\delta) \sqrt{v_e + v_i}]}$ in the Boltzmann limit. The first-order correction in Eq. (7) is found by first solving Eq. (8). After straightforward but lengthy calculations and setting $\epsilon = 1$, we obtain (here $g'$ means $dg/dn$):

$$
\frac{\partial F}{\partial t} + v M V(F) = \frac{eM}{l} \left( 1 + \frac{\epsilon}{e M} \frac{\partial F}{\partial x} \right) - D \left( \frac{\partial F}{\partial x} \right) e \frac{\partial^2 F}{\partial x^2} + A \left( \frac{\partial F}{\partial x} \right) J(t),
$$

where

$$
A = 1 + \frac{2eV_{M}F_{M}^{2}F_{M}^{2}-(1+2\tau_{e})F^{2}}{\epsilon l (v_{e}+v_{i})(F_{M}^{2}+F^{2})^{3}} n M,
$$

and

$$
\nu = v_{M}V M \left( A - \frac{\Delta B}{2 \epsilon} \frac{\partial F}{\partial x} \right),
$$

$$
D = \frac{\Delta^{2} l F_{M}}{8h e \tau_{e} (F_{M}^{2}+F^{2})} \left( 1 - \frac{4h v_{M} C}{\Delta l} \right),
$$

$$
B = \frac{5F_{M}^{2}-4F^{2}}{(F_{M}^{2}+4F^{2})^{2}} M
$$

$$
- \frac{4h v_{M} F_{M}^{2}(F_{M}^{2}-F^{2})(\tau_{e} + \tau_{e}^{-1})(n M)^{y}}{\Delta l (F_{M}^{2}+F^{2})^{3}},
$$

$$
C = - \frac{\tau_{e}(F_{M}^{2}-2F^{2})(n M)^{y}}{F_{M}^{2}+4F^{2}} + \frac{8h v_{M} [F M (n M)^{y}]}{\Delta l (F_{M}^{2}+F^{2})^{2}}.
$$

Here the density-dependent function $M(n/N_{D}) = I_{2}(\tilde{\mu}) I_{0}(M) / [I_{0}(\tilde{\mu}) I_{1}(M)]$ 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 (10), analyzed in studies of the Gunn effect a long time ago. Table I shows that the solution of the GDDE and Eq. (2) yield self-oscillations of the current with frequencies that agree with those measured by Schomburg et al. An often used DDE consists of Eq. (10) (with $M = 1$) plus a diffusion term obeying the Einstein relation.

<table>
<thead>
<tr>
<th>$d_{W}$ (Å)</th>
<th>$d_{B}$ (Å)</th>
<th>$N_{D}/l$ (cm$^{-2}$)</th>
<th>$\nu_{exp}$ (GHz)</th>
<th>$\nu_{num}$ (GHz)</th>
<th>$\Phi$ (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>51.3</td>
<td>8.7</td>
<td>$1.4 \times 10^{17}$</td>
<td>19.44</td>
<td>19.5</td>
<td>0.95</td>
</tr>
<tr>
<td>48</td>
<td>9</td>
<td>$8 \times 10^{16}$</td>
<td>29.12</td>
<td>29.1</td>
<td>1.07</td>
</tr>
<tr>
<td>40</td>
<td>10</td>
<td>$8 \times 10^{16}$</td>
<td>46.35</td>
<td>46.5</td>
<td>1.2</td>
</tr>
<tr>
<td>36.4</td>
<td>9.3</td>
<td>$10^{17}$</td>
<td>52.79</td>
<td>52.8</td>
<td>1.24</td>
</tr>
<tr>
<td>35.4</td>
<td>9.6</td>
<td>$9 \times 10^{16}$</td>
<td>65</td>
<td>65</td>
<td>1.73</td>
</tr>
</tbody>
</table>

The difference between the predictions of Eqs. (13) and (19) can be remarkable if the dimensionless parameter $\tilde{\epsilon}$ is relatively large and the dimensionless coefficient $\delta = \Delta / (2k_{B}T)$ is not small, as illustrated in Fig. 2. The parameter values in this figure correspond to the 5.13-nm GaAs/0.87-nm AlAs SL of Ref. 18, for which $\epsilon = 0.34; N_{D} = 0.84 \times 10^{11}$ cm$^{-2}$, $\Delta = 55$ meV, $\nu_{e} = \nu_{i} = 10^{13}$ Hz, $x_{f} / l = 0.75$. 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 $1.2F_{M}$, and $F = 2jl(eN_{D}v_{M})$ 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 Eq. (19).

For SL's with a smaller value of $\epsilon$, the difference between the predictions of the GDDE and the DDE (19) 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 $\tilde{\mu} = M$):

$$
\frac{\partial F}{\partial t} + \frac{eM}{l} V(F) = J(t) + \frac{k_{B}T v_{M}}{F^{3}} V(F) \frac{\partial F}{\partial x}.
$$

The table below shows the numerical values of the oscillation frequencies $\nu_{num}$ compared with the experimental value $\nu_{exp}$ for five of the SL's of Ref. 18, together with the corresponding applied voltage $\Phi$. $d_{W}$ and $d_{B}$ are well and barrier widths, respectively.

![FIG. 2. (Color online) (a) Current ($J_{o} = ev_{M}N_{D}/l$) vs time during self-oscillations for a 100-period SL at 300 K, 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 GDDE (1) and the dipole wave for the DDE, (2).]
\[ R(F) = \frac{e F D(F,0)}{k_B T V(F,0)} = \frac{\Delta I_0}{4k_B T I_1} \]

\[ R(F) = \frac{1 - 2 F^2 / 1 + 4 F^2}{1 + 2 F^2 / (1 + F^2)^2} \left[ \frac{\Delta I_0}{I_0} \right] \]

\[ + \frac{e^2 \Delta \ln N_D[1 - (1 + \tau_f^2) F^2]}{2 e h^2 (v_+ + v_I) I_0 (1 + F^2)^3} \]

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.

In the Boltzmann limit, \( \exp(\mu - \delta + \delta \cos k l) \ll 1 \), and we can substitute the modified Bessel functions \( I_{\nu}(\delta) \) instead of \( \mathcal{I}_n(M) \) in the previous formula. Moreover, Eqs. (3) and (4) give \( n_\alpha = e^{\mu - \delta} I_0(\delta) \rho_0 N_D \), where \( \rho_0 = m^* k_B T / (\pi h^2 N_D) \). For \( n = N_D \), the Boltzmann limit holds provided \( \rho_0 \gg 1 \). If we also have \( \delta = \Delta/(2k_B T) \ll 1 \), Eq. (20) becomes

\[ R(F) \sim 1 + \frac{\Delta^2}{8k_B^2 T^2} \left[ \frac{3 F^2}{2(F_M^2 + 4F^2)} - \frac{F_M^2 \tau_f^2}{(F_M^2 + F^2)^2} \right] \times \left[ \frac{k_B T N_D[F_M^2 - (1 + \tau_f^2) F^2]}{\epsilon l(F_M^2 + F^2)} + F^2 \right]. \]

Ignoring correcting terms, in this limit the right-hand side of Eq. (21) becomes 1 and the Einstein relation holds. Figure 3 shows the deviation from the Einstein relation at different temperatures, either using the Fermi-Dirac distribution in Eq. (1), using its Boltzmann limit, or the two-term approximation (21). Deviations are more appreciable at low temperatures. In the limit \( k_B T \gg \max(\Delta, \tau_f N_D/m^*) \), the GDDE (13) becomes the DDE (19) up to terms of order \( \epsilon \delta \) if we set \( A = 1 + O(\epsilon) \approx 1 \).

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 \( \epsilon \ll 1, k_B T \gg \max(\Delta, \tau_f N_D/m^*) \), which is not very realistic for many strongly coupled SL’s, 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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