Spatially Confined Bloch Oscillations in Semiconductor Superlattices

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Abstract. Bloch oscillations are coherent oscillations of the position of electrons (and therefore also of the electric current) inside energy bands of a crystal under an applied constant electric field. Their frequency is proportional to the lattice constant and to the field and therefore can be tuned by an applied voltage. Damped Bloch oscillations have been observed by optical means in undoped semiconductor superlattices which are artificial crystal structures formed by growing a succession of equal periods comprising layers of at least two different semiconductors. We model Bloch oscillations in a doped superlattice by using Boltzmann-Poisson equations and derive hydrodynamic equations for the electron, current and energy densities. For a superlattice with long scattering times, we show that the damping of Bloch oscillations is so small that nonlinearities may compensate it and provide stable oscillations of the current and energy densities. In this case, numerical solutions show that there are stable Bloch oscillations spatially confined to part of the superlattice, thereby having inhomogeneous field, charge, current density and energy density profiles. These Bloch oscillations disappear as scattering times become sufficiently short.

Keywords: Bloch oscillations, semiconductor superlattices, Boltzmann-BGK model, hydrodynamic limit and equations, waves, modulated oscillations
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INTRODUCTION

Bloch oscillations (BOs) are coherent time periodic oscillations of the position of electrons inside energy bands of a crystal under an applied constant electric field. They give rise to self-sustained oscillations of the current. Predicted by Zener in 1934, they are an immediate consequence of the Bloch theorem [1]. Scattering damps BOs and they can be experimentally observed in artificial periodic structures such as semiconductor superlattices (SLs), first proposed by Esaki and Tsu [1]. Besides their interest for theoretical physics, BOs have attracted the attention of many physicists and engineers because of their potential for designing infrared detectors, emitters or lasers which can be tuned in the THz frequency range simply by varying the applied electric field [1]. Another application is based on the fact that BOs give rise to a resonance peak in the absorption coefficient under dc+ac bias and a positive gain at THz frequencies [2, 3]. These applications are severely limited by scattering which rapidly damps BOs and, for a dc voltage biased SL, favors the formation of electric field domains (EFDs) whose dynamics yields Gunn-type self-sustained oscillations of lower frequency (GHz) [4, 5]. Recently, we have proposed a model that may contain both BOs and the slower Gunn-type oscillations due to EFD dynamics [6, 7]. Electron transport in a doped SL is described by a self-consistent Boltzmann-Poisson equation in which phonon scattering is modeled by a dissipative Bhatnagar-Gross-Krook (BGK) collision term [6, 7]. The local equilibrium distribution depends on the electron, current and energy densities. Previous models could describe Gunn-type oscillations but not stable BOs because their local distribution was a function of electron density only [5], and they could not describe BOs except as short transient stages (the electron density remains approximately constant during a BO). The model equations are

$$\partial_t f + v(k)\,\partial_x f + eF\hbar^{-1}\partial_k f = Q[f] \equiv -\nu(f - f^B), \tag{1}$$

$$\varepsilon\,\partial_x F = el^{-1}(n - N_D), \tag{2}$$

$$f^B(k;n,J_n,E) = n\,\frac{\pi\, e^{\tilde{u}kl + \tilde{\beta}\cos kl}}{\int_0^\pi e^{\tilde{\beta}\cos K}\cosh(\tilde{u}K)\,dK}, \tag{3}$$

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

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Here n, N_D, ε, $-e<0$, m^*, ν, and $-F$ are the 2D electron density, the 2D doping density, the permittivity, the electron charge, the effective mass of the electron, the constant collision frequency and the electric field, respectively. $v(k)=\Delta l\sin(kl)/(2\hbar)$ is the group velocity corresponding to the miniband tight binding dispersion relation $\mathscr{E}(k)=\Delta(1-\cos kl)/2$. For the sake of simplicity, we have assumed a Boltzmann local equilibrium (3), but it is easy to replace it by the Fermi-Dirac local distribution in the degenerate case. The distribution functions f and f^B have the same units as n and are $2\pi/l$-periodic in k (the function $\tilde{u}kl$ in (3) is extended periodically outside $-\pi<kl\leq\pi$). A quantum version of (1) can be obtained as indicated in Ref. [5].

The dimensionless multipliers $\tilde{\beta}(x,t)$ and $\tilde{u}(x,t)$ depend on J_n=$e\int_{-\pi/l}^{\pi/l}v(k)\,f\,dk/(2\pi)$ (electron current density) and on E=$l\int_{-\pi/l}^{\pi/l}[\Delta/2-\mathscr{E}(k)]f\,dk/(2\pi n)$ (mean energy). They are found by solving $\frac{e}{2\pi}\int_{-\pi/l}^{\pi/l}v(k)\,f^B\,dk=(1-\alpha_j)J_n$, and $\frac{l}{2\pi n}\int_{-\pi/l}^{\pi/l}\left(\frac{\Delta}{2}-\mathscr{E}\right)f^B dk=\alpha_e E_0+(1-\alpha_e)E$. α_e and α_j are constant restitution coefficients that take on values on the interval $[0,1]$ and measure the dissipation due to collisions in current density and energy, respectively. In fact, the collision operator satisfies $\int_{-\pi/l}^{\pi/l}Q[f]\,dk=0$ (charge continuity), $e\int_{-\pi/l}^{\pi/l}v(k)\,Q[f]\,dk/(2\pi)=-\nu\alpha_j J_n$, and $l\int_{-\pi/l}^{\pi/l}[\Delta/2-\mathscr{E}(k)]\,Q[f]\,dk/(2\pi n)=-\nu\alpha_e(E-E_0)$. Obviously for $\alpha_{e,j}=0$ the collisions conserve energy and momentum (elastic limit). E_0 is the mean energy at the lattice temperature of the global equilibrium which will be reached in the absence of bias and contact with external reservoirs.

HYDRODYNAMIC EQUATIONS

In the hyperbolic limit in which the collision and Bloch frequencies are comparable and dominate all other terms in (1), it is possible to derive closed equations of hydrodynamic type for the nondimensional variables n, F and A (the complex envelope of the BO solution) [8], provided the collisions are almost elastic. For the BO solution, the first harmonic of the distribution function is

$$f_1=nE-iJ_n=A(x,t)e^{-i\theta}+f_{1,S}(x,t),\quad \theta=\frac{1}{\delta}\int_0^t F(x,s)\,ds \tag{5}$$

where $f(x,k,t;\delta)=\sum_{j=-\infty}^{\infty}f_je^{ijk}$ (f is 2π-periodic in k), θ is the rapidly varying phase of the BO and $f_{1,S}=O(\delta)$ is a slowly varying function; see below. The small dimensionless parameter $\delta=e^2N_Dl\Delta/(2\varepsilon\hbar^2\nu^2)$ is the ratio between the scattering time and the dielectric relaxation time and the restitution coefficients are assumed to scale with it, $\alpha_{e,j}=\delta\gamma_{e,j}$. The nondimensional hydrodynamic equations for n, F and A are

$$\frac{\partial F}{\partial t}+\frac{\delta}{F^2+\delta^2\gamma_j\gamma_e}\left[\gamma_eE_0nF+\frac{F}{2}\frac{\partial}{\partial x}\mathrm{Im}\frac{f_{2,0}^{B(0)}}{1+2iF}-\frac{\delta\gamma_e}{2}\frac{\partial}{\partial x}\left(n-\mathrm{Re}\frac{f_{2,0}^{B(0)}}{1+2iF}\right)-F\mathrm{Re}\,h_S+\delta\gamma_e\mathrm{Im}\,h_S\right]=J(t), \tag{6}$$

$$\frac{\partial F}{\partial x}=n-1, \tag{7}$$

$$\frac{\partial A}{\partial t}=-\frac{\gamma_e+\gamma_j}{2}A+\frac{1}{2i}\frac{\partial}{\partial x}\left(\frac{f_{2,-1}^{B(0)}}{1+iF}\right), \tag{8}$$

$$h_S=\frac{f_{1,Su}}{n}\mathrm{Im}\frac{\partial f_{1,Su}}{\partial x}+(J+\mathrm{Im}f_{1,Su})\frac{\partial f_{1,Su}}{\partial F},\qquad f_{1,Su}=\frac{\delta\gamma_enE_0(\delta\gamma_j-iF)}{\delta^2\gamma_e\gamma_j+F^2}, \tag{9}$$

$$\begin{aligned}f_{1,S}&=nE_S-iJ_{n,S}=\frac{\delta}{F^2+\delta^2\gamma_j\gamma_e}[\gamma_enE_0(\delta\gamma_j-iF)-(\delta\gamma_j-iF)\mathrm{Re}h_S-(F+i\delta\gamma_e)\mathrm{Im}h_S\\&+\frac{F+i\delta\gamma_e}{2}\frac{\partial}{\partial x}\left(n-\mathrm{Re}\frac{f_{2,0}^{B(0)}}{1+i2F}\right)+\frac{\delta\gamma_j-iF}{2}\mathrm{Im}\frac{\partial}{\partial x}\left(\frac{f_{2,0}^{B(0)}}{1+i2F}\right)\Bigg].\end{aligned} \tag{10}$$

We have defined the nondimensional variables $\tilde{f}=f/N_D$, $\tilde{n}=n/N_D$, $\tilde{E}=2E/\Delta$, $\tilde{J}_n=J/[J_n]$, $\tilde{x}=x/[x]$, ...(where $[y]$ are the units in Table 1) and omitted tildes over variables. The dimensionless multipliers $\tilde{\beta}$ and $\tilde{u}$ in f^B are functions of the rapidly varying BO phase θ due to (5) and therefore, we can expand f^B in (3) in powers of δ,

TABLE 1. Hyperbolic scaling and nondimensionalization with $\nu = 10^{14}$ Hz.

f, n	F	$\mathscr{E}, E$	$v(k)$	J_n	x	k	t	δ
N_D	$\frac{\hbar\nu}{el}$	$\frac{\Delta}{2}$	$\frac{l\Delta}{2\hbar}$	$\frac{eN_D\Delta}{2\hbar}$	$\frac{\varepsilon\hbar\nu}{e^2N_D}$	$\frac{1}{l}$	$\frac{2\varepsilon\hbar^2\nu}{e^2N_Dl\Delta}$	$\frac{e^2N_Dl\Delta}{2\varepsilon\hbar^2\nu^2}$
$\frac{10^{10}}{\mathrm{cm}^2}$	$\frac{\mathrm{kV}}{\mathrm{cm}}$	meV	$\frac{10^4\mathrm{m}}{\mathrm{s}}$	$\frac{10^4\mathrm{A}}{\mathrm{cm}^2}$	nm	$\frac{1}{\mathrm{nm}}$	ps	–
4.048	130	8	6.15	7.88	116	0.2	1.88	0.0053

$f^B \sim f^{B(0)} + \delta f^{B(1)}$. The $f^{B(m)}$ $(m = 1,2)$ are now 2π-periodic functions of θ and k. Then we have the Fourier coefficients $f^{B(0)}_{j,m} = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} f^{B(0)}(k;n,f_1)\, e^{-ijk-im\theta}\, \frac{dk\,d\theta}{(2\pi)^2}$, in which we set $f_1 = A\, e^{-i\theta}$ ignoring $O(\delta)$ terms in (5).

To derive (6)-(8), we first obtain equations for $f_0 = n$ and $f_1 = nE - iJ_n$ by integrating (1) over k [6, 7]:

$$\frac{\partial f_0}{\partial t} - \mathrm{Im}\frac{\partial f_1}{\partial x} = 0, \tag{11}$$

$$\left(\delta\frac{\partial}{\partial t} + iF\right) f_1 = \delta\left[\gamma_e f_0 E_0 - \frac{\gamma_e+\gamma_j}{2} f_1 - \frac{\gamma_e-\gamma_j}{2} f_1^* - \frac{1}{2i}\frac{\partial}{\partial x}(f_0 - f_2)\right]. \tag{12}$$

From (11) and (7), we find an Ampère's law for F: $\partial F/\partial t = J(t) + \mathrm{Im} f_1$, where $J(t)$ is the total current density. We shall assume that the second moment f_2 is a known function of f_0 and f_1, $f_2 = g(f_0, f_1)$. Then we separate the rapidly and slowly varying parts of f_1 according to (5) and find equations for n, F and A by a method of nonlinear multiple scales with time scales θ and t. To find g, we carry out a Chapman-Enskog expansion [9, 8] for (1) (in dimensionless units) with a time derivative given by $F\,\partial f/\partial\theta + \delta\,\partial f/\partial t$, according to (5). The distribution function is supposed to be periodic in k and in θ. This procedure gives approximate formulas for $g = f_2$ from which (6)-(8) are obtained [8].

The hydrodynamic equations (6)-(8) have the spatially uniform solutions, $n = 1$, $J = -\mathrm{Im} f_{1,Su} = \delta\gamma_e E_0 nF/(\delta^2\gamma_e\gamma_j + F^2)$ [5], and $A = A_0 e^{-(\gamma_e+\gamma_j)t/2}$. (5) shows that the latter formula corresponds to a damped BO whose amplitude relaxes to 0. Even when we prepare the initial state with a coherent BO of complex amplitude A_0, ignoring space dependence will lead to disappearance of the BOs after a relaxation time $2/(\gamma_e + \gamma_j)$. Stabilization of the BOs may be caused only by the spatially dependent second term in the right hand side of (8).

NUMERICAL RESULTS

We now solve numerically the hydrodynamic equations with the boundary conditions [5]

$$\frac{\partial F}{\partial t} + \sigma_0 F\bigg|_{x=0} = J, \quad \frac{\partial F}{\partial t} + \sigma_1 nF\bigg|_{x=L} = J, \quad \frac{1}{L}\int_0^L F(x,t)\,dx = \phi, \quad \frac{\partial A}{\partial x}\bigg|_{x=0} = 0. \tag{13}$$

We obtain similar numerical results with $A(0,t) = 0$. Here $L = Nl/[x]$ and $\phi = eV/(\hbar\nu N)$ are dimensionless SL length and average field (proportional to the applied voltage V), respectively. We have used contact conductivities $\sigma_{0,1} = 12.1$ $(\Omega\,\mathrm{m})^{-1}$ which yield dimensionless conductivities $\sigma_{0,1} = 0.2$ (conductivity units are $[\sigma] = e^2 N_D\Delta l/(2\hbar^2\nu)$). Initially, $F(x,0) = \phi$ and $A(x,0) = A_0$ (constant). The latter condition means that we have prepared the SL in an initial state having a coherent BO with complex amplitude A_0.

We solve (6)-(8) with the parameter values indicated in Table 1 (which are similar to those in Ref. [10]) and different values of the restitution coefficients. We start with $\alpha_e = \alpha_j = 0.01$ so that $\nu\alpha_e = \nu\alpha_j = 10^{12}$ Hz. The 3D doping density $N_{3D} = 8\times 10^{16}$ cm^{-3} gives $N_D = N_{3D}l = 4.048\times 10^{10}$ cm^{-2} as in Table 1, and $\varepsilon = 12.85\,\varepsilon_0$. We find $\delta \approx 0.0053$ and $\gamma_{e,j} = \alpha_{e,j}/\delta = 1.8781$. We consider a 50-period ($N = 50$) dc voltage biased SL with lattice temperature 300 K. For $V = 0.2$ V (therefore $\phi = 0.06$), we observe that $|A(x,t)|$ first diminishes uniformly from $A_0 = 0.153$ to almost zero after a relaxation time $2/(\gamma_e+\gamma_j) \approx 0.53$ (about 1 ps). Later a small pulse is formed at about $x = L/4$ which subsequently extends to the remaining part of the sample and it grows more near its end. The BOs are confined to the second half of the sample that is closer to $x = L$ and are zero in the first half of the sample closer to $x = 0$. Thus the profile of $|A|$ has a compact support with a maximum near $x = L$. $|A(x,t)|$ is close to a periodic oscillation in time: small pulses are formed at the left of its support, climb up towards the maximum of the pulse which then diminishes and the same behavior repeats itself. Figure 1(a) shows four snapshots of $|A(x,t)|$ illustrating this behavior. The field profile depicted in Fig. 1(b) is almost stationary. The mean energy and electron current densities during one BO can be reconstructed by means of (5). At the two different SL locations marked in Fig. 1(b), the graphs of J_n versus time

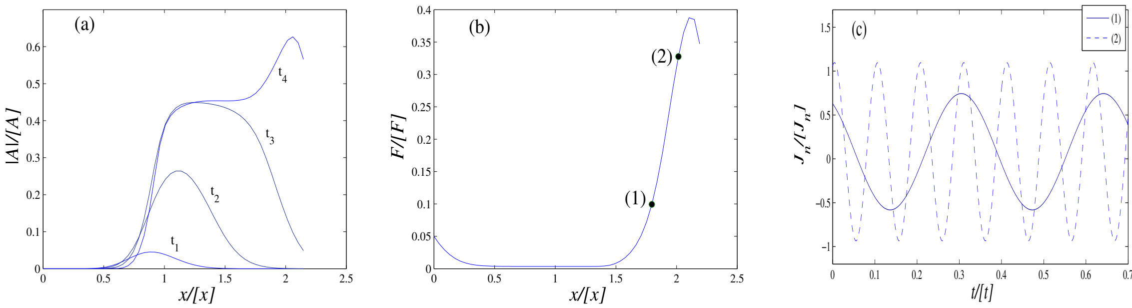

FIGURE 1. (a) Modulus of the BO complex amplitude vs space at times $t_1 = 7$, $t_2 = 9$, $t_3 = 11$, $t_4 = 13$. (b) Stationary field profile. (c) Current density at the two different points marked by (1) and (2) in (b) during BOs. Clearly, the frequency at point (2) is larger than at (1).

are shown in Fig. 1(c). This figure illustrates that the Bloch frequencies depend strongly on space and are higher near the collector where the field is larger.

For the scattering times reported in Ref. [10], the restitution coefficients are $\alpha_e = 0.09$ and $\alpha_j = 0.29$, but the BO amplitude becomes zero everywhere after a short relaxation time. There is a critical curve in the plane of restitution coefficients such that, for $(\gamma_e + \gamma_j)/2 > \gamma_{\text{crit}}$ ($\gamma_{\text{crit}} \approx 2.5$ for $\delta = 0.0053$), BOs disappear after a relaxation time but they persist for smaller values of $(\gamma_e + \gamma_j)$.

SUMMARY

We have analyzed the Boltzmann-BGK-Poisson equations with local equilibrium depending on the electron density, current density and energy density in the hyperbolic limit in which the BO period is much shorter than the dielectric relaxation time and collisions are almost elastic. In the long-time scale, there is a hydrodynamic regime described by coupled equations for the electric field, the electron density and the BO complex amplitude. When the restitution coefficients (equivalently the inverse of the scattering times) are sufficiently small and the initial state has been prepared so that there is a nonzero Bloch oscillation, there are stable spatially inhomogeneous profiles of current and energy densities displaying BOs confined to a fraction of the SL extent. It would be interesting to investigate whether confined Bloch oscillations may also be important for terahertz harmonic generation with underlying inhomogeneous charge and electric field profiles.

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