Nonlinear Electron Transport in Nanostructures

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Abstract. We propose novel BGK models for inelastic collisions in the kinetic theory of electron transport in semiconductor superlattices. The Chapman-Enskog method produces a drift-diffusion equation describing the behavior of the electric field F and the electron density n in an appropriate hyperbolic limit. Under voltage bias, stable solutions thereof include stable self-sustained oscillations of the current through the superlattice due to periodic injection of electric field pulses at one end of the device that move to the other end. For almost elastic collisions, the model has a local equilibrium that oscillates rapidly in time and the resulting balance equations describe for the first time the annihilation of the Bloch oscillations due to scattering.

Keywords: BGK kinetic equation; drift-diffusion equation; inelastic collisions; Chapman-Enskog method; self-sustained current oscillations; modulated hydrodynamics; modulated Bloch oscillations
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INTRODUCTION

Electron transport in nanostructures under strong applied fields is a fascinating subject. In semiconductor nanostructures, electrons are confined in one, two or all three spatial dimensions and, as a result, their transport properties are between those of bulk semiconductors and those of molecules. These structures are typically grown by molecular beam epitaxy or defined by lithographical patterned gate electrodes. Quantum dots confine electrons in all three spatial dimensions and resemble large atoms or molecules. In quantum wires, electrons are confined in two dimensions, whereas electrons are confined in one spatial dimensions in quantum wells and in superlattices. Applications to devices such as transistors, LEDs, solar cells, diode lasers, fast oscillators or infrared detectors and lasers are myriad [1, 2].

Here we will study electron transport in superlattices, i.e. artificial one dimensional crystals obtained by epitaxially growing many identical spatial periods of different semiconductors. In the simplest case, one period comprises several monolayers of two different semiconductors, for example GaAs and AlAs, as sketched in Fig. 1. Since the bandgaps of these semiconductors are different, the conduction band profile of the superlattice (SL) is periodic in its growth direction and electrons moving along this direction are subject to a periodic electric potential with periods of several nanometers. The lateral extension of the superlattice is much larger than its period. At room temperature and in conditions when the electron density varies slowly over several SL periods, electron transport is described by Boltzmann-type kinetic equations. As in the kinetic theory of gases, an important problem is to derive balance equations for macroscopic quantities (electron density, electric field, electric current density and mean energy) which describe the behavior of devices made out of SLs. Our focus here is to propose, derive and solve these macroscopic equations thereby showing interesting behavior such as self-sustained oscillations of the current through a SL.

The kinetic equations for electron transport in the lowest miniband of a SL with energy dispersion relation

$$\mathscr{E}(k)=\frac{\Delta}{2}(1-\cos kl), \quad \text{and group velocity} \quad v(k)=\frac{1}{\hbar}\frac{d\mathscr{E}}{dk}=\frac{\Delta l}{2\hbar}\sin kl \tag{1}$$

(assuming a tight-binding dispersion relation), are

$$\frac{\partial f}{\partial t}+v(k)\frac{\partial f}{\partial x}+\frac{eF}{\hbar}\frac{\partial f}{\partial k}=Q(f), \tag{2}$$

$$\varepsilon\frac{\partial F}{\partial x}=\frac{e}{l}(n-N_D), \tag{3}$$

$$n=\frac{l}{2\pi}\int_{-\pi/l}^{\pi/l}f(x,k,t)dk. \tag{4}$$

Here f, n, N_D, ε, $-e<0$, l and $F=\partial W/\partial x$ are the one-particle distribution function, the 2D electron density, the 2D doping density, the dielectric constant, the electron charge, the SL period, and minus the electric field, respectively. W

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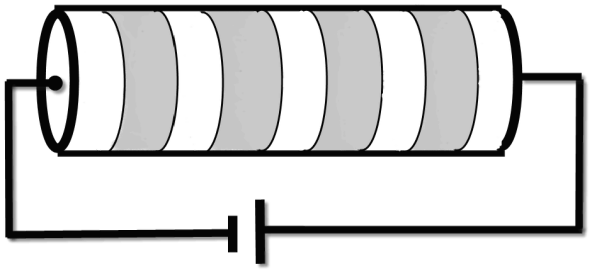

FIGURE 1. Sketch of a dc voltage biased superlattice made out of two different semiconductors. Shaded areas may represent AlAs (potential barriers) and white areas may represent GaAs (potential wells)

is the electric potential. Eq. (2) is the kinetic equation with a collision operator $Q(f)$ to be specified later. Eq. (3) is the Poisson equation for the 1D electric field. f is $2\pi/l$-periodic in k and therefore it can be expanded in a Fourier series:

$$f(x,k,t) = \sum_{j=-\infty}^{\infty} f_j(x,t)\, e^{ijkl}. \tag{5}$$

BGK COLLISION MODELS

Realistic collision models for semiclassical equations involve integrals of f over k with appropriate kernels. As in classical kinetic theory, many qualitative features of the kinetic equation are preserved if the collision kernel is simply $[f_{\rm eq}(k)-f]/\tau$, where $f_{\rm eq}$ is an appropriate local equilibrium distribution having the same moments ($n = f_0$ and perhaps current density and mean energy associated with f_1) as f. This is the idea of Bhatnagar-Gross-Krook (BGK) collision models in classical kinetic theory. Collisions in the kinetic theory of gases are elastic, thereby preserving mass, momentum and kinetic energy. In a SL, electrons are scattered by phonons, impurities, interface roughness, etc., and momentum and energy are typically not conserved by these processes. Thus electron density should be the zeroth harmonic of f and of the local equilibrium function, but the first harmonic of these two functions should be different. We propose the following Boltzmann local equilibrium function as f_{eq}:

$$f^B = n\frac{\pi\, e^{\tilde{u}kl+\tilde{\beta}\cos kl}}{\int_0^\pi e^{\tilde{\beta}\cos K}\cosh(\tilde{u}K)\, dK}, \tag{6}$$

in which $\tilde{u} = u/(k_BT)$ and $\tilde{\beta} = \Delta/(2k_BT)$ (u is a mean velocity and T is the electron temperature) are obtained in terms of J_n/n and E (the average of the dispersion relation is $n\Delta/2 - nE$), with

$$J_n = \frac{e}{2\pi}\int_{-\pi/l}^{\pi/l} v(k)\, f\, dk, \quad E = \frac{l}{2\pi n}\int_{-\pi/l}^{\pi/l}\left[\frac{\Delta}{2} - \mathscr{E}(k)\right] f\, dk, \tag{7}$$

by solving

$$\frac{e}{2\pi}\int_{-\pi/l}^{\pi/l} v(k)\, f^B\, dk = \alpha_j J_n, \quad \frac{l}{2\pi n}\int_{-\pi/l}^{\pi/l}\left[\frac{\Delta}{2} - \mathscr{E}(k)\right] f^B\, dk = \alpha_e E + (1-\alpha_e)E_0. \tag{8}$$

Note that $f_0^B = n$. In thermal equilibrium at the lattice temperature $T_0 = \Delta/(2k_B\tilde{\beta}_0)$, $J_n = 0$, $\tilde{u} = 0$, and $E = E_0 = I_1(\tilde{\beta}_0)/[2I_0(\tilde{\beta}_0)]$ gives the relation between E_0 and the lattice temperature in terms of modified Bessel functions.

When the following collision kernel is used in (2),

$$Q(f) = -\nu_e(f - f^B) - \frac{\nu_p}{2}[f(x,k,t) - f(x,-k,t)], \tag{9}$$

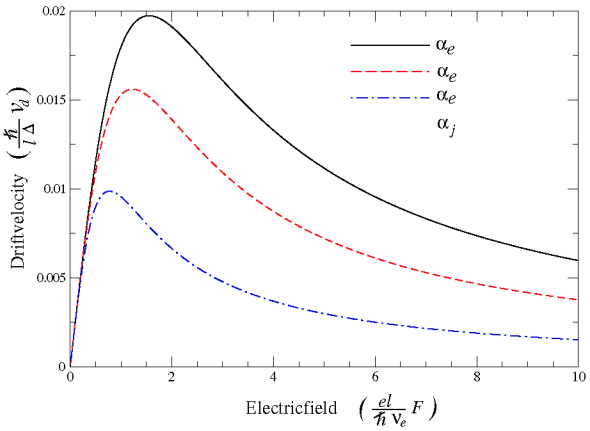

FIGURE 2. Drift velocity versus field for the inelastic case with $\alpha_j = 0$ and different values of the restitution coefficient α_e.

simple integration of 1 and e^{-ikl} times (2) with respect to k yield the moment equations:

$$\frac{e}{l}\frac{\partial n}{\partial t} + \frac{\partial J_n}{\partial x} = 0, \tag{10}$$

$$\frac{\partial J_n}{\partial t} + \frac{e\Delta^2 l}{8\hbar^2}\frac{\partial}{\partial x}(n - \mathrm{Re}\, f_2) - \frac{e^2 l\, nEF}{\hbar^2} = -[\nu_e(1-\alpha_j) + \nu_p]J_n, \tag{11}$$

$$\frac{\partial E}{\partial t} - \frac{lE}{en}\frac{\partial J_n}{\partial x} - \frac{\Delta^2 l}{8\hbar n}\frac{\partial}{\partial x}\mathrm{Im} f_2 + \frac{F J_n l}{n} = -\nu_e(1-\alpha_e)(E - E_0). \tag{12}$$

Inserting n from (3) in (10), we obtain the following form of Ampère's law: $\varepsilon\,\partial F/\partial x + J_n = J(t)$, where $J(t)$ is the space independent total current density. The first term in (9) corresponds to inelastic collisions in which energy and momentum are dissipated (e.g., optical phonon scattering), whereas the second term represents collisions which preserve energy but dissipate momentum (e.g. impurity or interface roughness scattering); cf. Ref. [3] for a discussion. Eq. (10) is the continuity equation indicating that charge is conserved. The right hand sides of (11) and (12) indicate that momentum and energy are dissipated in such a way that the current density will eventually decay to zero and the mean energy to the lattice energy E_0. α_j and α_e are restitution coefficients, similar to those used by Brey, Moreno and Dufty [4] in models of granular gases (in which energy is dissipated by collisions, but momentum is not).

EQUATIONS FOR THE MOMENTS OF f

For $0 < \alpha_{e,j} < 1$, (10) - (12) have the following spatially independent solutions

$$J_n = \frac{en}{l}\,v_d(\mathscr{F}), \quad v_d = \frac{2v_M\mathscr{F}}{1+\mathscr{F}^2}, \quad E = \frac{E_0}{1+\mathscr{F}^2}, \quad \mathscr{F} = \frac{F}{F_M}, \tag{13}$$

$$F_M = \frac{\hbar\nu_e\tau_e(1-\alpha_e)}{el}, \quad v_M = \frac{E_0 l}{2\hbar\tau_e} = \frac{I_1(\tilde{\beta}_0)\Delta l}{4I_0(\tilde{\beta}_0)\hbar\tau_e}, \quad \tau_e = \sqrt{\frac{(1-\alpha_j)\nu_e + \nu_p}{\nu_e(1-\alpha_e)}}, \tag{14}$$

where n and F are constant. Fig. 2(a) shows the dimensionless electron drift velocity $\hbar v_d/(\Delta l)$ as a function of the dimensionless field $eFl/(\hbar\nu_e)$ for different values of the restitution coefficients. Note that the maximum values of drift velocity and field decrease as α_e increases, thereby making elastic collisions dominant over inelastic ones. The average of the energy (1), $\Delta n/2 - nE$, increases with the field because E decreases according to (13).

For the special case of elastic collisions, $\alpha_e = \alpha_j = 1$, $\nu_p = 0$, the space independent solutions of (11) and (12) are

$$J_n = \frac{en}{\hbar}\,a\sin(\omega_B t + \varphi), \quad E = a\cos(\omega_B t + \varphi), \quad \omega_B = \frac{eFl}{\hbar}, \tag{15}$$

in which ω_B is the Bloch frequency and a and φ are real constants.

Equations (10) - (12) and (3) are not a closed system of equations because we do not know the second moments f_2 in terms of n, F, J_n and E. If we ignore spatial derivatives, (13) or (14) (in the case of elastic collisions) are stable solutions of (11) - (12) and can be used to set up a Chapman-Enskog procedure to determine f_2 in terms of n, F, J_n and E, thereby closing (11) and (12). The relevant limit is the hyperbolic one, in which the collision and Bloch frequencies are of the same order. Then collision and field dependent terms are of the same order, $\nu_e N_D$ (n and f are of the order of the doping density), and dominate all others in Eq. (2). The Poisson equation (3) then establishes that the unit of length is $[x] = \varepsilon[F]\,l/(eN_D) = \varepsilon\hbar\nu_e/(e^2N_D)$. Then the convective term $v(k)\,\partial f/\partial x$ is of order $[v]N_D/[x]$ with $[v] = \Delta l/\hbar$. This term is much smaller than the collision term if $[v]/[x] \ll \nu_e$, i.e., if $\delta = e^2N_D l\Delta/(\varepsilon\hbar^2\nu_e^2) \ll 1$. In this limit, we nondimensionalize (2) - (4) and (9) and implement the Chapman-Enskog method. There are two cases:

- In the inelastic case, f is a function of k and depends on space and time through the slowly varying variables n and F. The method yields J_n and E as functionals of n and F whose leading order in δ is given by the dimensionless version of (13). The resulting drift-diffusion equation closely resembles the semiclassical version of that in [3]. As in that reference, appropriate boundary conditions and voltage bias produce stable self-sustained oscillations of the current through the SL as solutions. These oscillations are due to the periodic formation of electric field pulses at the injecting contact that move towards the other end of the SL [2, 3].
- In the almost elastic case, $(1-\alpha_e)$ and $(1-\alpha_j+\nu_p/\nu_e)$ are of order δ. Then the leading order equations for the moments have solutions (15). We have to introduce a fast time scale, $\theta = \delta^{-1}\int_0^t F(x,s)\,ds$ (in nondimensional units) and implement a modified Chapman-Enskog method for the following nondimensional kinetic equation:

$$F\left(\frac{\partial f}{\partial\theta}+\frac{\partial f}{\partial k}\right)+\left(1+\frac{\nu_p}{2\nu_e}\right)f-\frac{\nu_p}{2\nu_e}f(x,-k,t)-f^B=-\delta\left(\frac{\partial f}{\partial t}+\frac{\sin k}{2}\frac{\partial f}{\partial x}\right). \tag{16}$$

To obtain dimensional variables from those in this equation, we have to multiply the nondimensional f, n, F, ... by its corresponding scale, namely $[f] = [n] = N_D$, $[F] = \hbar\nu_e/(el)$, ... The solution of (16) is 2π-periodic in k and in θ, and it depends on space and time through the slowly varying variables n, F and A, where $f_1 = 2(nE - iJ_n) = A\,e^{-i\theta}$. A is the slowly varying complex-valued envelope of the Bloch oscillations (15). The Chapman-Enskog method yields balance equations for F and A in addition to the nondimensional Poisson equation $\partial F/\partial x = n-1$. These equations indicate how A decays, thereby shedding light on how scattering processes annihilate Bloch oscillations.

In summary, we propose a novel BGK inelastic collision model for semiconductor superlattices. The Chapman-Enskog method yields drift-diffusion equations for inelastic collisions whereas for almost elastic collisions it yields coupled equations for field, electron density, residual values of mean energy and current density and the envelope of the Bloch oscillations. These equations describe the annihilation of the Bloch oscillations due to scattering. The local equilibrium of the Chapman-Enskog procedure oscillates rapidly in time, which is very different of the usual stationary local equilibrium in kinetic theory or the algebraically time decaying homogeneous cooling state in granular gases.

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