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Numerical methods for kinetic equations in semiconductor superlattices

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ABSTRACT

We compare three different numerical methods for solving the Boltzmann–Poisson kinetic equation describing electron transport in semiconductor superlattices. The associated initial-boundary value problem is computationally intensive, and it requires the use of efficient and accurate numerical methods and a large integration time to observe the Gunn-type self-oscillations of the current that characteristically appear among its stable solutions. The first two numerical methods solve the kinetic equation using finite differences and particles, respectively. The third method solves by finite differences a less costly drift–diffusion partial differential equation that can be derived from the Boltzmann–Poisson equation using the Chapman–Enskog perturbation method. We show the convergence of the methods by means of numerical simulations with parameter values corresponding to superlattices used in experiments. Comparing the results obtained with the three methods for a wide miniband superlattice used in experiments (for which the small dimensionless parameter in the Chapman–Enskog expansion is about 0.15), we show that the error of the Chapman–Enskog method is less than 0.8% despite a ten times shorter computation time. Thus, for this superlattice, the Chapman–Enskog perturbation method provides a very accurate solution with very low computational cost compared with directly solving the kinetic equation by either finite differences or particles methods.

1. Introduction

Semiconductor superlattices are periodic layered materials formed by epitaxial growth of layers belonging to two different semiconductors that have similar lattice constants [1]. They were synthesized following Esaki and Tsu's idea that these artificial crystals would be useful to observe high-frequency oscillations in the terahertz range such as Bloch oscillations [2]. In a doped superlattice (SL), self-sustained Bloch oscillations have not been found in experiments although they could exist under certain restrictive circumstances [3]. Self-sustained current oscillations of lower frequency (up to several gigahertz) have been observed in experiments and explained by theory [1]. They are produced by repeated formation of pulses of the electric field at the injecting contact of a dc voltage biased SL and their motion toward the collecting contact [1]. Thus they are transit-time oscillations whose frequency is inversely proportional to the SL length: they are similar to the Gunn effect in bulk semiconductors [4]. These Gunn-type oscillations have been observed in experiments with GaAs/AlAs SL (and with other SL based on III–V semiconductors) since 1996 and are the basis of fast oscillator devices [5].

To understand the electron transport responsible for self-sustained oscillations, mathematical models based on the Boltzmann transport equation have been proposed and used since the 1970s [6,1]. Aspects of electron transport can be understood by ignoring space charge effects and simplifying the model equations, but the study of self-sustained oscillations requires considering these effects. The earliest Boltzmann-type model was introduced by Ktitorov, Simin and Sindalovskii (KSS) in 1971 [6]. They assumed that only one miniband of the SL was populated by electrons and modeled the collision terms in the Boltzmann equation by one simple, energy-conserving, impurity collision term and by a relaxation-time term involving the distribution function in thermal equilibrium. Later Ignatov and Shashkin (IS) improved the relaxation-time term by assuming that the distribution function relaxes toward a local equilibrium containing the instantaneous value of the electron density [7]. Electron–electron interaction was ignored by these authors [6,7]. Their analyses were based on simplified reduced ordinary differential equations that can be easily derived from the kinetic equation if the space dependence is ignored [6–8].

To include space charge effects, it suffices to couple the kinetic equation for the distribution function to a Poisson equation for the electric potential created by electrons. The resulting Boltzmann–Poisson model with simplified KSS and IS collision terms

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was first studied by Bonilla, Escobedo and Perales (BEP) [9]. Using a Chapman–Enskog method, these authors derived a nonlinear drift–diffusion equation (DDE) for the electric field inside the SL in a high-electric field hydrodynamic limit. Then they added appropriate boundary and initial conditions and solved the resulting drift–diffusion problem numerically. Stable self-sustained oscillations are among the solutions found numerically [9]. A direct numerical solution of the kinetic Boltzmann–Poisson system considered by BEP also shows stable self-sustained oscillations for appropriate values of the voltage bias [10]. However, no one has compared, in terms of accuracy and computational cost, the numerical solution of the DDE with the one obtained by solving directly the kinetic equation. We tackle these problems in the present paper and their solution is a step toward more precise studies of stable current oscillations in superlattices and other low dimensional solid state systems.

We solve the BEP Boltzmann–Poisson kinetic equation model in two ways: by a previously used deterministic particle method [10–12], and also by an efficient and accurate implicit finite differences method. Particle methods are appropriate to study our system of equations because their solutions may present large gradients: the electric field pulses obtained by simulating the approximate DDE have a smooth leading front but a steep trailing back front [1]. The present work validates the Chapman–Enskog perturbation method used to derive the DDE for the present semiclassical Boltzmann–Poisson problem. The Chapman–Enskog method has also been used to analyze other interesting problems in nanoelectronics and spintronics described by related quantum kinetic equations for which no direct numerical solution is known [3,13,14].

The rest of the paper is as follows. In Section 2 we describe the model equations and derive the DDE by means of the Chapman–Enskog method. Sections 3–5 explain the numerical methods used: finite differences, particles and the scheme for the DDE, respectively. The analysis of the convergence of the numerical methods presented in Section 6 is based on numerical simulations. Finally, Section 7 contains our conclusions.

2. Model equations

The BEP Boltzmann–Poisson system for 1D electron transport in the lowest miniband of a strongly coupled SL is [9]:

$$\frac{\partial f}{\partial t} + v(k)\,\frac{\partial f}{\partial x} + \frac{eF}{\hbar}\,\frac{\partial f}{\partial k} = -\nu_{en}\left(f - f^{FD}\right) - \frac{\nu_{imp}}{2}\left(f - f(x,-k,t)\right) \quad (1)$$

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

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

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

with $x \in [0, L]$ and f periodic in k with period $2\pi/l$. Here f, f^{FD}, n, N_D, $\mathcal{E}$, l, $-F$, ε, m^*, k_B, T, ν_{en}, ν_{imp} and $-e < 0$ are the one-particle distribution function, the 1D local equilibrium distribution function, the 2D electron density, the 2D doping density, the miniband dispersion relation, the SL period, the electric field, the SL permittivity, the effective mass of the electron, the Boltzmann constant, the lattice temperature, the constant frequency of the inelastic collisions responsible for energy relaxation, the constant frequency of the elastic impurity collisions and the electron charge, respectively. Both the exact and the local equilibrium Fermi–Dirac distribution functions have the same electron density according to (3). The chemical potential μ is a function of the electron density n that can be obtained by inserting (4) into (3) and solving for $\mu = \mu(n)$. The first term in the right hand side of Eq. (1) represents energy relaxation toward a 1D effective Fermi–Dirac distribution $f^{FD}(k;\mu)$ (local equilibrium) due to, e.g. phonon scattering. A similar collision model with a Boltzmann local distribution function was proposed by Ignatov and Shashkin [7]. The second term in the right hand side of Eq. (1) accounts for impurity elastic collisions, which conserve energy but dissipate momentum [6,9,1]. Transfer of lateral momentum due to impurity scattering is ignored in this model; the effects of lateral momentum transfer have been analyzed by Gerhardts using a simple collision model [15].

There are more realistic semiclassical and quantum treatments of collisions [16]. However the resulting kinetic equations are much more difficult to handle and have not been solved with boundary and initial conditions corresponding to current self-oscillations. These equations have not been amenable to singular perturbation reductions precisely because their collision terms are so unwieldy. In marked contrast to this situation, the simple collision model used in (1) allows to find approximate solutions in different important limits. Self-sustained oscillations of the current appear in the limit of strong electric fields such that the term proportional to the electric field and the collision terms have the same order and dominate all others. Keeping only the electric field and the collision terms in (1) produces an equation that can be solved to yield a modified local equilibrium distribution. That distribution is the basis of any perturbation analysis. Replace the KSS–IS collision by a more realistic model either semiclassical [15,17] or quantum mechanical [16], and no analytical expression for the modified local equilibrium distribution has been found. In the case of small electric fields in which collisions dominate all other terms in the kinetic equation, perturbative schemes produce useful reduced equations even for more realistic collision models. For instance, if the elastic collisions dominate over inelastic ones and over all other terms in a one-band 3D semiconductor kinetic equation, the Hilbert expansion produces in the parabolic limit a reduced kinetic equation usually called the Spherical Harmonic Expansion (SHE) model [17]. A Chapman–Enskog expansion further reduces the SHE model to an energy-transport system of equations [17]. It would be interesting to see whether SHE ideas yield reduced model equations in the limit of strong electric fields producing comparable field-dependent and elastic collision terms in the kinetic equation. For superlattices, the KSS–IS collision model can be fitted so that the frequencies ν_{en} and ν_{imp} yield current–voltage curves similar to those found in experiments or calculated by Monte Carlo simulations in idealized situations (infinite superlattices, constant electric fields, space-independent conditions) [16]. Thus calibrated, the KSS–IS collision model provides a good description of electron transport in superlattices at a given temperature.

We assume the simple tight-binding miniband dispersion relation:

$$\mathcal{E}(k) = \frac{\Delta}{2}\,(1 - \cos(kl))\,, \quad (5)$$

where Δ is the first miniband width. The group velocity is then given by:

$$v(k) = \frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial k} = \frac{\Delta\, l}{2\hbar}\,\sin(kl). \quad (6)$$

The tight-binding expression (5) keeps only the first harmonic in a Fourier cosine expansion of the dispersion relation. We show elsewhere that keeping more terms does not change substantially