
Quantum kinetic and drift-diffusion equations for semiconductor superlattices

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Summary. A nonlocal (quantum) drift-diffusion equation for the electric field and the electron density is derived from a Wigner-Poisson equation modelling quantum vertical transport in strongly coupled semiconductor superlattices, by using a consistent Chapman-Enskog procedure. Numerical solutions for a device consisting of a n-doped superlattice placed in a $n^+ - n - n^+$ diode under a constant voltage bias are presented and compared with those obtained by using a semiclassical approximation.

Key words: superlattices, Chapman-Enskog, quantum drift-diffusion eq.

Industrial uses of semiconductor superlattices (SLs) include fast nanoscale oscillators, terahertz and infrared detectors and quantum cascade lasers. The Wigner-Poisson system for 1D electron transport in the lowest miniband of a strongly coupled SL is:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{i}{\hbar} \left[\mathcal{E} \left(k + \frac{1}{2i} \frac{\partial}{\partial x} \right) - \mathcal{E} \left(k - \frac{1}{2i} \frac{\partial}{\partial x} \right) \right] f \\ + \frac{ie}{\hbar} \left[W \left(x + \frac{1}{2i} \frac{\partial}{\partial k}, t \right) - W \left(x - \frac{1}{2i} \frac{\partial}{\partial k}, t \right) \right] f = Q[f], \end{aligned} \quad (1)$$

$$\varepsilon \frac{\partial^2 W}{\partial x^2} = \frac{e}{l} (n - N_D), \quad (2)$$

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

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

Here f , n , N_D , $\mathcal{E}(k)$, l , k_B , T , W , ε , m^* and $e > 0$ are the one-particle Wigner function, the 2D electron density, the 2D doping density, the miniband dispersion relation, the SL period, the Boltzmann constant, the lattice temperature, the electric potential, the SL permittivity, the effective mass of the electron, and minus the electron charge, respectively. The left-hand side of Eq. (1)

can be straightforwardly derived from the Schrödinger-Poisson equation for the wave function in the miniband using the definition of the 1D Wigner function: $f(x, k, t) = \sum_{j=-\infty}^{\infty} \int \psi(x + jl/2, y, z, t) \psi(x - jl/2, y, z, t) e^{ijk l} dx_{\perp}$ [$\psi(x, x_{\perp}, t) = \sum_{q, q_{\perp}} a(q, q_{\perp}, t) \phi_q(x) e^{iq_{\perp} \cdot x_{\perp}}$, $x_{\perp} = (y, z)$, is a superposition of the Bloch states corresponding to the miniband]. The collision term $-Q[f]$ in Eq. (1) is the sum of $\nu_e (f - f^{FD})$, which represents energy relaxation towards a 1D effective Fermi-Dirac (FD) distribution $f^{FD}(k; n)$ (local equilibrium), and $\nu_i [f(x, k, t) - f(x, -k, t)]/2$, which accounts for impurity elastic collisions [Bonilla et al. (2003)]. For simplicity, the collision frequencies ν_e and ν_i are fixed constants. Exact and FD distribution functions have the same electron density, thereby preserving charge continuity as in the Bhatnagar-Gross-Krook (BGK) collision models [Bhatnagar et al. (1954)]. Then the chemical potential μ depends on n and is found by inverting the exact relation (3).

It is convenient to derive the charge continuity equation and a nonlocal Ampère's law for the current density. The Wigner function f is periodic in k ; its Fourier expansion is $\sum_{j=-\infty}^{\infty} f_j(x, t) e^{ijk l}$. Defining $F = \partial W / \partial x$ (*minus* the electric field) and the average $\langle F \rangle_j(x, t) = \frac{1}{jl} \int_{-jl/2}^{jl/2} F(x + s, t) ds$, it is possible to obtain the following equivalent form of the Wigner equation

$$\frac{\partial f}{\partial t} + \sum_{j=-\infty}^{\infty} \frac{ijl}{\hbar} e^{ijk l} \left(\mathcal{E}_j \frac{\partial}{\partial x} \langle f \rangle_j + e \langle F \rangle_j f_j \right) = Q[f], \quad (5)$$

where $\mathcal{E}(k) = \Delta(1 - \cos kl)/2$ is the tight-binding dispersion relation (Δ is the miniband width) and $v(k) = \frac{\Delta l}{2\hbar} \sin kl$ is the miniband group velocity. Integrating this equation over k yields the charge continuity equation $\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \sum_{j=1}^{\infty} \frac{2jl}{\hbar} \langle \text{Im}(\mathcal{E}_{-j} f_j) \rangle_j = 0$, from which we can eliminate the electron density by using the Poisson equation and integrating over x , thereby obtaining the nonlocal Ampère's law for the total current density $J(t)$:

$$\varepsilon \frac{\partial F}{\partial t} + \frac{2e}{\hbar} \sum_{j=1}^{\infty} j \langle \text{Im}(\mathcal{E}_{-j} f_j) \rangle_j = J(t). \quad (6)$$

To derive the QDDE, we shall assume that the electric field contribution in Eq. (5) is comparable to the collision terms and that they dominate the other terms (*the hyperbolic limit*) [Bonilla et al. (2003)]. Let v_M and F_M be the electron velocity and field positive values at which the (zeroth order) drift velocity reaches its maximum. In this limit, the time t_0 it takes an electron with speed v_M to traverse a distance $x_0 = \varepsilon F_M l / (e N_D)$, over which the field variation is of order F_M , is much longer than the mean free time between collisions, $\nu_e^{-1} \sim \hbar / (e F_M l) = t_1$. We therefore define the *small parameter* $\epsilon = t_1 / t_0 = \hbar v_M N_D / (\varepsilon F_M^2 l^2)$ and formally multiply the first two terms on the left side of (1) or (5) by ϵ [Bonilla et al. (2003)]. After obtaining the number of desired terms, we set $\epsilon = 1$. The solution of Eq. (5) for $\epsilon = 0$ is calculated in terms of its Fourier coefficients as

$$f^{(0)}(k; F) = \sum_{j=-\infty}^{\infty} \frac{(1 - ij\mathcal{F}/\tau_e) f_j^{FD}}{1 + j^2 \mathcal{F}^2} e^{ijkl}, \quad (7)$$

where $\mathcal{F} = \langle F \rangle_1 / F_M$, $F_M = \frac{\hbar}{e l} \sqrt{\nu_e(\nu_e + \nu_i)}$ and $\tau_e = \sqrt{(\nu_e + \nu_i) / \nu_e}$.

The Chapman-Enskog ansatz for the Wigner function is [Bonilla et al. (2003)]:

$$f(x, k, t; \epsilon) = f^{(0)}(k; F) + \sum_{m=1}^{\infty} f^{(m)}(k; F) \epsilon^m, \quad (8)$$

$$\epsilon \frac{\partial F}{\partial t} + \sum_{m=0}^{\infty} J^{(m)}(F) \epsilon^m = J(t). \quad (9)$$

The coefficients $f^{(m)}(k; F)$ depend on the ‘slow variables’ x and t only through their dependence on the electric field and the electron density. The electric field obeys a reduced evolution equation (9) in which the functionals $J^{(m)}(F)$ are chosen so that the $f^{(m)}(k; F)$ are bounded and $2\pi/l$ -periodic in k . Differentiating the Ampère’s law (9) with respect to x , we obtain the charge continuity equation. 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 $f^{(0)}$. Inserting (8) and (9) in (5), we find the hierarchy:

$$\mathcal{L}f^{(1)} = - \left(\frac{\partial f^{(0)}}{\partial t} + \sum_{j=-\infty}^{\infty} \frac{ijl\mathcal{E}_j e^{ijkl}}{\hbar} \frac{\partial}{\partial x} \langle f^{(0)} \rangle_j \right) \Big|_0 \quad (10)$$

$$\mathcal{L}f^{(2)} = - \left(\frac{\partial f^{(1)}}{\partial t} + \sum_{j=-\infty}^{\infty} \frac{ijl\mathcal{E}_j e^{ijkl}}{\hbar} \frac{\partial}{\partial x} \langle f^{(1)} \rangle_j \right) \Big|_0 - \frac{\partial}{\partial t} f^{(0)} \Big|_1, \quad (11)$$

and so on, where $\mathcal{L}u(k) \equiv ie\hbar^{-1} \sum_{j=-\infty}^{\infty} jl \langle F \rangle_j u_j e^{ijkl} + (\nu_e + \nu_i/2)u(k) + \nu_i u(-k)/2$, and the subscripts 0 and 1 in the right hand side of these equations mean that $\epsilon \partial F / \partial t$ is replaced by $J - J^{(0)}(F)$ and by $-J^{(1)}(F)$, respectively.

The solvability conditions for the linear hierarchy of equations yield $J^{(m)} = \frac{2e}{\hbar} \sum_{j=1}^{\infty} j \langle \text{Im}(\mathcal{E}_{-j} f_j^{(m)}) \rangle_j$, which can also be obtained by insertion of Eq. (8) in (6). In the tight-binding dispersion relation case, the leading order of the Ampère’s law (9) is

$$\epsilon \frac{\partial F}{\partial t} + \frac{ev_M}{l} \langle n \mathcal{M} V(\mathcal{F}) \rangle_1 = J(t), \quad (12)$$

$$V(\mathcal{F}) = \frac{2\mathcal{F}}{1 + \mathcal{F}^2}, \quad v_M = \frac{\Delta l \mathcal{I}_1(M)}{4\hbar\tau_e \mathcal{I}_0(M)}, \quad \mathcal{M} \left(\frac{n}{N_D} \right) = \frac{\mathcal{I}_1(\tilde{\mu}) \mathcal{I}_0(M)}{\mathcal{I}_1(M) \mathcal{I}_0(\tilde{\mu})}, \quad (13)$$

$$\mathcal{I}_m(s) = \int_{-\pi}^{\pi} \cos(mk) \ln(1 + e^{s - \delta + \delta \cos k}) dk, \quad (14)$$

provided $\delta = \Delta/(2k_B T)$ and $\tilde{\mu} \equiv \mu/(k_B T)$. Here M (calculated graphically in Fig. 1 of Ref. [Bonilla et al. (2003)]) is the value of the dimensionless chemical potential $\tilde{\mu}$ at which (3) holds with $n = N_D$. The drift velocity $v_M V(\mathcal{F})$ has the Esaki-Tsu form with a peak velocity that becomes $v_M \approx \Delta I_1(\delta)/[4\hbar\tau_e I_0(\delta)]$ in the Boltzmann limit [Ignatov et al. (1987)] ($I_n(\delta)$ is the modified Bessel function of the n th order).

To find the first-order correction in (9), we first solve (10) and find $J^{(m)}$ for $m = 1$. The calculation yields the first correction to Eq. (12) (here $'$ means differentiation with respect to n): [Bonilla et al. (2003)]

$$\varepsilon \frac{\partial F}{\partial t} + \frac{ev_M}{l} \mathcal{N} \left(F, \frac{\partial F}{\partial x} \right) = \varepsilon \left\langle D \left(F, \frac{\partial F}{\partial x}, \frac{\partial^2 F}{\partial x^2} \right) \right\rangle_1 + \langle A \rangle_1 J(t), \quad (15)$$

$$A = 1 + \frac{2ev_M}{\varepsilon F_M l (\nu_e + \nu_i)} \frac{1 - (1 + 2\tau_e^2) \mathcal{F}^2}{(1 + \mathcal{F}^2)^3} n \mathcal{M}, \quad (16)$$

$$\mathcal{N} = \langle n V \mathcal{M} \rangle_1 + \langle (A - 1) \langle n V \mathcal{M} \rangle_1 \rangle_1 - \frac{\Delta l \tau_e}{F_M \hbar (\nu_e + \nu_i)} \left\langle \frac{B}{1 + \mathcal{F}^2} \right\rangle_1, \quad (17)$$

$$D = \frac{\Delta^2 l^2}{8\hbar^2 (\nu_e + \nu_i) (1 + \mathcal{F}^2)} \left(\frac{\partial^2 \langle F \rangle_1}{\partial x^2} - \frac{4\hbar v_M \tau_e C}{\Delta l} \right) \quad (18)$$

$$B = \left\langle \frac{4\mathcal{F}_2 n \mathcal{M}_2}{(1 + 4\mathcal{F}_2^2)^2} \frac{\partial \langle F \rangle_2}{\partial x} \right\rangle_1 + \mathcal{F} \left\langle \frac{n \mathcal{M}_2 (1 - 4\mathcal{F}_2^2)}{(1 + 4\mathcal{F}_2^2)^2} \frac{\partial \langle F \rangle_2}{\partial x} \right\rangle_1, \quad (19)$$

$$- \frac{4\hbar v_M (1 + \tau_e^2) \mathcal{F} (n \mathcal{M})'}{\Delta l \tau_e (1 + \mathcal{F}^2)} \left\langle n \mathcal{M} \frac{1 - \mathcal{F}^2}{(1 + \mathcal{F}^2)^2} \frac{\partial \langle F \rangle_1}{\partial x} \right\rangle_1,$$

$$C = \left\langle \frac{(n \mathcal{M}_2)'}{1 + 4\mathcal{F}_2^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1 - 2\mathcal{F} \left\langle \frac{(n \mathcal{M}_2)' \mathcal{F}_2}{1 + 4\mathcal{F}_2^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1, \quad (20)$$

$$+ \frac{8\hbar v_M (1 + \tau_e^2) (n \mathcal{M})' \mathcal{F}}{\Delta l \tau_e (1 + \mathcal{F}^2)} \left\langle \frac{(n \mathcal{M})' \mathcal{F}}{1 + \mathcal{F}^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1.$$

Here $\mathcal{M}_2(n/N_D) \equiv \mathcal{I}_2(\tilde{\mu}) \mathcal{I}_0(M)/[\mathcal{I}_1(M) \mathcal{I}_0(\tilde{\mu})]$ and $\mathcal{F}_2 \equiv \langle F \rangle_2/F_M$. If the electric field and the electron density do not change appreciably over two SL periods, $\langle F \rangle_j \approx F$, the spatial averages can be ignored, and the *nonlocal* QDDE (15) becomes the *local* generalized DDE (GDDE) obtained from the semiclassical theory [Bonilla et al. (2003)]. The boundary conditions for the QDDE (15) (which contains triple spatial averages) need to be specified on the intervals $[-2l, 0]$ and $[Nl, Nl + 2l]$, not just at the points $x = 0$ and $x = Nl$, as in the case of the parabolic GDDE. Similarly, the initial condition has to be defined on the extended interval $[-2l, Nl + 2l]$.

Fig. 1 shows the evolution of the current during the self-sustained oscillations that appear when the QDDE (15) and (2) are solved for boundary conditions $\varepsilon \partial F / \partial t + \sigma F = J$ at each point of the intervals $[-2l, 0]$ and $[Nl, Nl + 2l]$ and appropriate dc voltage bias. The contact conductivity σ is selected so that σF intersects $e N_D v_M V(F/F_M)/l$ on its decreasing branch, as in the theory of the Gunn effect [Bonilla (2002)]. Parameter values correspond to a 157-period 3.64 nm GaAs/0.93 nm AlAs SL at 5K, with $N_D = 4.57 \times 10^{10} \text{ cm}^{-2}$,

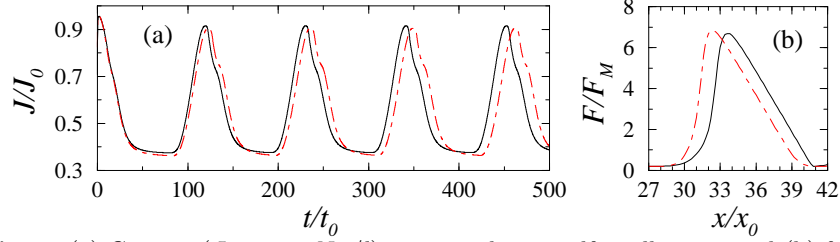


Fig. 1. (a) Current ($J_0 = ev_M N_D / l$) vs. time during self-oscillations, and (b) fully developed dipole wave. Solid line: QDDE, dashed line: GDDE. Parameter values: $x_0 = 16$ nm, $t_0 = 0.24$ ps, $J_0 = 1.10 \times 10^5$ A/cm².

$\nu_i = 2\nu_e = 18 \times 10^{12}$ Hz under a dc voltage bias of 1.62 V. Cathode and anode contact conductivities are 2.5 and 0.62 $\Omega^{-1}\text{cm}^{-1}$, respectively.

We observe that the field profile of the dipole wave during self-oscillations is sharper in the case of the GDDE than in the case of the QDDE. The local spatial averages appearing in the QDDE have a smoothing effect on the sharp gradients of the electric field. This smoothing effect produces rounder and smaller dipole waves in the QDDE, as compared to the same solution for the GDDE. The equal-area rule as in the theory of the Gunn effect hints that smaller waves are faster [Bonch-Bruevich et al. (1975)], resulting in a slightly larger frequency for the self-oscillations in the QDDE (37.6 GHz) than in the case of the GDDE (36.8 GHz).

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