

WIGNER–POISSON AND NONLOCAL DRIFT-DIFFUSION MODEL EQUATIONS FOR SEMICONDUCTOR SUPERLATTICES

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A Wigner–Poisson kinetic equation describing charge transport in doped semiconductor superlattices is proposed. Electrons are assumed to occupy the lowest miniband, exchange of lateral momentum is ignored and the electron–electron interaction is treated in the Hartree approximation. There are elastic collisions with impurities and inelastic collisions with phonons, imperfections, etc. The latter are described by a modified BGK (Bhatnagar–Gross–Krook) collision model that allows for energy dissipation while yielding charge continuity. In the hyperbolic limit, nonlocal drift-diffusion equations are derived systematically from the kinetic Wigner–Poisson–BGK system by means of the Chapman–Enskog method. The nonlocality of the original quantum kinetic model equations implies that the derived drift-diffusion equations contain spatial averages over one or more superlattice periods. Numerical solutions of the latter equations show self-sustained oscillations of the current through a voltage biased superlattice, in agreement with known experiments.

1. Introduction

Nonlinear charge transport in semiconductor superlattices has been widely studied in the last decade.^{1,2} A superlattice (SL) is a convenient approximation to a quasi-one-dimensional crystal that was originally proposed by Esaki and Tsu to observe Bloch oscillations, i.e. the periodic coherent motion of electrons in a miniband in the presence of an applied electric field. When the materials were grown, many interesting nonlinear phenomena were observed, including self-oscillations of the current through the SL due to motion of electric field pulses, multistability of stationary solutions, and so on.^{1,2} In the effort to describe quantitatively transport in these materials, a large number of quantum and semiclassical equations, hydrodynamic and drift-diffusion models have been proposed. However, systematic derivations of reduced balance equations (hydrodynamic or drift-diffusion equations) are scarce.

Hydrodynamic equations have been derived by Lei and co-workers^{3,4} and their numerical solutions describe self-oscillations of the current in different regimes.⁵ They write operator Heisenberg equations, and average them to obtain a hierarchy of equations for moments such as electron density, current and energy. These equations are then closed by using a Fermi–Dirac local equilibrium ansatz, which clearly does not amount to a systematic procedure, nor gives a clue to the validity of the resulting hydrodynamic equations. A similar closure procedure has been recently developed for the case of quantum particles in an arbitrary external three-dimensional potential by Degond and Ringhofer,⁶ who have used the maximum entropy principle to select their local equilibrium. These authors employ an operator form of a local Maxwellian in their examples, which therefore do not obey the Pauli exclusion principle. Earlier, Huang and Wu⁷ found a local Fermi–Dirac distribution function as a basis of their hydrodynamic equations by using a different definition of entropy.

For SL drift-diffusion models, systematic derivation procedures do exist. Many authors have used the Einstein relation to write a field-dependent diffusion coefficient from the electron drift velocity. The latter was obtained by Ignatov and Shashkin⁸ from a simple solution of a Bhatnagar–Gross–Krook (BGK) kinetic equation.⁹ Recently, we have used the Chapman–Enskog method to derive a generalized drift-diffusion equation (GDDE) from a BGK–Poisson system.¹⁰ Interestingly, the Einstein relation does not hold, except in a very particular high-temperature limit.¹⁰ Earlier, Cercignani, Gamba and Levermore had used essentially the same method to obtain reduced balance equations for a semiclassical BGK–Poisson semiconductor system treating the band dispersion relation in the parabolic approximation.¹¹ The aim of this paper is to extend these methods to quantum kinetic equations. To this end, we shall derive a Wigner–Poisson system of equations for a SL having only one populated miniband, ignore changes in lateral momentum and model the collisions in the BGK approximation. The resulting quantum kinetic equation is

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{i}{\hbar} \left[\mathcal{E}_1 \left(k + \frac{1}{2i} \frac{\partial}{\partial x} \right) - \mathcal{E}_1 \left(k - \frac{1}{2i} \frac{\partial}{\partial x} \right) \right] f \\ + \frac{ie}{\hbar} \left[W \left(x + \frac{1}{2i} \frac{\partial}{\partial k}, t \right) - W \left(x - \frac{1}{2i} \frac{\partial}{\partial k}, t \right) \right] f \\ = -\nu_{\text{en}} (f - f^{\text{FD}}) - \nu_{\text{imp}} \frac{f(x, k, t) - f(x, -k, t)}{2}, \end{aligned} \tag{1.1}$$

$$\varepsilon \frac{\partial^2 W}{\partial x^2} = \frac{e}{l} (n - N_D), \tag{1.2}$$

$$n = \frac{l}{2\pi} \int_{-\pi/l}^{\pi/l} f(x, k, t) dk = \frac{l}{2\pi} \int_{-\pi/l}^{\pi/l} f^{\text{FD}}(k; n) dk, \tag{1.3}$$

$$\begin{aligned} f^{\text{FD}}(k; n) = \frac{m^* k_B T}{\pi^2 \hbar^2} \left\{ \tan^{-1} \left(\frac{\Gamma}{\mathcal{E}_1(k)} \right) \right. \\ \left. + \int_0^\infty \frac{\Gamma}{[E - \mathcal{E}_1(k)]^2 + \Gamma^2} \ln \left[1 + \exp \left(\frac{\mu - E}{k_B T} \right) \right] dE \right\}. \end{aligned} \tag{1.4}$$

Here f : one-particle Wigner function, n : the 2D electron density, N_D : the 2D doping density, $\mathcal{E}_1(k)$: the miniband dispersion relation, d_B : the barrier width, d_W : the well width, $l = d_B + d_W$: the SL period, W : the electric potential, ε : the SL permittivity, m^* : the effective mass of the electron, k_B : the Boltzmann constant, T : the lattice temperature, Γ : the energy broadening of the equilibrium distribution due to collisions, ν_{en} : the frequency of the inelastic collisions responsible for energy relaxation, ν_{imp} : the frequency of the elastic impurity collisions and $-e < 0$: the electron charge. The chemical potential μ is a function of n resulting from solving Eq. (1.3) with the integral of the collision-broadened 3D Fermi–Dirac distribution over the lateral components of the wave vector (k, k_y, k_z) , which is given by Eq. (1.4). Note that, following Ignatov and Shashkin,⁸ we have not included the effects of the electric potential in our Fermi–Dirac distribution. As discussed later, the model equations we use can be improved by including scattering processes with change of lateral momentum and an electric field-dependent local equilibrium. However, the resulting model could only be treated numerically and the qualitative features of our derivation and nonlocal drift-diffusion equation would be lost in longer formulas.

The Wigner–Poisson–Bhatnagar–Gross–Krook (WPBGK) system (1.1) to (1.4) should be solved for a Wigner function which is $2\pi/l$ -periodic in k and satisfies appropriate initial and boundary conditions. If we integrate (1.1) over k and use the periodicity condition, only the first two terms on its left-hand side yield nonzero contributions which, in fact provide the charge continuity equation as we shall see later. Equation (1.1) contains two pseudo-differential operators, depends on the unknown electric potential W and is nonlocal in x . However, the fact that f is $2\pi/l$ -periodic in k makes it possible to use a modification of the Chapman–Enskog method along the lines of that used in Refs. 11 and 10 for the semiclassical case and earlier in Refs. 12 and 13 for nonlinear Fokker–Planck equations. The result is a generalized drift-diffusion equation for the electric field which is nonlocal in space because it contains averages of the electric field over one or more SL periods. The nonlocality of the *quantum drift-diffusion equation* (QDDE) is a direct consequence of the nonlocality of the Wigner equation (1.1).

In this paper, we derive the WPBGK system, deduce the nonlocal QDDE by means of the Chapman–Enskog method and solve it numerically to illustrate the resulting self-sustained oscillations of the current through a finite superlattice subject to an appropriate dc voltage bias. The rest of the paper is organized as follows. In Sec. 2 we derive the WPBGK system. In Sec. 3, we study the hyperbolic limit of the WPBGK system and use the Chapman–Enskog method to derive the reduced equation to leading order. This equation is hyperbolic, and we would like to regularize possible singularities. Diffusive terms are obtained in Sec. 3 by calculating the first-order terms in the Chapman–Enskog expansion. The resulting QDDE is discussed in Sec. 4 and solved numerically for appropriate voltage bias conditions. Finally, Sec. 5 contains a discussion of our results.

2. Derivation of the Quantum Kinetic Equation

Let us consider an n -doped SL formed by periodic alternation of two different semiconductors such as GaAs (quantum well W) and AlAs (barrier B). The SL cross section S is much larger than l^2 , the square of the SL period. For n -doped SLs, we can restrict ourselves to studying electronic transport in the conduction band of the SL. We shall assume that the SL is under a dc voltage bias, which is equivalent to an external electric field directed along the SL growth direction. The corresponding Hamiltonian is

$$H = H_0 + H_{e-e} + H_{sc}. \quad (2.1)$$

We have separated the electron–electron interaction H_{e-e} and other scattering processes (impurity, phonon, . . .) H_{sc} from the one-electron Hamiltonian H_0 . Typically, the electron–electron interaction is treated in the Hartree approximation. Then we can find the spectrum of the Hamiltonian $H_0 + H_{e-e}$ by solving a nonlinear stationary Schrödinger–Poisson system of equations. Their solutions yield a basis in which quantum kinetic equations describing the scattering processes out of equilibrium can be written, as shown below. The envelope wave function is¹⁴

$$\varphi_\nu(\mathbf{x}, \mathbf{k}) \equiv \varphi_\nu(x, \mathbf{x}_\perp, k, \mathbf{k}_\perp) = \frac{1}{\sqrt{S}} e^{i\mathbf{k}_\perp \cdot \mathbf{x}_\perp} \varphi_\nu(x, k, \mathbf{k}_\perp). \quad (2.2)$$

At zero external field, φ_ν satisfies

$$\left[\mathcal{E}_c + V_c(x) - eW(x) - \frac{\hbar^2}{2} \frac{\partial}{\partial x} \frac{1}{m(x)} \frac{\partial}{\partial x} + \frac{\hbar^2 \mathbf{k}_\perp^2}{2m(x)} \right] \varphi_\nu = \mathcal{E}_\nu(\mathbf{k}) \varphi_\nu, \quad (2.3)$$

$$\varepsilon(x) \frac{\partial^2 W}{\partial x^2} = e[n_0 - N_{3D}(x)]. \quad (2.4)$$

Here \mathcal{E}_c is the conduction band edge of material W (GaAs, well), $W(x)$ is the electric potential due to the electron–electron interaction, $N_{3D}(x) = N_D(x)/l$ is the 3D doping density, and

$$m(x) = \begin{cases} m_W & \text{if } x \text{ corresponds to a quantum well } W, \\ m_B & \text{if } x \text{ corresponds to a barrier } B \end{cases} \quad (2.5)$$

$$\varepsilon(x) = \begin{cases} \varepsilon_W & \text{if } x \text{ corresponds to a quantum well } W, \\ \varepsilon_B & \text{if } x \text{ corresponds to a barrier } B \end{cases} \quad (2.6)$$

are the masses and permittivities of the well and barrier. If V_c corresponds to the conduction-band offset between the well and barrier material, we have

$$V_c(x) = \begin{cases} 0 & \text{if } x \text{ corresponds to a quantum well } W, \\ V_c & \text{if } x \text{ corresponds to a barrier } B. \end{cases} \quad (2.7)$$

Moreover, the 3D equilibrium electron density is

$$n_0(x) = \frac{1}{Sl} \sum_{\nu, k, \mathbf{k}_\perp} |\varphi_\nu(x, k, \mathbf{k}_\perp)|^2 n_F(\nu, k, \mathbf{k}_\perp), \quad (2.8)$$

where n_F denotes the Fermi function of the miniband ν . The boundary conditions at the well–barrier interfaces are that φ_ν and $m(x)^{-1} \partial \varphi_\nu / \partial x$ are both continuous.

The electronic spectrum is continuous, consisting of *minibands* of energies $\mathcal{E}_\nu(k; \mathbf{k}_\perp)$ with $\nu = 1, 2, 3, \dots$ (doubly degenerate because of spin) with an associated basis of spatially extended Bloch wave functions $\varphi_\nu(x, k; \mathbf{k}_\perp) = e^{ikx} u_\nu(x, k; \mathbf{k}_\perp)$.¹⁴

Although we can discuss the effects of scattering using the previous basis of electronic states that solve a nonlinear Schrödinger–Poisson system, we will for simplicity ignore the difference in mass and permittivity between barriers and wells and assume that the doping density is uniform. Of course in real devices, only the central parts of the wells are doped and the effective masses are different in wells and barriers.¹⁵ These differences can be treated with the formulation sketched here (see for example, the Galdrikian–Birbir work for GaAs quantum wells, AlGaAs barriers and a nonuniform doping density¹⁶), but then we would have to rely more heavily in numerical solutions than we intend to do, while obtaining qualitatively similar results (the AlAs barriers are much larger than the AlGaAs barriers and therefore the change in the energy levels due to electrostatic effects is much less important in the GaAs/AlAs SLs we consider in this paper than in Galdrikian and Birbir’s work). With these simplifications, the model [Eqs. (2.3)–(2.7)] becomes the Kronig–Penney model with $m_W = m_B = m^*$, $\varepsilon_W = \varepsilon_B = \varepsilon$, and $N_{3D}(x) = N_{3D}$ (constant). The Schrödinger–Poisson problem is simply $[H_0 - \mathcal{E}_\nu(\mathbf{k})] \varphi_\nu(\mathbf{x}, \mathbf{k}) = 0$ with $n_0 = N_{3D}$, and its solutions have the form

$$\varphi_\nu(\mathbf{x}, \mathbf{k}) = \frac{1}{\sqrt{S}} e^{i\mathbf{k}_\perp \cdot \mathbf{x}_\perp} \varphi_\nu(x, k), \quad \mathcal{E}_\nu(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}_\perp^2}{2m^*} + \mathcal{E}_\nu(k). \quad (2.9)$$

The Bloch functions are $2\pi/l$ -periodic in k , satisfying the orthogonality condition

$$\int_{-\infty}^{\infty} \varphi_\mu^*(x, k) \varphi_\nu(x, k') dx = \delta_{\mu\nu} \delta(k - k'), \quad (2.10)$$

and the closure condition

$$\int_{-\infty}^{\infty} \varphi_\mu^*(x, k) \varphi_\nu(x', k) dk = \delta_{\mu\nu} \delta(x - x'), \quad (2.11)$$

provided the integral of $|\varphi_\nu|^2$ over one SL period is unity.

Scattering different from electron–electron scattering is usually treated by writing equations for the density matrix, its Wigner transform, or the non-equilibrium Green’s function (NGF).^{17,18,1} Whatever the chosen formulation, the equations for the one-electron functions depend on two-electron and higher functions, and we have the usual infinite hierarchy of coupled equations, which is well known in classical kinetic theory. Typically, the hierarchy is closed by assuming some dependence of the two-electron functions on one-electron functions, which is suggested by perturbation theory in the limit of weak scattering.¹⁸ Assuming weak scattering, the differences between the equations corresponding to the different formulations are small. The trouble is that the kinetic equations are often used in the opposite *hydrodynamic* limit, in which collisions due to scattering are dominant. Then the results of using different formalisms are not equivalent, which has resulted in some discussion and confusion. In this paper, we shall not discuss the difference between

formulations in a precise way. Instead, we shall write kinetic equations for the one-electron density matrix or Wigner function leaving the collision terms unspecified as much as we can, and discuss how to obtain reduced theories for electric field, electron density and current, and so on. These theories are easier to analyze and to solve numerically, and they are the ones commonly used to understand nonlinear phenomena in SLs.

To find a kinetic equation, we start writing equations for the coefficients $a_{\nu,\mathbf{k}}(t)$ in the expansion of the wave function

$$\psi(\mathbf{x}, t) = \sum_{\nu,\mathbf{k}} a_{\nu,\mathbf{k}}(t) \varphi_{\nu}(\mathbf{x}, \mathbf{k}) \equiv \sum_{\nu} \psi_{\nu}(\mathbf{x}, t). \tag{2.12}$$

If we ignore the scattering term H_{sc} in Eq. (2.1), the coefficients $a_{\nu,\mathbf{k}}(t)$ become

$$i\hbar \frac{\partial}{\partial t} a_{\nu,\mathbf{k}} = \mathcal{E}_{\nu}(\mathbf{k}) a_{\nu,\mathbf{k}} - e \sum_{\nu',\mathbf{k}'} \langle \nu\mathbf{k} | W | \nu'\mathbf{k}' \rangle a_{\nu',\mathbf{k}'}. \tag{2.13}$$

The equations for the *band wave functions* ψ_{ν} of Eq. (2.12) can be obtained from this equation after some algebra

$$i\hbar \frac{\partial}{\partial t} \psi_{\nu} = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial \mathbf{x}_{\perp}^2} \psi_{\nu} + \sum_{m=-\infty}^{\infty} E_{\nu}(m) \psi_{\nu}(x + ml, \mathbf{x}_{\perp}, t) - e \sum_{\nu'} \int \Phi_{\nu}(\mathbf{x}, \mathbf{x}') W(\mathbf{x}') \psi_{\nu'}(\mathbf{x}', t) d\mathbf{x}', \tag{2.14}$$

$$\Phi_{\nu}(\mathbf{x}, \mathbf{x}') = \sum_{\mathbf{k}} \varphi_{\nu}(\mathbf{x}, \mathbf{k}) \varphi_{\nu}^*(\mathbf{x}', \mathbf{k}), \tag{2.15}$$

$$\mathcal{E}_{\nu}(k) = \sum_{m=-\infty}^{\infty} E_{\nu}(m) e^{imkl}. \tag{2.16}$$

Note that Eq. (2.2) implies

$$\begin{aligned} \Phi_{\nu}(\mathbf{x}, \mathbf{x}') &= \delta(\mathbf{x}_{\perp} - \mathbf{x}'_{\perp}) \phi_{\nu}(x, x'), \\ \phi_{\nu}(x, x') &= \sum_{\mathbf{k}} \varphi_{\nu}(x, k) \varphi_{\nu}^*(x', k), \end{aligned} \tag{2.17}$$

and the closure condition in Eq. (2.11) yields

$$\sum_{\nu} \Phi_{\nu}(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'). \tag{2.18}$$

Thus $\Phi_{\nu}(\mathbf{x}, \mathbf{x}')$ can be considered as the projection of the delta function $\delta(\mathbf{x} - \mathbf{x}')$ onto the band ν .

After second quantization, the band density matrix is defined by

$$\rho_{\mu,\nu}(\mathbf{x}, \mathbf{y}, t) = \langle \psi_{\mu}^{\dagger}(\mathbf{x}, t) \psi_{\nu}(\mathbf{y}, t) \rangle, \tag{2.19}$$

so that the 2D electron density is (the factor 2 is due to spin degeneracy)

$$n(\mathbf{x}, t) = 2l \sum_{\mu,\nu} \langle \psi_{\mu}^{\dagger}(\mathbf{x}, t) \psi_{\nu}(\mathbf{x}, t) \rangle = 2l \sum_{\mu,\nu} \rho_{\mu,\nu}(\mathbf{x}, \mathbf{x}, t). \tag{2.20}$$

Using Eqs. (2.19) and (2.20), we can derive the following evolution equation for the band density matrix

$$\begin{aligned}
 & i\hbar \frac{\partial}{\partial t} \rho_{\mu,\nu} + \frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial \mathbf{y}_\perp^2} - \frac{\partial^2}{\partial \mathbf{x}_\perp^2} \right) \rho_{\mu,\nu} \\
 & - \sum_{m=-\infty}^{\infty} [E_\nu(m) \rho_{\mu,\nu}(\mathbf{x}, y + ml, \mathbf{y}_\perp, t) - E_\mu(m) \rho_{\mu,\nu}(x - ml, \mathbf{x}_\perp, \mathbf{y}, t)] \\
 & + e \sum_{\nu'} \int W(\mathbf{z}) [\Phi_\nu(\mathbf{y}, \mathbf{z}) \rho_{\mu\nu'}(\mathbf{x}, \mathbf{z}, t) - \Phi_\mu(\mathbf{z}, \mathbf{x}) \rho_{\nu'\nu}(\mathbf{z}, \mathbf{y}, t)] = Q[\rho], \quad (2.21)
 \end{aligned}$$

with $Q[\rho] \equiv 0$ in the absence of scattering. The Hartree potential satisfies the Poisson equation

$$\varepsilon \frac{\partial^2 W}{\partial x^2} = \frac{e}{l} (n - N_D) \quad (2.22)$$

(recall that $e > 0$ and that W is the electric potential. The charge density is thus equal to the negative of the right-hand side of this equation). When considering scattering, the right-hand side of Eq. (2.21) is equal to a nonzero functional of the band density matrix $Q[\rho]$, whose form depends on the closure assumption we have made to close the density matrix hierarchy. In the semiclassical limit, the kernel of the collision term $Q[\rho]$ is usually found by using perturbation theory in the impurity potential, electron-phonon interaction, etc. For the time being, we shall not try to formulate collision models. Instead and in order to make contact with the kinetic equations in the semiclassical limit, we shall rewrite Eq. (2.21) in terms of the band Wigner function

$$w_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) = \int \rho_{\mu,\nu} \left(\mathbf{x} + \frac{1}{2} \xi, \mathbf{x} - \frac{1}{2} \xi, t \right) e^{i\mathbf{k} \cdot \xi} d\xi. \quad (2.23)$$

The evolution equation for the Wigner function is

$$\begin{aligned}
 & \frac{\partial}{\partial t} w_{\mu,\nu} + \frac{\hbar \mathbf{k}_\perp}{m^*} \cdot \frac{\partial}{\partial \mathbf{x}_\perp} w_{\mu,\nu} + \frac{i}{\hbar} \sum_{m=-\infty}^{\infty} e^{imkl} \left[E_\nu(m) w_{\mu,\nu} \left(x + \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right. \\
 & \left. - E_\mu(m) w_{\mu,\nu} \left(x - \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] + \frac{ie}{\hbar} \sum_{\nu'} \int \left[W \left(z + \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right. \\
 & \times \phi_\mu(z, x) e^{ik(x-z)} w_{\nu'\nu} \left(\frac{x+z}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) - W \left(z - \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \\
 & \left. \times \phi_\nu(x, z) e^{-ik(x-z)} w_{\mu,\nu'} \left(\frac{x+z}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] dz = Q_{\mu,\nu}[w], \quad (2.24)
 \end{aligned}$$

in which the collision term is again left unspecified. Notice that the 2D electron density is

$$n(\mathbf{x}, t) = \frac{2l}{8\pi^3} \sum_{\mu,\nu} \int w_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}, \quad (2.25)$$

due to Eq. (2.20) and the definition in Eq. (2.23). From Eqs. (2.24) and (2.25), we obtain the charge continuity equation

$$\frac{e}{l} \frac{\partial n}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{J} = 0, \tag{2.26}$$

$$\mathbf{J}_\perp = \frac{2e}{8\pi^3} \int \frac{\hbar \mathbf{k}_\perp}{m^*} \sum_{\mu,\nu} w_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) d\mathbf{k}, \tag{2.27}$$

$$\begin{aligned} \frac{\partial J}{\partial x} = & \frac{ie}{4\pi^3 \hbar} \sum_{\mu,\nu,m} \int e^{imkl} \left[E_\nu(m) w_{\mu,\nu} \left(x + \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right. \\ & \left. - E_\mu(m) w_{\mu,\nu} \left(x - \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] d\mathbf{k}, \end{aligned} \tag{2.28}$$

provided our collision model satisfies $\int \sum_{\mu,\nu} Q_{\mu,\nu} d\mathbf{k} = 0$.

A related formulation of the band Wigner functions (without collision terms) is due to Demeio *et al.*¹⁹ One difficulty with our formulation is that the Wigner function in Eq. (2.23) is not $2\pi/l$ -periodic in k . This can be corrected by using the following definition

$$\begin{aligned} f_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) &\equiv \sum_{s=-\infty}^{\infty} w_{\mu,\nu} \left(\mathbf{x}, k + \frac{2\pi s}{l}, \mathbf{k}_\perp, t \right) \\ &= \sum_{j=-\infty}^{\infty} e^{ijkl} \int \rho_{\mu,\nu} \left(x + \frac{jl}{2}, \mathbf{x}_\perp + \frac{1}{2}\xi_\perp, x - \frac{jl}{2}, \mathbf{x}_\perp - \frac{1}{2}\xi_\perp, t \right) \\ &\quad \times e^{i\mathbf{k}_\perp \cdot \xi_\perp} d\xi_\perp. \end{aligned} \tag{2.29}$$

To derive this equation, we have used the identity

$$\sum_{j=-\infty}^{\infty} \delta(\xi - jl) = \frac{1}{l} \sum_{s=-\infty}^{\infty} e^{i2\pi \xi s/l}, \tag{2.30}$$

together with the definition of Eq. (2.23). From Eqs. (2.25) and (2.29), we obtain the 2D electron density in terms of $f_{\mu,\nu}$

$$n(\mathbf{x}, t) = \frac{2l}{8\pi^3} \sum_{\mu,\nu} \int_{-\pi/l}^{\pi/l} \int f_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) dk d\mathbf{k}_\perp. \tag{2.31}$$

Similarly, the transversal current density can be obtained from Eqs. (2.27) and (2.29)

$$\mathbf{J}_\perp = \frac{2e}{8\pi^3} \int_{-\pi/l}^{\pi/l} \int \frac{\hbar \mathbf{k}_\perp}{m^*} \sum_{\mu,\nu} f_{\mu,\nu}(\mathbf{x}, \mathbf{k}, t) dk d\mathbf{k}_\perp. \tag{2.32}$$

The current density along the growth direction has the form

$$J = \frac{2e\hbar}{8\pi^3 m^*} \sum_{\mu,\nu,s} \int_{-\pi/l}^{\pi/l} \int \left(k + \frac{2\pi s}{l} \right) w_{\mu,\nu} \left(\mathbf{x}, k + \frac{2\pi s}{l}, \mathbf{k}_\perp, t \right) dk d\mathbf{k}_\perp, \tag{2.33}$$

from which we can also derive Eq. (2.28).

The definition of periodic band Wigner function is related to that adopted by Bechouche *et al.*²⁰ These authors have rigorously proved that the collisionless Wigner–Poisson equations for a crystal become the crystal Vlasov–Poisson equations in the semiclassical limit assuming that the initial conditions are concentrated in isolated bands. Scattering other than electron–electron scattering is not considered in these works. A similar work for a stratified material can be found in Ref. 21.

To find a Wigner–Poisson description of transport in a single miniband, we sum all the Wigner equations (2.24) over the band indices and use the closure condition in Eq. (2.18), so as to find an equation for $w(\mathbf{x}, \mathbf{k}, t) = \sum_{\mu, \nu} w_{\mu, \nu}(\mathbf{x}, \mathbf{k}, t)$:

$$\begin{aligned} \frac{\partial}{\partial t} w + \frac{\hbar \mathbf{k}_\perp}{m^*} \cdot \frac{\partial}{\partial \mathbf{x}_\perp} w + \frac{i}{\hbar} \sum_{m=-\infty}^{\infty} e^{imkl} \sum_{\mu, \nu} \left[E_\nu(m) w_{\mu, \nu} \left(x + \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right. \\ \left. - E_\mu(m) w_{\mu, \nu} \left(x - \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] + \frac{ie}{\hbar} \left[W \left(x + \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right. \\ \left. - W \left(x - \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right] w = \sum_{\mu, \nu} Q_{\mu, \nu}[w]. \end{aligned} \quad (2.34)$$

Let us now assume that only the first miniband is populated and that there are no transitions between minibands, $w(\mathbf{x}, \mathbf{k}, t) \approx w_{1,1}(\mathbf{x}, \mathbf{k}, t)$. This approximation is commonly used when describing strongly coupled SLs with wide minibands. Then Eq. (2.34) becomes

$$\begin{aligned} \frac{\partial}{\partial t} w + \frac{\hbar \mathbf{k}_\perp}{m^*} \cdot \frac{\partial}{\partial \mathbf{x}_\perp} w + \frac{i}{\hbar} \sum_{m=-\infty}^{\infty} e^{imkl} E_1(m) \left[w \left(x + \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right. \\ \left. - w \left(x - \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] + \frac{ie}{\hbar} \left[W \left(x + \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right. \\ \left. - W \left(x - \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right] w = Q_{1,1}[w]. \end{aligned} \quad (2.35)$$

This yields the following equation for the periodic Wigner function in Eq. (2.29)

$$\begin{aligned} \frac{\partial}{\partial t} f + \frac{\hbar \mathbf{k}_\perp}{m^*} \cdot \frac{\partial}{\partial \mathbf{x}_\perp} f + \frac{i}{\hbar} \sum_{m=-\infty}^{\infty} e^{imkl} E_1(m) \left[f \left(x + \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right. \\ \left. - f \left(x - \frac{ml}{2}, \mathbf{x}_\perp, \mathbf{k}, t \right) \right] + \frac{ie}{\hbar} \left[W \left(x + \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right. \\ \left. - W \left(x - \frac{1}{2i} \frac{\partial}{\partial k}, \mathbf{x}_\perp \right) \right] f = Q[f]. \end{aligned} \quad (2.36)$$

The dispersion relation $\mathcal{E}_1(k)$ is an even periodic function of k with period $2\pi/l$ that can be written as $\mathcal{E}_1(k) = \Delta_1[1 - \cos(kl)]/2$ plus a constant in the tight-binding approximation (Δ_1 denotes the width of the first miniband). Moreover, the field

$\mathbf{F} = \partial W / \partial \mathbf{x}$ (note that the real electric field is $-\mathbf{F}$) satisfies

$$\varepsilon \left(\frac{\partial F}{\partial x} + \frac{\partial}{\partial \mathbf{x}_\perp} \cdot \mathbf{F}_\perp \right) = \frac{e}{l} (n - N_D), \tag{2.37}$$

$$n(x, \mathbf{x}_\perp, t) = \frac{l}{4\pi^3} \int_{-\pi/l}^{\pi/l} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, \mathbf{x}_\perp, k, \mathbf{k}_\perp, t) dk d\mathbf{k}_\perp. \tag{2.38}$$

We want to explicitly derive reduced balance equations from the kinetic equation. For this purpose, we need a sufficiently simplified description of scattering. Scattering processes such as phonon scattering change the energy and momentum of the electrons leading the distribution function toward thermal equilibrium. We can describe these processes by a BGK collision model⁹

$$Q_{\text{en}}[f] = -\nu_{\text{en}} (f - f^{\text{FD}}), \tag{2.39}$$

$$f^{\text{FD}}(\mathbf{k}; n) = \int_0^\infty \frac{\Gamma/\pi}{\left[E - \mathcal{E}_1(k) - \frac{\hbar^2 \mathbf{k}_\perp^2}{2m^*} \right]^2 + \Gamma^2} \frac{dE}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)}, \tag{2.40}$$

$$n(\mathbf{x}, t) = \frac{l}{4\pi^3} \int_{-\pi/l}^{\pi/l} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^{\text{FD}}(k, \mathbf{k}_\perp; n) dk d\mathbf{k}_\perp. \tag{2.41}$$

Here Γ measures the finite width of the spectral function in thermal equilibrium due to scattering.¹ As $\Gamma \rightarrow 0$, the first factor in Eq. (2.40) becomes a delta function, and we recover the usual Fermi–Dirac distribution function with a chemical potential μ . The chemical potential $\mu = \mu(x, \mathbf{x}_\perp, t)$ is a function of the exact electron density n of Eq. (2.38) that is calculated by solving Eq. (2.41). With these definitions, the integral of $Q_{\text{en}}[f]$ over momentum vanishes, and the equation of charge continuity holds, as we shall show below. Notice that we have not included the electric potential in (2.40). Then the equilibrium Wigner function does not include the \hbar^2 corrections to the semiclassical Fermi–Dirac distribution corresponding to the effective Hamiltonian $\mathcal{E}_1(-i\partial/\partial x) - (\hbar^2/2m^*)\partial^2/\partial \mathbf{x}_\perp^2 - eW(x)$ (recall that the electron charge is $-e$): these corrections vanish if we set $W = 0$.^{6,22} Omitting the electric potential W is certainly an imperfection of our BGK collision model, which could perhaps be corrected using field-dependent collision models as in Ref. 6. However, the resulting technical complications would encumber our derivation of drift-diffusion type equations. Thus we prefer to adopt the same line as in previous works^{8,10} and leave the study of field-dependent and broadened collision models for the future.

Other processes, such as impurity scattering, conserve the energy of the electron, change only its momentum, and also preserve charge continuity. Gerhardtts²³ used the following model

$$Q_{\text{imp}}[f] = -\frac{\tilde{\nu}_{\text{imp}}}{4\pi^3} \int_{-\pi/l}^{\pi/l} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \delta[E(k, \mathbf{k}_\perp) - E(k', \mathbf{k}'_\perp)] \times [f(k, \mathbf{k}_\perp) - f(k', \mathbf{k}'_\perp)] dk' d\mathbf{k}'_\perp, \tag{2.42}$$

which can be rewritten as a relaxation to a weighted, energy-conserving mean value of the Wigner function: $Q_{\text{imp}}[f] = -\nu_G (f - \Phi_f[E(\mathbf{k})])$, provided $\Phi_f[E] = \int \delta[E - E(\mathbf{k}')] f(\mathbf{k}') d^3\mathbf{k}' / [4\pi^3 g(E)]$, $g(E) = \int \delta[E - E(\mathbf{k}')] d^3\mathbf{k}' / (4\pi^3)$ is the density of states, and $\nu_G = \tilde{\nu}_{\text{imp}} g(E(\mathbf{k}))$. Note that we have dropped the dependence of the Wigner function on space and time. This collision term couples the vertical motion of the electron to the lateral degrees of freedom. For SLs, scattering processes involving acoustic phonons, impurities and interface roughness may modify the lateral momentum. Liu *et al.*²⁴ have calculated and measured the scattering times in weakly coupled double barrier heterostructures and obtained energies smaller than 10 meV. This energy is also a generous upper bound for the energy exchanged in impurity scattering processes in strongly coupled SLs, as indicated in Wacker's review (his smallest scattering time is 0.0666 ps¹). In any case, 10 meV is much less than the typical energy exchange in the direction parallel to the electric field, of more than 1 eV (which can be estimated from the width of the Brillouin zone, $2\pi/l$). Thus, we may reasonably assume that the variation of the energy in the lateral direction is negligible, $E(k, \mathbf{k}_\perp) - E(k', \mathbf{k}'_\perp) \approx \mathcal{E}_1(k) - \mathcal{E}_1(k')$, and therefore

$$\begin{aligned}
 Q_{\text{imp}}[f] &\approx -\frac{\tilde{\nu}_{\text{imp}}}{2\pi} \int_{-\pi/l}^{\pi/l} \delta[\mathcal{E}_1(k) - \mathcal{E}_1(k')] [f(k) - f(k')] dk' \\
 &= -\frac{\tilde{\nu}_{\text{imp}}}{2\pi |\mathcal{E}'_1(k)|} [f(k) - f(-k)] \equiv -\frac{\nu_{\text{imp}}}{2} [f(k) - f(-k)], \quad (2.43)
 \end{aligned}$$

$$f(x, k, t) = \frac{1}{2\pi^2 S} \iint f(x, \mathbf{x}_\perp, k, \mathbf{k}'_\perp, t) d\mathbf{k}'_\perp d\mathbf{x}_\perp. \quad (2.44)$$

Here $\mathcal{E}'_1(k) = d\mathcal{E}_1/dk$. The approximate collision term in Eq. (2.43) was introduced by Ktitorov *et al.*²⁵ In terms of the 1D Wigner function in Eq. (2.44), we can derive from Eqs. (2.36)–(2.44) the 1D WPBGK system (1.1)–(1.4) (which is independent of \mathbf{x}_\perp if we assume that the initial Wigner function does not depend on \mathbf{x}_\perp). The Gerhardt's collision model is still better than the approximation (2.43) because his collision model explains the observed temperature dependence of the field at which the drift velocity has its lowest local maximum.²³ However, the simpler 1D WPBGK model is much more convenient for analytical calculations. The semiclassical limit of the WPBGK system has been analyzed in Ref. 10 in order to derive a reduced drift-diffusion model in the hydrodynamic limit. Particular solutions of the semiclassical model have been found by different authors. Ignatov and Shashkin⁸ found the stationary, space-independent semiclassical solution of Eq. (1.1) for a Boltzmann distribution function, the *Boltzmann limit* of Eq. (1.4), and studied its linear stability to plane wave disturbances in the field.

Before we proceed, it is convenient to derive the charge continuity equation and a form of Ampère's law for the current density from Eq. (1.1). Since the Wigner function is periodic in k , we can write the second and third terms on the right-hand side of Eq. (1.1) in terms of its Fourier series

$$f(x, k, t) = \sum_{j=-\infty}^{\infty} f_j(x, t) e^{ijk_l}. \quad (2.45)$$

We have

$$W\left(x \pm \frac{1}{2i} \frac{\partial}{\partial k}, t\right) f = \sum_{j=-\infty}^{\infty} W\left(x \pm \frac{jl}{2}, t\right) f_j e^{ijkl}, \tag{2.46}$$

and therefore,

$$\begin{aligned} &W\left(x + \frac{1}{2i} \frac{\partial}{\partial k}, t\right) f - W\left(x - \frac{1}{2i} \frac{\partial}{\partial k}, t\right) f \\ &= \sum_{j=-\infty}^{\infty} [W(x + jl/2, t) - W(x - jl/2, t)] f_j e^{ijkl} \\ &= \sum_{j=-\infty}^{\infty} jl \langle F \rangle_j f_j e^{ijkl}. \end{aligned} \tag{2.47}$$

Here we have defined the average

$$\langle F \rangle_j(x, t) = \frac{1}{jl} \int_{-jl/2}^{jl/2} F(x + s, t) ds. \tag{2.48}$$

Note that differentiating an average, we obtain a finite difference

$$\frac{\partial}{\partial x} \langle g \rangle_j = \left\langle \frac{\partial g}{\partial x} \right\rangle_j = \frac{g(x + jl/2) - g(x - jl/2)}{jl}. \tag{2.49}$$

Then the second term in Eq. (1.1) is

$$\begin{aligned} &\frac{i}{\hbar} \sum_{j=-\infty}^{\infty} \left[f\left(x + \frac{jl}{2}, k, t\right) - f\left(x - \frac{jl}{2}, k, t\right) \right] E_1(j) e^{ijkl} \\ &= \sum_{j=-\infty}^{\infty} \frac{ijl}{\hbar} e^{ijkl} E_1(j) \frac{\partial}{\partial x} \langle f \rangle_j, \end{aligned} \tag{2.50}$$

which in the case of the tight-binding dispersion relation $\mathcal{E}_1(k) = \Delta_1(1 - \cos kl)/2$ becomes $v(k) \partial \langle f \rangle_1 / \partial x$, with the usual miniband group velocity

$$v(k) \equiv \frac{1}{\hbar} \frac{d\mathcal{E}_1}{dk} = \frac{\Delta_1 l}{2\hbar} \sin(kl). \tag{2.51}$$

Inserting Eqs. (2.47) and (2.50) into Eq. (1.1), we obtain the following equivalent form of the Wigner equation, which is particularly suitable for treating SL problems

$$\begin{aligned} &\frac{\partial f}{\partial t} + \sum_{j=-\infty}^{\infty} \frac{ijl}{\hbar} e^{ijkl} \left(E_1(j) \frac{\partial}{\partial x} \langle f \rangle_j + e \langle F \rangle_j f_j \right) \\ &= -\nu_{\text{en}}(f - f^{\text{FD}}) - \nu_{\text{imp}} \frac{f(x, k, t) - f(x, -k, t)}{2}. \end{aligned} \tag{2.52}$$

We now integrate this equation over k , thereby getting the charge continuity equation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \sum_{j=1}^{\infty} \frac{2jl}{\hbar} \langle \text{Im}(E_1(-j)f_j) \rangle_j = 0. \tag{2.53}$$

We can eliminate the electron density from Eq. (2.53) by using the Poisson equation (1.2) and integrating the result over x , thereby obtaining the nonlocal Ampère’s law

$$\varepsilon \frac{\partial F}{\partial t} + \frac{2e}{\hbar} \sum_{j=1}^{\infty} j \langle \text{Im}(E_1(-j)f_j) \rangle_j = J(t). \tag{2.54}$$

Here $J(t)$ is the total current density. Equations (2.52), (2.53) and (2.54) are spatially nonlocal versions of the corresponding semiclassical equations. The charge continuity and Ampère’s equations have their traditional form as derived from semiclassical Boltzmann equations, except that the electron current is averaged over the SL periods. This nonlocality will be transmitted to the QDDE.

3. Derivation of the QDDE in the Hyperbolic Limit of the Kinetic Equation

To derive the QDDE, we shall assume that the electric field contribution in Eq. (2.52) is comparable to the collision terms and that they dominate the other terms (*the hyperbolic limit*).¹⁰ 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 $x_0 = \varepsilon F_M l / (eN_D)$, over which the field variation is of order F_M , is much longer than the mean free time between collisions, $\nu_{\text{en}}^{-1} \sim \hbar / (eF_M l) = t_1$. We therefore define the *small parameter* $\lambda = t_1 / t_0 = \hbar v_M N_D / (\varepsilon F_M^2 l^2)$ and formally multiply the first two terms on the left of (1.1) and of (2.52) by λ .¹⁰ After obtaining the number of desired terms, we set $\lambda = 1$.

The solution of Eq. (2.52) for $\lambda = 0$ is the stationary space-independent solution that is easily found as a Fourier series

$$f^{(0)}(k; n) = \sum_{j=-\infty}^{\infty} f_j^{(0)} e^{ijkl}, \quad f_j^{(0)} = \frac{1 - ij\mathcal{F}_j / \tau_e}{1 + j^2 \mathcal{F}_j^2} f_j^{\text{FD}}, \tag{3.1}$$

in which

$$\mathcal{F}_j = \frac{\langle F \rangle_j}{F_M}, \quad F_M = \frac{\hbar \sqrt{\nu_{\text{en}}(\nu_{\text{en}} + \nu_{\text{imp}})}}{el}, \quad \tau_e = \sqrt{\frac{\nu_{\text{en}} + \nu_{\text{imp}}}{\nu_{\text{en}}}}. \tag{3.2}$$

Since f^{FD} is an even function of k , its Fourier coefficient f_j^{FD} is real. Note that Eq. (1.3) implies $f_0^{(0)} = f_0^{\text{FD}} = n$.

The Chapman–Enskog ansatz consists of writing the distribution function as an expansion in powers of the book-keeping parameter λ (recall that we have to set

$\lambda = 1$ after retaining the desired number of terms)¹⁰

$$f(x, k, t; \lambda) = f^{(0)}(k; F) + \sum_{m=1}^{\infty} f^{(m)}(k; F) \lambda^m, \tag{3.3}$$

$$\varepsilon \frac{\partial F}{\partial t} + \sum_{m=0}^{\infty} J^{(m)}(F) \lambda^m = J(t). \tag{3.4}$$

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 (which are related through the Poisson equation). The field obeys a reduced evolution equation (3.4), 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 Ampère’s law (3.4) with respect to x , we obtain the charge continuity equation. Moreover, the condition

$$\int_{-\pi/l}^{\pi/l} f^{(m)}(k; n) dk = 2\pi f_0^{(m)}/l = 0, \quad m \geq 1, \tag{3.5}$$

ensures that $f^{(m)}$ for $m \geq 1$ does not contain contributions proportional to the zeroth-order term $f^{(0)}$. Note that the insertion of Eq. (3.3) in Ampère’s law (2.54) yields

$$J^{(m)} = \frac{2e}{\hbar} \sum_{j=1}^{\infty} j \langle \text{Im} [E_1(-j) f_j^{(m)}] \rangle_j, \tag{3.6}$$

which is also obtained by means of the above mentioned boundedness condition.

Inserting Eqs. (3.3) and (3.4) into Eq. (2.52) and equating all coefficients of λ^m in the resulting series to zero, we find the hierarchy

$$\mathcal{L}f^{(1)} = - \left(\frac{\partial}{\partial t} + v(k) \frac{\partial}{\partial x} \right) f^{(0)} \Big|_0, \tag{3.7}$$

$$\mathcal{L}f^{(2)} = - \left(\frac{\partial}{\partial t} + v(k) \frac{\partial}{\partial x} \right) f^{(1)} \Big|_0 - \frac{\partial}{\partial t} f^{(0)} \Big|_1, \tag{3.8}$$

and so on. We have defined

$$\mathcal{L}u(k) \equiv \frac{ie}{\hbar} \sum_{j=-\infty}^{\infty} j l \langle F \rangle_j u_j e^{ijk l} + \left(\nu_{\text{en}} + \frac{\nu_{\text{imp}}}{2} \right) u(k) + \frac{\nu_{\text{imp}} u(-k)}{2}, \tag{3.9}$$

and the subscripts 0 and 1 on the right-hand side of these equations mean that $\varepsilon \partial F / \partial t$ is replaced by $J - J^{(0)}(F)$ and $-J^{(1)}(F)$, respectively.

The linear equation $\mathcal{L}u = S$ has a bounded $2\pi/l$ -periodic solution provided $\int_{-\pi/l}^{\pi/l} S dk = 0$. Equation (3.7) and this solvability condition yield Eq. (3.6) for $m = 0$. The solution of Eq. (3.7) is

$$f^{(1)}(k; F) = \sum_{j=-\infty}^{\infty} \frac{\text{Re} S_j^{(1)} + i \tau_e^{-2} \text{Im} S_j^{(1)} - ij \mathcal{F}_j S_j^{(1)} / \tau_e}{(1 + j^2 \mathcal{F}_j^2) \nu_{\text{en}}} e^{ijk l}, \tag{3.10}$$

in which $S_j^{(1)}$ is the j th Fourier coefficient of the right-hand side of Eq. (3.7). Using Eq. (3.10), we can now explicitly write two terms in Eq. (3.4), thereby obtaining

the following QDDE for the field and the electron density given by the Poisson equation (1.2) (with $\partial^2 W/\partial x^2 = \partial F/\partial x$). For the tight-binding dispersion relation, the QDDE is

$$\begin{aligned} \varepsilon \frac{\partial F}{\partial t} + \frac{eN_D}{l} \mathcal{N} \left(F, \frac{\partial F}{\partial x} \right) \\ = \varepsilon \left\langle D \left(F, \frac{\partial F}{\partial x}, \frac{\partial^2 F}{\partial x^2} \right) \right\rangle_1 + \left\langle A \left(F, \frac{\partial F}{\partial x} \right) \right\rangle_1 J(t), \end{aligned} \quad (3.11)$$

$$A = 1 + \frac{2ev_M}{\varepsilon F_M l (\nu_{\text{en}} + \nu_{\text{imp}})} \frac{1 - (1 + 2\tau_e^2) \mathcal{F}^2}{(1 + \mathcal{F}^2)^3} n\mathcal{M}, \quad (3.12)$$

$$\begin{aligned} \mathcal{N} = \langle nV\mathcal{M} \rangle_1 + \langle (A - 1) \langle \langle nV\mathcal{M} \rangle_1 \rangle_1 \\ - \frac{l\tau_e \Delta_1}{F_M \hbar (\nu_{\text{en}} + \nu_{\text{imp}})} \left\langle \frac{B}{1 + \mathcal{F}^2} \right\rangle_1, \end{aligned} \quad (3.13)$$

$$V(\mathcal{F}) = \frac{2\mathcal{F}}{1 + \mathcal{F}^2}, \quad v_M = \frac{l\mathcal{I}_1(M)\Delta_1}{4\hbar\tau_e\mathcal{I}_0(M)}, \quad (3.14)$$

$$D = \frac{l^2 \Delta_1^2}{8\hbar^2 (\nu_{\text{en}} + \nu_{\text{imp}}) (1 + \mathcal{F}^2)} \left(\frac{\partial^2 \langle F \rangle_1}{\partial x^2} - \frac{4\hbar v_M \tau_e C}{l\Delta_1} \right), \quad (3.15)$$

$$\begin{aligned} B = \left\langle \frac{4\mathcal{F}_2 n\mathcal{M}_2}{(1 + 4\mathcal{F}_2^2)^2} \frac{\partial \langle F \rangle_2}{\partial x} \right\rangle_1 \\ + \mathcal{F} \left\langle \frac{n\mathcal{M}_2 (1 - 4\mathcal{F}_2^2)}{(1 + 4\mathcal{F}_2^2)^2} \frac{\partial \langle F \rangle_2}{\partial x} \right\rangle_1 \\ - \frac{4\hbar v_M (1 + \tau_e^2) \mathcal{F} (n\mathcal{M})'}{l\tau_e (1 + \mathcal{F}^2) \Delta_1} \left\langle n\mathcal{M} \frac{1 - \mathcal{F}^2}{(1 + \mathcal{F}^2)^2} \frac{\partial \langle F \rangle_1}{\partial x} \right\rangle_1 \end{aligned} \quad (3.16)$$

$$\begin{aligned} C = \left\langle \frac{(n\mathcal{M}_2)'}{1 + 4\mathcal{F}_2^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1 - 2\mathcal{F} \left\langle \frac{(n\mathcal{M}_2)' \mathcal{F}_2}{1 + 4\mathcal{F}_2^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1 \\ + \frac{8\hbar v_M (1 + \tau_e^2) (n\mathcal{M})' \mathcal{F}}{l\tau_e (1 + \mathcal{F}^2) \Delta_1} \left\langle \frac{(n\mathcal{M})' \mathcal{F}}{1 + \mathcal{F}^2} \frac{\partial^2 F}{\partial x^2} \right\rangle_1. \end{aligned} \quad (3.17)$$

$$\mathcal{M}(n/N_D) = \frac{\mathcal{I}_1(\tilde{\mu}) \mathcal{I}_0(M)}{\mathcal{I}_0(\tilde{\mu}) \mathcal{I}_1(M)}, \quad \mathcal{M}_2(n/N_D) = \frac{\mathcal{I}_2(\tilde{\mu}) \mathcal{I}_0(M)}{\mathcal{I}_0(\tilde{\mu}) \mathcal{I}_1(M)}, \quad (3.18)$$

$$\begin{aligned} \mathcal{I}_m(\tilde{\mu}) = \frac{1}{\pi} \int_{-\pi}^{\pi} \cos(mk) \left[\tan^{-1} \left(\frac{\tilde{\Gamma}/\delta}{1 - \cos k} \right) \right. \\ \left. + \int_0^{\infty} \frac{\tilde{\Gamma}}{(\tilde{E} - \delta + \delta \cos k)^2 + \tilde{\Gamma}^2} \ln \left(1 + e^{\tilde{\mu} - \tilde{E}} \right) d\tilde{E} \right] dk. \end{aligned} \quad (3.19)$$

Here g' denotes dg/dn , $\delta = \Delta_1/(2k_B T)$, $\tilde{\mu} = \mu/(k_B T)$, $\tilde{\Gamma} = \Gamma/(k_B T)$, $\mathcal{F} = \mathcal{F}_1$, and $n = N_D$ at the particular value of the dimensionless chemical potential $\tilde{\mu} = M$. 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 (3.11) becomes the *local* generalized DDE (GDDE) obtained from the semiclassical theory.¹⁰ The boundary conditions for the QDDE (3.11), which contains triple spatial averages, need to be specified for the intervals $[-2l, 0]$ and $[Nl, Nl + 2l]$,

and not just at the points $x = 0$ and $x = Nl$ (N denotes the number of SL periods spanning the device), as in the case of the parabolic semiclassical GDDE. Similarly, the initial condition has to be defined on the extended interval $[-2l, Nl + 2l]$. Note that the spatial averages in the nonlocal QDDE give rise to finite differences of partial derivatives in the diffusion terms, and therefore lead to a type of equations for which little seems to be known.

4. Numerical Solution of the QDDE

In this section, we solve the nonlocal QDDE (3.11) together with the voltage bias condition

$$\int_0^{Nl} F(x, t) dx = \phi F_M Nl, \quad (4.1)$$

for the field F and the total current density J . As boundary conditions in the intervals $[-2l, 0]$ and $[Nl, Nl + 2l]$, we adopt

$$J - \varepsilon \frac{\partial F}{\partial t} = \sigma F, \quad (4.2)$$

at all points $[-2l, 0]$ of the Ohmic injecting contact and zero-flux boundary conditions at the receiving contact $[Nl, Nl + 2l]$. The contact conductivity σ is selected so that $eN_D v_M V(F/F_M)$ and σF intersect on the second branch of $V(\mathcal{F})$, in which $dV/d\mathcal{F} < 0$. This is a typical boundary condition yielding self-sustained oscillations in drift-diffusion SL models.^{2,10} We have used a constant initial condition $F = \phi F_M$ in our numerical simulations. The SL parameters we have used correspond to a 157-period 3.64 nm GaAs/0.93 nm AlAs SL²⁶ at 14 K, with $\Delta = 72$ meV, $N_D = 4.57 \times 10^{10} \text{ cm}^{-2}$, $\nu_{\text{imp}} = 2\nu_{\text{en}} = 18 \times 10^{12} \text{ Hz}$ under a dc voltage bias of 1.62 V ($\phi = 1$). Cathode and anode contact conductivities are 2.5 and 0.62 $\Omega^{-1} \text{ cm}^{-1}$, respectively, and the effective mass is $m^* = (0.067d_W + 0.15d_B)m_0/l$, where $m_0 = 9.109534 \times 10^{-31} \text{ kg}$ is the electron rest mass.

Our numerical solution shows that the current and the field profile become stationary for $\phi < 0.75$ (1.2 V). For larger values of the dimensionless voltage ϕ , the initial field profile evolves toward a stable time-periodic solution for which J oscillates with time and the field profile shows recycling and motion of a pulse from $x = 0$ to the SL end. Figure 1 shows the self-oscillations of the current for 1.62 V ($\phi = 1$) and the corresponding field pulse at different times. In this figure, we compare the solution of the GDDE corresponding to the semiclassical BGK–Poisson kinetic equation and the solution of the QDDE for $\Gamma = 0$ (no collision broadening) and for $\Gamma = 18$ meV which is of the same order as the collision frequencies.

Self-oscillations in the QDDE have a frequency of $\nu_Q = 25.5$ GHz, faster than in the GDDE, $\nu_G = 20.6$ GHz (relative frequency $(\nu_Q - \nu_G)/\nu_G = 23.8\%$). When $\Gamma = 0$, the frequency is $\nu_{Q^*} = 21$ GHz, and the relative frequency $(\nu_{Q^*} - \nu_G)/\nu_G = 1.94\%$.

Collision broadening shortens the period of the current oscillations and therefore it reinforces the effects of the nonlocal terms in the QDDE due to quantum effects.

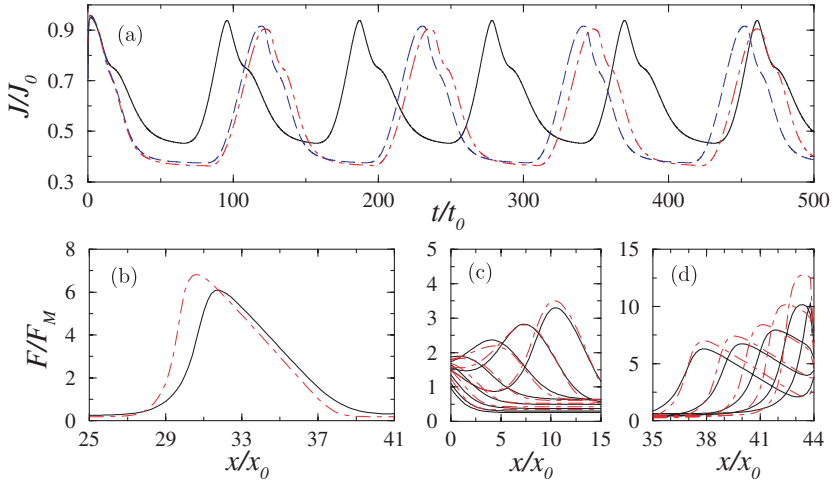


Fig. 1. (a) Current ($J_0 = ev_M N_D / l$) vs. time ($t_0 = \varepsilon F_M / J_0$) during self-oscillations for a voltage biased GaAs/AlAs SL, as described by the QDDE (solid line), the QDDE with $\Gamma = 0$ (long-dashed line) and by the GDDE (dot-dashed line). (b) Comparison between the fully developed dipole wave for the QDDE (solid line) and the dipole wave for the GDDE (dashed line). (c) Dipole wave at different times during the stage in which it is shed from the injecting contact. (d) Same as (c) for the stage in which the dipole disappears at the anode, located at $Nl/x_0 \approx 44$. Parameter values are $x_0 = v_M t_0 = 16$ nm, $t_0 = 0.43$ ps, $J_0 = 6.07 \times 10^5$ A/cm², $\phi = 1$.

5. Discussion

We have derived a nonlocal drift-diffusion model for a strongly coupled superlattice with one miniband by applying the Chapman–Enskog procedure to a simple WPBGK quantum kinetic equation. Our local equilibrium function is a collision-broadened Fermi–Dirac distribution inspired in the well-known thermal equilibrium of the Kadanoff–Baym equations,^{17,1} but the effects of the electric field on the collision operator have been ignored. For the case of a quantum particle in an external potential, Degond and Ringhofer⁶ have proposed a different form of the BGK collision model, in which the density matrix corresponding to local equilibrium is a Maxwellian operator obtained by minimizing the Boltzmann entropy subject to moment constraints. Their formulation includes the effects of the electric field on the collisions, and the chemical potential is a nonlocal functional of the electron density, not a function given by solving Eq. (1.3) for μ . This functional relation introduces additional nonlocalities in the balance equations resulting from the Chapman–Enskog procedure. See Ref. 27, in which quantum drift-diffusion and energy-transport models are derived for the case of a particle in an external potential undergoing collisions according to their BGK model. Notice that the BGK collision models used by these authors conserve kinetic energy, which is a somewhat unrealistic feature for semiconductors.

In this paper, we have treated the case of a one-dimensional SL with one miniband. We have used a Wigner–Poisson equation with relaxation towards a

broadened local Fermi–Dirac distribution and a simple elastic impurity collision term. We have derived a nonlocal drift-diffusion equation and solved it numerically to show that our model displays the self-oscillations of the current which are observed in experiments. There are several directions in which we could extend our results. Firstly, it would be interesting to derive quantum hydrodynamic models by using a more general BGK collision model and compare it with the models by Lei and collaborators.^{3–5} Our approximation $f^{(0)}$ is possibly closer to the real electron distribution than the parametrized local equilibrium used by Lei *et al.*, which has been criticized by other authors.¹ Unlike Lei’s, our approximation $f^{(0)}$ takes explicitly into account the effect of the electric field (and therefore the modified “equilibrium” $f^{(0)}$ corrects somewhat the effect of having neglected the electric potential in our collision model). Secondly, it would be important to consider the case of a SL with several minibands, although figuring out a reasonable local equilibrium distribution to include in the BGK collision model is probably harder. Thirdly, there are many interesting mathematical questions arising from these derivations. To mention one, the trailing edge of the pulse in Fig. 1 is rather sharp. In related work with drift-diffusion models of the Gunn effect, it is known that this trailing edge is close to a shock wave of the zeroth-order hyperbolic drift equation.²⁸ Obviously, the diffusive terms in the QDDE regularize this shock, and so do the collision terms in the kinetic equation (even if we think in terms of the semiclassical kinetic equation). What is the relation between these two regularizations? Cafilisch has considered a related problem in gas dynamics.²⁹ We hope that our work paves the way to tackling these problems in the future.

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