

## Nonlinear electronic transport in semiconductor superlattices

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Nonlinear charge transport in strongly coupled semiconductor superlattices is described by single or two-miniband Wigner-Poisson kinetic equations with BGK collision terms. Balance equations for miniband populations and electric field are derived using the Chapman-Enskog method. Numerical solutions show stable self-oscillations of the current through a voltage biased superlattice.

Keywords: Quantum drift-diffusion equations, Chapman-Enskog method, Rashba spin-orbit interaction, modified Kane model.

### 1. Introduction

Semiconductor superlattices are essential ingredients in fast nanoscale oscillators, quantum cascade lasers and infrared detectors. A superlattice (SL) is a quasi-one dimensional crystal originally proposed by Sivan et al. to observe Bloch oscillations, i.e. the periodic coherent motion of electrons in a miniband when an electric field is applied. In these materials, there are many interesting nonlinear phenomena, such as self-oscillations of the current through the SL, due to charge dipole motion, multistability of stationary charge and field profiles, etc. See the review [1].

Nonlinear charge transport in SLs has been investigated in the last decade using balance equations for electron densities and electric field.

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These equations are either proposed using phenomenological arguments or derived from microscopic theories.<sup>1,2</sup> Systematic derivations are scarce. For a single miniband  $S$  the Chapman-Enskog method applied to a semiclassical Boltzmann equation shows collision term is of Hartnag-Ross type in a general equilibrium situation<sup>3</sup> and an alternative method can be applied to a linearized Boltzmann equation.<sup>4</sup> For a semiclassical parabolic band Boltzmann equation system the method has earlier been used to obtain balance equations.<sup>5</sup> The Boltzmann equation system contains two pseudodifferential operators in solving the Boltzmann equation and the electric potential. The leading order approximation in the parabolic limit balances collisions and electric potential and its solution is not obvious because the potential is an a priori unknown solution of the Boltzmann equation. These are simpler because their linearizations are periodic in the reciprocal lattice the potential terms become multiplication operators in Fourier space and the leading order approximation is straightforward to solve.<sup>4</sup>

For sufficiently high applied electric fields electrons may populate higher minibands then be scattered to the lowest etc. Moreover  $S$  with tilted magnetic impurities subject to a magnetic field may present spin polarization effects whose understanding is crucial to develop spintronic devices.<sup>6</sup> Even though magnetic impurities spin polarization could appear due to Rashba spin-orbit interaction.<sup>7</sup> Hence we consider electron spin each miniband is split into two minibands  $S$  become two minibands  $S$ . We shall systematically derive alternative balance equations by the method.

## 2. Single miniband superlattice

The linearized Boltzmann-Hartnag-Ross Boltzmann equation for 1D electron transport in the lowest miniband of a strong coupled  $S$  is:

$$\frac{df}{dt} - \frac{i}{\hbar} E(k) \frac{1}{2i} \frac{1}{x} - E(k) - \frac{1}{2i} \frac{1}{x} f$$

$$= -W(x) \frac{1}{2i} \frac{1}{k}, t - W(x) - \frac{1}{2i} \frac{1}{k}, t f$$

$$Q f = -e f - f^{FD} = i \frac{f(x, k, t) - f(x, -k, t)}{2}, \quad 2.1$$

$$\frac{2W}{x^2} = \frac{e}{\hbar} n - N_D, \quad 2.2$$

with

$$n = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x, k, t) dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} f^{FD}(k, n) dk, \quad 2.3$$

$$f^{FD}(k, n) = \frac{m^* k_B T}{2\pi} \ln \left[ 1 + \exp \left( \frac{\mu - E(k)}{k_B T} \right) \right]. \quad 2.4$$

where  $f$  is the one particle distribution function,  $n$  is the electron density,  $E(k)$  is the energy dispersion relation,  $\mu$  is the chemical potential,  $m^*$  is the effective mass of the electron,  $k_B$  is the Boltzmann constant,  $T$  is the lattice temperature,  $\ln$  is the natural logarithm, and  $\exp$  is the exponential function. The terms  $d_B$  and  $d_W$  are the barrier width and the well width, respectively.

The right hand side of Eq. 2.1 can be straightforwardly derived from the Schrödinger equation or the wave function in the miniband using the definition of the one particle distribution function:

$$f(x, k, t) = \frac{2l}{S} \int_{j=-\infty}^{\infty} \psi_j(x, y, z, t) \psi_j^*(x - \frac{j l}{2}, y, z, t) e^{ijkl} dx dy. \quad 2.5$$

The second antiwave function is a superposition of the Bloch states corresponding to the miniband and  $S$  is the cross section.<sup>4</sup> The right hand side in Eq. 2.1 is the sum over  $j$  of  $f - f^{FD}$  which represents energy relaxation to a steady state Fermi distribution  $f^{FD}(k, n)$  local equilibrium which is the Fermi distribution integrated over the lateral components of the wave vector  $k_x, k_y, k_z$  and  $\frac{1}{2} [f(x, k, t) + f(x, -k, t)]$  which accounts for impurity elastic collisions.<sup>3</sup> For simplicity the collision rates  $\tau_e$  and  $\tau_i$  are taken as constants. Exact Fermi distribution functions have the same electron density thereby preserving charge continuity.  $\mu$  is determined from solving Eq. 2.3 with Eq. 2.4.

The system Eq. 2.1 to 2.4 should have a periodic in  $k$  solution satisfying appropriate initial and boundary conditions:

$$f(x, k, t) = \sum_{j=-\infty}^{\infty} f_j(x, t) e^{ijkl}. \quad 2.$$

where  $F_j = W/l$  minus the electric field and the average

$$F_j(x, t) = \frac{1}{2l} \int_{-l/2}^{l/2} F(x + s, t) ds, \quad 2.$$

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it is possible to obtain the following integral form of the integro-differential equation<sup>4</sup>

$$\frac{df}{dt} = \sum_{j=-\infty}^{\infty} \frac{|ij|}{x} e^{ijkl} E_j \frac{f_j}{x} - e F_j f_j - Q f. \quad 2.8$$

Integrating 2.8 over  $k$  yields the charge continuity equation

$$\frac{dn}{dt} = \sum_{j=1}^{\infty} \frac{2j|}{x} m E_{-j} f_{j-} = 0. \quad 2.9$$

Here we can eliminate the electron density by using the Poisson equation and then integrate over  $x$  thereby obtaining the nonlocal Ampere's law or the total current density  $J(t)$ :

$$\frac{F}{t} = \frac{2e}{x} \sum_{j=1}^{\infty} j m E_{-j} f_{j-} = J(t). \quad 2.10$$

Therefore the above shall assume that the electric field contribution in 2.8 is comparable to the collision terms and that they dominate the other terms *the hyperbolic limit*.<sup>3</sup> Let  $v_M$  and  $F_M$  be the electron velocity and electric field at which the electron drift velocity reaches its maximum. In this limit the time  $t_0$  it takes an electron with speed  $v_M$  to traverse a distance  $x_0 = F_M | / e N_D$  over which the field variation is of order  $F_M$  is much longer than the mean free time between collisions  $\tau_e^{-1} / e F_M | = t_1$ . Therefore we define the *small parameter*  $\epsilon = t_1 / t_0 = v_M N_D / F_M^2 |^2$  and formally multiply the first two terms on the left side of 2.1 or 2.8 by  $\epsilon$ .<sup>3,4</sup> The result is

$$\frac{df}{dt} = \sum_{j=-\infty}^{\infty} \frac{|ij|}{x} e^{ijkl} E_j \frac{f_j}{x} - Q f - \sum_{j=-\infty}^{\infty} \frac{|ej|}{x} e^{ijkl} F_j f_j. \quad 2.11$$

The solution of 2.11 or 2.10 is calculated in terms of its Fourier coefficients as

$$f^{(0)}(k, F) = \sum_{j=-\infty}^{\infty} \frac{1 - ij F_j / e f_j^{FD}}{1 - j^2 F_j^2} e^{ijkl}, \quad 2.12$$

where  $F_j = F_j / F_M = F_M / e e_i / e l$  and  $f_j^{FD} = f_j^{FD} / e e_i / e$ . The ansatz for the integro-differential equation is:<sup>4</sup>

$$f(x, k, t) = f^{(0)}(k, F, n) + \sum_{m=1}^{\infty} f^{(m)}(k, F, n) e^{-m t}, \quad 2.13$$

$$\frac{F}{t} = \sum_{m=0}^{\infty} J^{(m)}(F, n) e^{-m t} = J(t). \quad 2.14$$

The coefficients  $f^{(m)}(k, F, n)$  depend on the slow variables  $x$  and  $t$  only through their dependence on  $F$  and  $n$  which obey 2.2 and 2.14. The nonlocal  $J^{(m)}(F, n)$  are chosen so that the  $f^{(m)}(k, F, n)$  are both even and  $2/\lambda$  periodic in  $k$ . Keeping the desired number of terms and setting  $\lambda = 1$  in 2.14 yields the sought expansion. Inserting 2.13 and 2.14 in 2.11 yields the hierarchy:

$$L f^{(1)} = -\frac{f^{(0)}}{t} + \sum_{j=-\infty}^{\infty} \frac{ij |E_j| e^{ijkl}}{X} f^{(0)}_j \quad 2.15$$

$$L f^{(2)} = -\frac{f^{(1)}}{t} + \sum_{j=-\infty}^{\infty} \frac{ij |E_j| e^{ijkl}}{X} f^{(1)}_j - \frac{1}{t} f^{(0)}_1, \quad 2.16$$

and so on. Here

$$L u(k) = \frac{ie^{-\infty}}{-\infty} \sum_j |F_j| u_j e^{ijkl} = \frac{i}{2} u(k) - \frac{i}{2} u(-k), \quad 2.17$$

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

Inserting the expansion 2.13 into 2.3 we obtain the compatibility condition  $f_0^{(m)} = 0$  or  $m > 0$  which implies that  $L f^{(m)} = 0$  or  $m > 0$ . These solvability conditions yield  $J^{(m)} = 2e^{-\infty} \sum_{j=1}^{\infty} j^m E_{-j} f_j^{(m)}$  which can also be obtained by insertion of 2.12 in 2.10.

We shall particularly refer results to the tight binding dispersion relation  $E(k) = 1 - \cos k/2$  is the miniband with an  $v(k) = |\sin k|/2$  is the group velocity having non-zero Fourier coefficients  $E_0 = 1/2$ ,  $E_{\pm 1} = -1/4$ . The leading order Ampere's law 2.14 is

$$\frac{F}{t} = \frac{ev_M}{l} nM \frac{2F_1}{1 - F_1^2} J(t), \quad 2.18$$

where  $v_M = \frac{1}{l} \int_{-\pi}^{\pi} |v(k)| dk = \frac{1}{l} \int_{-\pi}^{\pi} |\sin k| dk = \frac{4}{l}$ ,  $M = \frac{1}{l} \int_{-\pi}^{\pi} \frac{1}{1 - \cos k} dk = \frac{1}{l} \int_{-\pi}^{\pi} \frac{1}{2k_B T} \mu dk = \frac{\mu}{k_B T}$ .  $\mu = Mk_B T$  calculated graphically in Fig. 1 of Sec. 3 solves 2.3 with  $N_D$ .

The solution of 2.15 yields  $J^{(1)}$  in 2.14 which is the first correction to the 2.18. The details can be found in references 4 and 8 or the numerical procedure. An important point is that the nonlocal terms in the hierarchy require that both boundary conditions be imposed on the intervals  $[-2l, 0]$  and  $[Nl, Nl + 2l]$  or a  $N$  period  $S$ . Fig. 1 shows the current self-oscillations that appear when the system is solved with both boundary conditions  $F/t = F - J$  at each point of the intervals  $[-2l, 0]$  and  $[Nl, Nl + 2l]$ .

an appropriate an c oltage bias. arameter al es correspon to a  
 15 perio 3.4 nm aAs 0.93 nm AlAs S at 5 ith  $N_D = 4.5 \times 10^{10}$   
 $\text{cm}^{-2}$  i  $2e = 18 \times 10^{12}$  n era c oltage bias o 1.2 hich iel  
 $x_0 = 1$  nm  $t_0 = 0.24$  ps  $J_0 = e v_M N_D / l = 1.10 \times 10^5$  A  $\text{cm}^2$ . atho e  
 an ano e contact con tti ities are 2.5 an 0.2  $\text{cm}^{-1}$  respecti el .

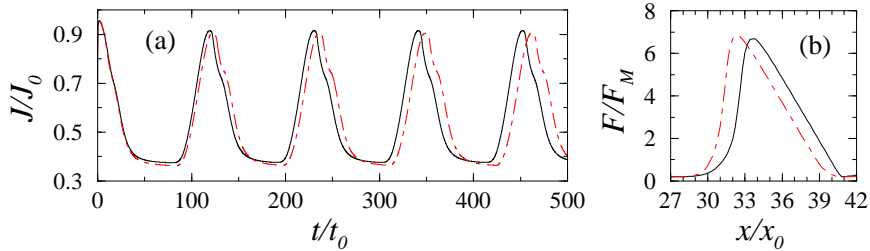


Fig. 1. (a) Current vs. time during self-oscillations, and (b) fully developed dipole wave. Solid line: QDDE, dashed line: GDDE.

### 3. Wigner description of a two-miniband superlattice

e shall consi er a  $2 \times 2$  amiltonian  $H(x, -i \partial / \partial x)$  in hich

$$H(x, k) = \begin{pmatrix} h_0 k - eW(x) \sigma_0 & h_1 k \cdot \sigma \\ 1 - \cos kl - eW(x) \sigma_0 & -i \sin kl \\ i \sin kl & -1 - \cos kl - eW(x) \sigma_0 \end{pmatrix} \quad (3.1)$$

hen  $h_0 = 1 - \cos kl$ ,  $h_1 = 0$ ,  $h_2 = \sin kl$ ,  $h_3 = 1 - \cos kl$ ,  $g$  an

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3.2)$$

he amiltonian 3.1 correspon s to the simplest  $2 \times 2$  ane mo el  
 in hich the a ratic an linear terms  $kl^2/2$  an  $kl$  are replace b  
 $1 - \cos kl$  an  $\sin kl$  respecti el . For a S ith t o miniban s  $2g$  is the  
 miniban gap an  $\pm g$  an  $\pm g$  pro i e  $\pm g$  an  
 $\pm g$  are the miniban i ths. n the case o a lateral S  $g = 0$  an  $h_2 \sigma_2$   
 correspon s to the precession term in the ashba spin orbit interaction.<sup>7</sup>

he other term the inters bban co pling open s on the moment m in  
 the y irection an e ha e not incl e it here. Small mo i cations o  
 3.1 represent a single miniban S ith il te magnetic imp ities in the  
 presence o a magnetic el  $B: g = h_2 = 0$  an  $h_1 = B$ .<sup>6</sup> As in the  
 case o a single miniban S  $W(x)$  is the electric potential.

The energy minibands  $E^\pm(k)$  are the eigenvalues of the free Hamiltonian  $H_0(k) = \hbar_0(k) \sigma_0 + \hbar(k) \cdot \sigma$  and are given by

$$E^\pm(k) = \hbar_0(k) \pm |\hbar(k)|. \tag{3.3}$$

The corresponding spectral projections are  $P^\pm(k) = \sigma_0 \pm \hbar(k) \cdot \sigma / 2$  with  $\hbar/|\hbar(k)|$  so that we can write  $H_0(k) = E^+(k)P^+(k) + E^-(k)P^-(k)$ . We shall now write the equations or theigner matrix written in terms of the Pauli matrices  $\sigma_i$ :

$$f(x, k, t) = \sum_{i=1}^3 f^i(x, k, t) \sigma_i + f^0(x, k, t) \sigma_0 + f(x, k, t) \cdot \sigma. \tag{3.4}$$

Theigner components are real and can be related to the coefficients of the hermitianigner matrix by  $f_{11} = f^0 + f^3$ ,  $f_{12} = f^1 - if^2$ ,  $f_{21} = f^1 + if^2$ ,  $f_{22} = f^0 - f^3$ . Hereinafter we shall use the eigenvalue notations

$$f = \begin{pmatrix} f^0 & f^1 \\ f & f^2 \\ & f^3 \end{pmatrix}. \tag{3.5}$$

The populations of the minibands with energies  $E^\pm$  are the moments:

$$n^\pm(x, t) = \frac{1}{2} \int_{-\pi}^{\pi} f^0(x, k, t) \pm \hbar(k) \cdot f(x, k, t) dk, \tag{3.6}$$

and the total electron density is  $n^+ - n^-$ .

We shall restrict ourselves to the Ashcroft case  $\hbar_3 = 0$  from now on. Hence  $(0, 1, 0)$  and  $n^\pm$  are the densities of electrons having spin  $\pm$ . After some algebra we can obtain the following equations for theigner components

$$\frac{df^0}{dt} = -\sin(kl) f^0 - \frac{\cos(kl)}{2} (f^2 - f^0) - Q^0 f, \tag{3.7}$$

$$\frac{df}{dt} = \frac{\sin(kl)}{2} (f^2 - f^0) - f - f^0 \cos(kl) + \hbar(k) \times f \sin(kl) - f - Q f, \tag{3.8}$$

$$\frac{d^2 W}{dx^2} = \frac{e}{l} (n^+ - n^-) - N_D, \tag{3.9}$$

$$f^i(x, k, t) = \sum_{j=-\infty}^{\infty} \frac{e^{ijl}}{i} F(x, t)_j e^{ijkl} f_j^i(x, t). \tag{3.10}$$

the collision model contains two terms: a term which tries to send  $f^0 \pm f^2$  to its local equilibrium approximate Boltzmann statistics at  $T = 300$  K and a scattering term which tries to equilibrate  $n^+$  and  $n^-$ .<sup>6</sup>

$$Q^0 f = -\frac{f^0 - f^0_0}{\tau}, \quad Q f = -\frac{f - f_0}{\tau_{sc}}, \quad 3.11$$

$$Q^0 = \frac{1}{2} \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right), \quad Q = \frac{1}{2} \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right), \quad 3.12$$

$$n^\pm = n^\pm_0 \exp \left( -\frac{E^\pm - \mu^\pm}{k_B T} \right), \quad 3.13$$

$$\frac{1}{2} \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right) n^\pm = \pm k n^\pm dk. \quad 3.14$$

in 3.13  $\mu^\pm = \mu^\pm_0$  solve 3.14. The collision model satisfies charge continuity. In fact 3.1 to 3.9 yield:

$$\frac{1}{t} \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right) \left[ \sin kl f^0 \pm f^2 + \cos kl f^2 \pm f^0 \right] dk = \frac{1}{2} \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} \right) \left[ Q^0 f \pm Q^2 f \right] dk = \frac{n^+ - n^-}{\tau_{sc}}, \quad 3.15$$

here we have employed  $\int f^{0,2} dk = 0$ . Hence we obtain:

$$\frac{1}{t} (n^+ - n^-) = -\frac{1}{\tau} \int \left[ \sin kl f^0 + \cos kl f^2 \right] dk = 0. \quad 3.1$$

Since  $\int v dx = \int v dx = 1/x = 3.1$  provides charge continuity. From 3.9 and 3.1 we get Ampere's law  $J_t$  is the total current density:

$$\frac{F}{t} = \frac{eI}{\tau} \int \left[ \sin kl f^0 + \cos kl f^2 \right] dk = J_t. \quad 3.1$$

#### 4. Quantum drift-diffusion equations

In the simpler case of a lateral Si with the precession term of Rashba spin-orbit interaction but no intersubband coupling we can obtain explicit rate equations for  $n^\pm$  by means of the method. The general case 3.1 will be treated elsewhere. First of all we should identify the order of magnitude of the terms in the equations 3.1 and 3.8 in the hyperbolic limit. Recall that in this limit the collision frequencies  $1/\tau$  and the lock frequencies  $eF_M/\hbar$  are of the same order about  $10^{10}$  or the Si of Section 2. The scattering time  $\tau_{sc}$  is much longer than the collision time and we

shall consider /  $\text{sc}$   $O$  1. From 3. an 3.8 we can write the scale equations as follows:

$$L f = f - f - \frac{f}{t} f, \quad 4.1$$

$$f = \frac{0}{\text{sc}} \frac{0}{f} - \sin kl - f - \cos kl - \frac{0}{f^0} \quad 4.2$$

$$- \sin kl + \frac{0}{f^3} - f^1$$

where the balance equations are set the following ansatz:

$$f(x, k, t) = f^{(0)}(k, n^+, n^-, F) + \sum_{m=1}^{\infty} f^{(m)}(k, n^+, n^-, F) e^{-i m t}, \quad 4.3$$

$$\frac{F}{t} = \sum_{m=0}^{\infty} J_m(n^+, n^-, F) e^{-i m t}, \quad 4.4$$

$$\frac{n^{\pm}}{t} = \sum_{m=0}^{\infty} A_m^{\pm}(n^+, n^-, F) e^{-i m t}. \quad 4.5$$

$A_m^{\pm}$  and  $J_m$  are related through the Poisson equation 3.9 so that

$$A_m^+ = A_m^- = -\frac{1}{e} \frac{J_m}{x}. \quad 4.$$

Inserting 4.3 to 4.5 into 4.2 we get

$$L f^{(0)} = \dots, \quad 4.$$

$$L f^{(1)} = -\frac{f^{(0)}}{t} - f^{(0)}, \quad 4.8$$

$$L f^{(2)} = -\frac{f^{(1)}}{t} - f^{(1)} - \frac{f^{(0)}}{t}, \quad 4.9$$

and so on. The subscripts 0 and 1 in the right hand side of these equations mean that we replace  $F/t|_m = J_m(n^{\pm})/t|_m = A_m^{\pm}$ . Moreover inserting 4.3 into 3.1 yields the following compatibility conditions:

$$f_0^{(m)0} = f_0^{(m)2} = 0, \quad L f^{(m)0} = L f^{(m)2} = 0, \quad m = 1, 2, \dots \quad 4.10$$



The following values of the parameters are typical of a GaAs AlGaAs  
 S :  $10 \text{ meV}$ ,  $2.1 \text{ meV}$ ,  $l = 5 \text{ nm}$ ,  $T = 300 \text{ K}$ ,  $\tau = 10^{-13} \text{ s}$   
 $\tau_{sc} = 10^{-12} \text{ s}$ ,  $N_D = 10^{10} \text{ cm}^{-2}$ . Figure 2 shows the electron velocity  
 $v = \hbar k / eN_D$  measured in units of  $v_M = \hbar / m^* l$ ,  $\times 10^6 \text{ cm/s}$  as  
 a function of the electric field measured in units of  $F_M = 13.2 \text{ kV/cm}$  at which the  
 electron velocity reaches its maximum for a homogeneous solution of (4.14) -  
 (4.17) with constant  $F$  and  $n^+ = n^- = N_D/2$ . We observe that there is  
 a local maximum followed by a region of negative slope (negative differential  
 velocity) which suggests a spin-split instability as in Section 2:  
 self-sustained oscillations of the current through the S due to motion of  
 charge dipole moments in the presence of a high voltage bias.<sup>1,2,4</sup>

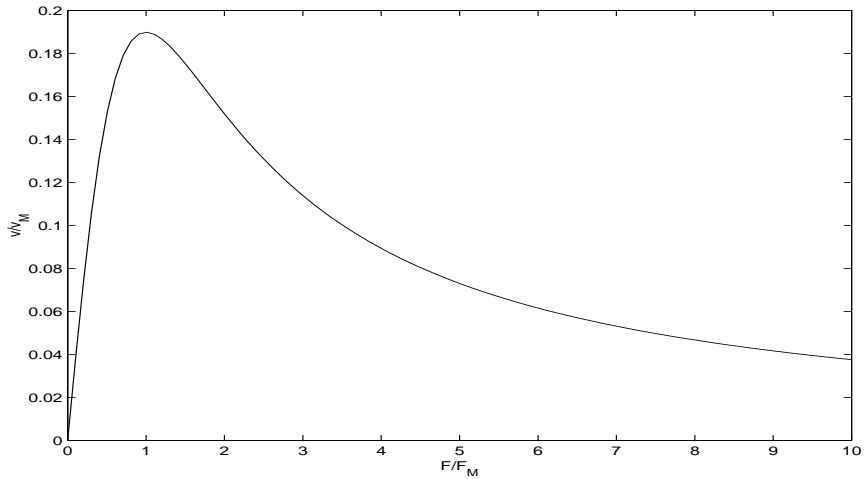


Fig. 2. Electron velocity vs. field for a homogeneous solution of (4.14) - (4.17).

### 5. Conclusions

For strongly coupled S's having only one populated miniband we have  
 written a tight-binding system of equations and derived an analytical  
 method for the calculation of the electron velocity through the  
 tight-binding method. With appropriate voltage bias an analytical solution of this  
 equation yields self-sustained oscillations of the current due to receding  
 and motion of charge dipole moments. For S's having two populated mini-  
 bands coupled through a Rashba spin-orbit interaction we have introduced

a periodic version of the one-dimensional and their corresponding systems of equations. Using the method we have derived important relations for the miniband populations which contain generation recombination terms. The spatially homogeneous solution of these equations provides an electron velocity which has a region of negative slope as a function of  $\mu$ . This hints to the possible existence of oscillator instabilities and self-oscillations of the current due to motion of charge in the presence of a high voltage bias.

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