A Mathematical Walk into the Paradox of Bloch Oscillations

Luigi Barletti

Dipartimento di Matematica e Informatica “Ulisse Dini”, Università degli Studi di Firenze, Firenze, Italy

ABSTRACT
We mathematically describe the apparently paradoxical phenomenon that the electric current in a semiconductor can flow because of collisions, and not despite them. A model of charge transport in a one-dimensional semiconductor crystal is considered, where each electron follows the periodic Hamiltonian trajectories, determined by the semiconductor band structure, and undergoes non-elastic collisions with a phonon bath. Starting from the detailed phase-space model, a closed system of ODEs is obtained for averaged quantities. Such a simplified model is nevertheless capable of describing transient Bloch oscillations, their damping and the consequent onset of a steady current flow, which is in good agreement with the available experimental data.

KEYWORDS
Bloch oscillations; semiconductors; collisions; transport; diffusion

1. Introduction
Microelectronics, whose fundamental importance for the modern civilization needs not to be stressed, is based on electronic currents flowing in semiconductor materials. Such currents are the macroscopic manifestation of the microscopic dynamics of electrons inside the semiconductor and of their interaction with external perturbations, such as electrostatic fields, light, heat, mechanical pressure, etc. Understanding the behavior of electrons in semiconductors has become therefore one of the most important branches of physics, which is known as solid-state physics. This is very well known. But what is probably less known is the curious phenomenon underlying all of this: the current can flow because of collisions, and not despite them. The aim of these notes is to illustrate this apparent paradox by means of a simple mathematical model of electron transport in a semiconductor crystal under the action of an external electrostatic field.

A semiconductor is a crystalline solid made by ions periodically arranged in space and held together by covalent bonds. So, what a “free” (non-bond)
an electron feels inside a semiconductor crystal is a periodic electrostatic potential generated by the crystal ions. Now, according to the basic laws of quantum mechanics, the possible energies $E$ of a particle with potential energy $W$ are given by the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m} \Delta \psi + W \psi = E \psi$$

which is the eigenvalue equation for the quantum Hamiltonian $-\frac{\hbar^2}{2m} \Delta + W$. For example, in the case of a free particle ($W=0$) one finds a continuum of possible energies (namely, $E \geq 0$), while in the case of a harmonic trap ($W$ is a harmonic potential) one finds a sequence of discrete levels. When $W$ is a periodic potential, which is the case under consideration, one finds that the possible energies form a sequence of intervals, called energy bands, alternated with forbidden bands. Therefore, the periodic case is, so to say, a mix of the free and the trapped particle cases. Moreover, and this point will be central for all that follows, each energy band is a periodic function $E_n(p)$ of the electron momentum $p$. Here, $n$ is an integer labeling the bands.

What we have said so far is not much different from what could be said for metals. What distinguishes a semiconductor from a metal is that a semiconductor possesses a energy gap, that is a forbidden band which is placed more or less at the level of the Fermi energy. This means (by simplifying a little) that the energy bands below the gap are statistically "fully occupied" and cannot contribute to the conduction of current (Ashcroft and Mermin 1976). On the contrary, the energy band just above the Fermi level is only partially occupied and its electrons can produce a current (not for nothing it is called conduction band). The fact that in a semiconductor the conduction band is energetically isolated will allow us to consider, in first approximation, only this energy band in the mathematical model that will be discuss hereafter. This is why our model applies to semiconductors and not to metals, even though many of the considerations that will be made are also true for metals.

Let us then consider an electron in the conduction band and assume that a constant electrostatic force is exerted on it (e.g., by applying a voltage). Such electron will be uniformly accelerated, or, more precisely, its momentum $p$ will increase (or decrease, according to the direction of the force) linearly with time. But the energy band is a periodic function of $p$ and then, by the conservation of energy, also the potential energy of the external field must vary periodically. This requires a periodic variation of the electron position, which is therefore forced to move back and forth. Such periodic motion is called Bloch oscillations, hereafter abbreviated with BO. Since it is extremely difficult to observe the BO in bulk
semiconductors (the Fourier reciprocity between space and momentum periods makes the latter too large to be entirely spanned by electrons), they have been observed in artificial semiconductor “superlattices” (Dekorsy et al. 1995; Leo et al. 1992). We will come back on this point in Section 5.

Then, the purely conservative Hamiltonian dynamics of an electron in a semiconductor is an oscillatory motion which would prevent the onset of any current. So, how is it possible that an electric current can actually flow in a semiconductor? The answer is in the obstacles that the electron finds on his path. Such obstacles can be of various kind, the most important being the phonons, i.e., the thermal vibrations of the crystal lattice. The interaction (“collision”) with a phonon is an inelastic process which makes the electron (instantaneously and locally, in first approximation) change momentum and loose energy, thus jumping on a different Hamiltonian trajectory. If the collisions are frequent enough (but not too much), they will allow the electron to jump from one trajectory to another, which is what really makes it advance in the direction of the field: see Figure 1. This is indeed the mechanism that makes currents possible.

The ideas that have been just sketched will be made more precise in the rest of the paper with the introduction of a transport model that includes both the BO dynamics and the collisions. In Section 2 we introduce the transport model, which consists of a semiclassical Boltzmann equation for the electronic density in phase-space. After non-dimensionalisation, in Section 3 a system of fluid-dynamic, Euler-like, equations is derived from the transport equation. The closure of such system is then obtained in the limit where the number of collision, compared to the time that the electron momentum takes to span the BO period, goes to infinity. This leads to a

![Figure 1: A pictorial representation of the BO paradox: an electron, which would be otherwise trapped on a Hamiltonian periodic trajectory in phase-space (dashed curves), jumps from one trajectory to another thanks to inelastic collisions (dashed arrows). This produces an average advance toward the direction of the field (here rightward).](image-url)
drift-diffusion equation and, therefore, to the existence of a current. In Section 4, we take space-averages of the fluid variables and find a system of ODEs which has the form of a forced and damped harmonic oscillator. The dynamics described by this system consists of an oscillatory transient, dominated by BO, the oscillation damping and the consequent onset of a steady current flow. The obtained solution is then discussed in relation with the available experimental data in the last section, Section 5.

2. The transport model

Let us consider a simple model of a semiconductor by assuming that the crystal lattice has only one spatial dimension ad that the charge transport takes place in a single conduction band $\mathcal{E}(p)$. Moreover, let us assume that the energy of the electrons in this band takes the form:

$$\mathcal{E}(p) = E_0 \left(1 - \cos \left(\frac{p}{p_0}\right)\right)$$

which is known as Kronig-Penney dispersion relation (Bransden and Joachain 2000). This is equivalent to assuming that the lattice periodic potential has the shape of a “square wave.” This is a simplification in general but, in the case of a semiconductor superlattice (see Section 5), it can be very close to the real situation. We remark that this energy is a periodic function of the electron momentum $p$, with a period of $2\pi p_0$ and an amplitude of $E_0$. In a semiclassical perspective, the electron velocity as a function of $p$ is given by

$$\frac{\partial \mathcal{E}}{\partial p} = \frac{E_0}{p_0} \sin \left(\frac{p}{p_0}\right)$$

and the electron effective mass (Barletti and Ben Abdallah 2011) is given by

$$\frac{1}{m^*} = \left. \frac{\partial^2 \mathcal{E}}{\partial p^2} \right|_{p=0} = \frac{E_0}{p_0^2}.$$  

Note that the effective mass is, indeed, a quantity that plays the role of the mass in the quadratic approximation of the energy:

$$\mathcal{E}(p) \approx \frac{p^2}{2m^*}$$

(physically speaking, for low energies, a particle in a periodic potential behaves as a free particle but with a different mass).

On the other hand, we assume that the electron is also subject to an external electrostatic field with a linear profile of the form
This of course corresponds to a constant force $F$ exerted by an applied voltage $V$ such that $qV = -FL$, where $q$ is the elementary charge and $L$ is the device length.

In this picture, the electron (classical) Hamiltonian can be written as

$$H(x,p) = E(p) + U(x) = E_0 \left(1 - \cos \left(\frac{p}{p_0}\right)\right) - Fx,$$

where $p$ is a periodic variable, of period $2\pi p_0$, and $x \in [0,L]$. The corresponding Hamilton equations are

$$\begin{cases} \dot{x} &= \frac{\partial H}{\partial p} = \frac{E_0}{p_0} \sin \left(\frac{p}{p_0}\right), \\ \dot{p} &= -\frac{\partial H}{\partial x} = F, \end{cases}$$

(6)

describing the unperturbed BO motion of the electron.

### 2.1. Transport equation

Let $f(x,p,t)$, $x \in [0,L]$, $p \in [-\pi p_0, +\pi p_0]$, $t \geq 0$, be the electron phase-space density function at time $t$. As the crystal has only one spatial dimension, the spatial electron density $\rho$ can be expressed as

$$\rho(x,t) = \int_{-\pi p_0}^{\pi p_0} f(x,p,t) \, dp$$

(7)

and the electronic current density can be expressed as

$$j(x,t) = \frac{E_0}{p_0} \int_{-\pi p_0}^{\pi p_0} \sin \left(\frac{p}{p_0}\right) f(x,p,t) \, dp.$$

(8)

The non-collisional, semiclassical transport equation for $f$ is the Liouville equation for the Hamiltonian $H$, namely,

$$\frac{\partial f}{\partial t} + x \frac{\partial f}{\partial x} + p \frac{\partial f}{\partial p} = \frac{\partial f}{\partial t} + \frac{E_0}{p_0} \sin \left(\frac{p}{p_0}\right) \frac{\partial f}{\partial x} + F \frac{\partial f}{\partial p} = 0.$$

(9)

This simply expresses the fact that the phase-space distribution is constant along the hamiltonian trajectories of the system. In particular, the distribution remains constant on the phase-space curves of constant energy $E$:

$$E_0 \left(1 - \cos \left(\frac{p}{p_0}\right)\right) - Fx = E.$$

(10)

Equation (9) describes a purely hamiltonian evolution of the electron population. In semiconductors, however, electrons undergo non-elastic
interactions with the lattice vibrations (phonons). A complete description of the interactions between electrons and phonons would require a detailed scattering operator that includes the different branches of the phonon dispersion relations (Camiola, Mascali, and Romano 2020). Here, for the sake of simplicity, we shall assume that such interactions can be described by means of a space-homogeneous, linearized Boltzmann collisional operator of the following form:

\[ \frac{1}{\tau_0} \int_{-\pi p_0}^{\pi p_0} b_0(p, p') \left[ M(p)f(x, p', t) - M(p')f(x, p, t) \right] dp', \]  

where \( \tau_0 \) is the typical collision time (1/\( \tau_0 \) is the collision frequency), \( b_0(p, p') = b_0(p', p) \) is the scattering kernel (i.e., the probability of the electron momentum \( p' \) to be scattered to a new momentum \( p \), following a collision) and

\[ M(p) = \frac{1}{\sqrt{2\pi m^* k_B T}} e^{-\frac{p^2}{2 m^* k_B T}} \]

is the Maxwellian distribution. In the last expression, \( m^* \) is the effective electron mass (3), \( k_B \) is the Boltzmann constant and \( T \) is the temperature of the phonon bath. Note that the collisions term described by (11) can be interpreted as follows: electrons collide with a typical frequency 1/\( \tau_0 \) and the effect of collisions is to re-distribute the electron momenta according to a maxwellian (thermal) distribution at the temperature of the phonon bath.

The complete transport model is now obtained by adding the collision term (11) to the Liouville Equation (9), which results in the transport equation

\[ \frac{\partial f}{\partial t} + \frac{E_0}{p_0} \sin \left( \frac{p}{p_0} \right) \frac{\partial f}{\partial x} + F \frac{\partial f}{\partial p} = \frac{1}{\tau_0} \int_{-\pi p_0}^{\pi p_0} b_0(p, p') \left[ M(p)f(p') - M(p')f(p) \right] dp', \]

(in the integral, the space and time variable have been omitted). This equation is a variant of what is sometimes called “semiclassical Boltzmann equation” (Ashcroft and Mermin 1976).

An important remark is necessary here. The choice of a Maxwellian as the thermal distribution may seem in contradiction with the periodicity of the variable \( p \). Actually, the correct equilibrium distribution would be

\[ c e^{-\frac{E(p)}{k_B T}}, \]

where \( c \) is the suitable normalization constant and \( E(p) \) is given by (1), which is indeed periodic. However, in standard situations, the thermal electron momentum \( p_{th} = \sqrt{m^* k_B T} \) is much smaller than \( p_0 \), which means that it is reasonable to assume
\[
\frac{p_{th}}{p_0} = \frac{\sqrt{m^* k_B T}}{p_0} = \sqrt{\frac{k_B T}{E_0}} \ll 1
\]  

(recalling the definition (3) of the effective mass \(m^*\)). Under such condition, \(E(p)\) is very close to its quadratic approximation \(\frac{p^2}{2m}\), which leads to the Maxwellian (12). This also means that the Maxwellian is narrow enough to be practically zero at the period endpoints \(\pm \pi p_0\) and, therefore, it can be reasonably considered as periodic.

### 2.2. The evolution problem

For physical and mathematical consistency, Equation (13) must be supplemented with suitable conditions on the inflow part of the boundary:

\[
\begin{cases}
    f(0, p, t) = \phi_l(p), & \text{if } p > 0, \\
    f(L, p, t) = \phi_r(p), & \text{if } p < 0,
\end{cases}
\]

where \(\phi_l(p)\) and \(\phi_r(p)\) are the assigned inflows of electrons from the left and from the right, respectively. Typically, they are chosen as maxwellian distributions, at the temperature \(T\), with densities corresponding to the electronic densities of the metallic contacts (Frensley 1987).

Moreover, since \(p\) is a periodic coordinate, we also have to impose the periodicity condition on the momentum boundary:

\[
f(x, \pi p_0, t) = f(x, -\pi p_0, t).
\]

Finally, we have to assign the density function at the initial time (say, \(t = 0\)):

\[
f(x, p, 0) = f_{in}(x, p).
\]

It can be proven that, under suitable regularity assumptions on the data, the initial-boundary value problem (13)-(15)-(16)-(17) is well-posed as an evolution problem in the Banach space \(L^1(\mathbb{R}_x \times \mathbb{R}_p)\) of integrable functions on phase-space (Barletti 2000; Belleni-Morante 1979; Tilli 2011). Such evolution problem can be formally written as

\[
\begin{cases}
    \dot{f}(t) = Af(t) + Bf(t), \\
    f(0) = f_{in}
\end{cases}
\]

where

\[
Af = \frac{E_0}{p_0} \sin \left( \frac{p}{p_0} \right) \frac{\partial f}{\partial x} + E \frac{\partial f}{\partial p}
\]

is the Liouville operator (defined on a suitable domain that contains the boundary conditions (15)-(16)) and
is the collisional operator. Under reasonable assumptions on the scattering kernel \( b_{0}(p, p') \), \( B \) is a bounded perturbation and the solution to the evolution problem can be represented as a Dyson-Phillips series (here written in the simpler case of homogeneous boundary conditions \( \phi_{I} = \phi_{R} = 0 \)):

\[
f(t) = T(t) f_{\text{in}}
\]

\[
+ \int_{0}^{t} T(t - s_{1}) B T(s_{1}) f_{\text{in}} ds_{1}
\]

\[
+ \int_{0}^{t} \int_{0}^{s_{1}} T(t - s_{1}) B T(s_{1} - s_{2}) B T(s_{2}) f_{\text{in}} ds_{1} ds_{2}
\]

\[
\vdots
\]

Here, \( T(t) \) is the evolution semigroup generated by \( A \), representing therefore the non-collisional dynamics (pure streaming along the hamiltonian trajectories), and each term of the series corresponds to the contributions of electrons that have undergone \( 0, 1, 2, \ldots \) collisions in the time interval \( [0, t] \). Equation (19) has to be considered as the rigorous mathematical representation of the dynamics pictured in Figure 1.

### 2.3. Non-dimensionalisation

We shall now write Equation (13) in non-dimensional form. Let \( x_{0}, p_{0}, t_{0} \) and \( f_{0} \) by reference length, momentum, time and density, respectively (the reference momentum is the same \( p_{0} \) appearing in the energy band (1)). The corresponding non-dimensional variables are given by

\[
\hat{x} = x/x_{0}, \quad \hat{p} = p/p_{0}, \quad \hat{t} = t/t_{0},
\]

and the non-dimensional distribution function is given by

\[
\hat{f}(\hat{x}, \hat{p}, \hat{t}) = f(x_{0} \hat{x}, p_{0} \hat{p}, t_{0} \hat{t})/f_{0}.
\]

Making these substitutions into (13) and multiplying by \( t_{0} \) yields

\[
f_{0} \frac{\partial \hat{f}}{\partial \hat{t}} + \frac{t_{0} f_{0} E_{0}}{p_{0} x_{0}} \sin(\hat{p}) \frac{\partial \hat{f}}{\partial \hat{x}} + \frac{f_{0} t_{0} F}{p_{0}} \frac{\partial \hat{f}}{\partial \hat{p}}
\]

\[
= \frac{t_{0} f_{0} p_{0}}{\tau_{0}} \int_{-\pi}^{\pi} b_{0}(p_{0} \hat{p}, p_{0} \hat{p}') \left[ \mathcal{M}(p_{0} \hat{p}) \hat{f}(\hat{p}') - \mathcal{M}(p_{0} \hat{p}') \hat{f}(\hat{p}) \right] d\hat{p}',
\]

(20)

where we also performed the change of integration variable \( \hat{p}' = p'/p_{0} \).

Now, it is natural to chose as reference length \( x_{0} = L \), the device length, while it is clear than the choice of \( f_{0} \) is irrelevant, because of the linearity of the equation. Moreover, the reference time is chosen to be
\[ t_0 = \frac{p_0}{F}. \]

This can be interpreted as follows: since the electron is uniformly accelerated by the constant force \( F \), and then \( F \) is the proportionality constant between momentum variations and time variations, \( 2\pi t_0 \) represents the time it takes for the electron momentum to span the energy-band period \( 2\pi p_0 \). Let us now introduce the non-dimensional scattering kernel

\[ b(\hat{p}, \hat{p}') = b_0(p_0\hat{p}, p_0\hat{p}') \]

and the non-dimensional Maxwellian

\[ M(\hat{p}) = \frac{p_0}{\sqrt{2\pi m^* k_B T}} e^{-\frac{\hat{p}^2}{2m^* k_B T}} = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{\sigma^2}{2}}, \quad (21) \]

where, obviously,

\[ \sigma^2 = \frac{m^* k_B T}{p_0^2} = \frac{k_B T}{E_0} \]

(note that the condition \( 14 \) translates into \( \sigma \ll 1 \)). Then, Equation \( 20 \) can be rewritten as follows

\[ \frac{\partial f}{\partial t} + \alpha \sin(p) \frac{\partial f}{\partial x} + \frac{\partial f}{\partial p} = \frac{1}{\tau} \int_{-\pi}^{\pi} b(p, p') [M(p)f(p') - M(p')f(p)] dp', \quad (22) \]

where, for the sake of clearness, we have dropped the hats everywhere (so that the new, non-dimensional variables are now indicated by the same symbols as the dimensional ones) and we have defined the non-dimensional parameters

\[ \alpha = \frac{t_0 E_0}{p_0 L} = \frac{E_0}{FL}, \quad \tau = \frac{\tau_0}{t_0} = \frac{\tau_0 F}{p_0}. \quad (23) \]

Note that \( \alpha \) is the ratio between the width of the energy band and the energy of the external field, and \( \tau \) is the scaled collision time, namely, the ratio between the typical collision time and the band-spanning time.

### 3. Fluid equations

In order to arrive at a macroscopic description, i.e., a fluid-dynamical description based on local averages, such as density and current, we shall take moments of the non-dimensional transport Equation \( 22 \) with respect to the momentum variable \( p \).
3.1. An Euler-like system

First of all, we calculate the integral with respect to $p \in [-\pi, \pi]$ of both sides of the transport Equation (22). In particular, since $b(p, p') = b(p', p)$, at the right-hand side we obtain

$$\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} b(p, p') [M(p)f(p') - M(p')f(p)] dp' dp = 0. \quad (24)$$

This reflects the fact that collisions locally conserve the number of particles. Then, the $p$-average of (22) yields the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0, \quad (25)$$

where

$$\rho(x, t) = \int_{-\pi}^{\pi} f(x, p, t) dp, \quad j(x, t) = \int_{-\pi}^{\pi} \alpha \sin (p) f(x, p, t) dp \quad (26)$$

are the non-dimensional counterparts of (7) and (8). We remark that Equation (25) has been obtained by assuming the periodicity of $f$ as a function of $p$ (making the boundary term vanish in the integration by parts).

To obtain an equation for $j$, we iterate the procedure by multiplying both sides of Equation (22) by $\alpha \sin (p)$ and taking the $p$-average. In particular, by assuming that $b$ is an even function,

$$b(p, p') = b(-p, p'), \quad (27)$$

at the right-hand side we obtain

$$\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} b(p, p') [M(p)f(p') - M(p')f(p)] dp' dp = -\frac{1}{\tau} \int_{-\pi}^{\pi} \alpha \gamma(p) \sin (p) f(p) dp,$$

where

$$\gamma(p) = \int_{-\pi}^{\pi} b(p, p') M(p') dp'. \quad (28)$$

Then:

$$\frac{\partial j}{\partial t} + \frac{\partial}{\partial x} \int_{-\pi}^{\pi} \alpha^2 \sin^2 (p) f(x, p, t) dp - \kappa(x, t) = -\frac{1}{\tau} \int_{-\pi}^{\pi} \alpha \gamma(p) \sin (p) f(p) dp, \quad (29)$$

where we introduced the new macroscopic quantity

$$\kappa(x, t) = \int_{-\pi}^{\pi} \alpha \cos (p) f(x, p, t) dp. \quad (30)$$

Recalling (1), we see that $\kappa$ is closely related to the local energy density.
In order to obtain an Euler-like system for the macroscopic quantities $\rho$, $j$ and $\kappa$, we iterate once again the procedure by taking the $p$-average of Equation (22) multiplied by $\alpha \cos(p)$. This yields
\[
\frac{\partial k}{\partial t} + \frac{\partial}{\partial x} \int_{-\pi}^{\pi} \alpha^2 \sin(p) \cos(p) f(x, p, t) \, dp + j = Q(f),
\]
where
\[
Q(f) = \int_{-\pi}^{\pi} \frac{\alpha}{\tau} \cos(p) \int_{-\pi}^{\pi} b(p, p') [M(p)f(p') - M(p)f(p)] \, dp' \, dp.
\]
Equations (25) (29), and (31) constitute an Euler-like system of macroscopic equations for the unknowns $\rho$, $j$ and $\kappa$. It is not closed, since it still depends on several averages of $f$ which, in general, cannot be expressed in terms of $\rho$, $j$ and $\kappa$.

In order to get a more explicit system, we introduce a further simplification by assuming that the scattering is isotropic, i.e.,
\[
b(p, p') = 1.
\]
In this case, the collisional term at the right-hand side of the transport Equation (22) takes the simple relaxation-time form
\[
\frac{1}{\tau} \int_{-\pi}^{\pi} [M(p)f(p') - M(p)f(p)] = \frac{1}{\tau} [M(p)\rho - f(p)],
\]
also known as BGK (Bhatnagar-Gross-Krook (Bhatnagar, Gross, and Krook 1954)) operator (as usual, the variables $x$ and $t$ are omitted in the description of collisions). It is readily seen that, with such assumption, system (25)-(29)-(31) assumes the simpler form
\[
\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0,
\]
\[
\frac{\partial j}{\partial t} + \frac{\partial}{\partial x} \int_{-\pi}^{\pi} \alpha^2 \sin^2(p) f(x, p, t) \, dp - \kappa = -\frac{j}{\tau},
\]
\[
\frac{\partial k}{\partial t} + \frac{\partial}{\partial x} \int_{-\pi}^{\pi} \alpha^2 \sin(p) \cos(p) f(x, p, t) \, dp + j = \frac{\varepsilon \rho - \kappa}{\tau},
\]
where $\varepsilon$ is a constant that (in the assumption $\sigma \ll 1$) is given by
\[
\varepsilon = \int_{-\pi}^{\pi} \alpha \cos(p) M(p) \, dp \approx \int_{-\infty}^{+\infty} \alpha \cos(p) M(p) \, dp = \alpha e^{-\sigma^2/2}.
\]
Of course, this system is still not closed, since the currents in Equations (36) and (37) are extra moments of $f$. However we can notice that the system contains (and in the space-homogeneous case reduces to) a damped harmonic oscillator with a forcing term, namely
\[
\begin{aligned}
\frac{\partial j}{\partial t} - \kappa &= -\frac{j}{\tau}, \\
\frac{\partial k}{\partial t} + j &= \frac{\varepsilon\rho - \kappa}{\tau},
\end{aligned}
\]
which is a manifestation of Bloch oscillations. Indeed, such a feature of this peculiar Euler system comes from the fact that the velocity is a sinusoidal function of \( p \), which is exactly what makes the term \(+j\) appear in Equation (37) (coming form the second derivative of the velocity). We will come back on this point in Section 4, but first let us investigate the behavior of the system for long times.

### 3.2. Diffusion asymptotics

By looking at the right-hand side of Equation (36) one notices that collisions tend to relax the current to zero, which is obviously due to the fact that the collisions we are describing conserve the mass but not the momentum. So, it is natural to consider the diffusion asymptotics, which is obtained by looking at the system on a time scale which is much larger than the typical collision time (Jüngel 2009). The diffusive scaling is therefore obtained by assuming \( \tau \ll 1 \) and by rescaling the time as follows:

\[
t \mapsto \frac{1}{\tau} t.
\]

The BGK transport equation and the Euler system are then re-written with such a rescaled time:

\[
\begin{aligned}
\tau^2 \frac{\partial f}{\partial t} + \tau x \sin(p) \frac{\partial f}{\partial x} + \tau \frac{\partial f}{\partial p} &= M(p)\rho - f(p), \\
\tau \frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} &= 0, \\
\tau^2 \frac{\partial j}{\partial t} + \tau \frac{\partial}{\partial x} \int_{-\pi}^{\pi} x^2 \sin^2(p) f(x, p, t) \, dp - \tau \kappa &= -j, \\
\tau^2 \frac{\partial k}{\partial t} + \tau \frac{\partial}{\partial x} \int_{-\pi}^{\pi} x^2 \sin(p) \cos(p) f(x, p, t) \, dp + \tau j &= \varepsilon \rho - \kappa.
\end{aligned}
\]

The unknowns are now expanded in powers of the small parameter \( \tau \)

\[
\begin{aligned}
f &= f^{(0)} + \tau f^{(1)} + \tau^2 f^{(2)} + \cdots, & \rho &= \rho^{(0)} + \tau \rho^{(1)} + \tau^2 \rho^{(2)} + \cdots, \\
j &= j^{(0)} + \tau j^{(1)} + \tau^2 j^{(2)} + \cdots, & \kappa &= \kappa^{(0)} + \tau \kappa^{(1)} + \tau^2 \kappa^{(2)} + \cdots,
\end{aligned}
\]

and these expansions are inserted in Equations (39)–(42). At leading order we obtain

\[
\begin{aligned}
f^{(0)} &= M \rho^{(0)}, & j^{(0)} &= 0, & \kappa^{(0)} &= \varepsilon \rho^{(0)}
\end{aligned}
\]
which are mutually consistent, since \( f^{(0)} \) is the equilibrium Maxwellian which does not carry any current. At order \( s \) in (40)–(42) we get

\[
\frac{\partial q^{(0)}}{\partial t} + \frac{\partial j^{(1)}}{\partial x} = 0,
\]

\[
j^{(1)} = -\frac{\partial}{\partial x} \int_{-\pi}^{\pi} x^2 \sin^2(p) f^{(0)}(x, p, t) \, dp + \kappa^{(0)},
\]

\[
\kappa^{(1)} = -\frac{\partial}{\partial x} \int_{-\pi}^{\pi} x^2 \sin(p) \cos(p) f^{(0)}(x, p, t) \, dp - j^{(0)} + \varepsilon \rho^{(1)}.
\]

The first two identities, together with (43), tell us that, up to \( O(\tau) \), \( \rho \) obeys the drift-diffusion equation

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial \rho}{\partial x} - \varepsilon \rho \right),
\]

where the diffusion coefficient is given by

\[
D = \int_{-\pi}^{\pi} x^2 \sin^2(p) M(p) \, dp \approx \int_{-\infty}^{+\infty} x^2 \sin^2(p) M(p) \, dp = x^2 \frac{1 - e^{-2\pi^2}}{2}.
\]

The third identity reduces to \( \kappa^{(1)} = \varepsilon \rho^{(1)} \), because \( f^{(0)} \) is an even function of \( p \) and \( j^{(0)} = 0 \), and will be of no use here. It is an easy exercise to compute the stationary solution of Equation (45), by assuming that at both sides of the semiconductor the electron density has a constant value \( \rho_c \) (e.g., the electronic density in the metal contacts). This leads to a classical ohmic law for the stationary diffusion current \( J_{\text{diff}} \):

\[
J_{\text{diff}} = \varepsilon \rho_c,
\]

or, substituting back the dimensional variables,

\[
J_{\text{diff}} = \frac{F \tau_0 E_0 \rho_c}{p_0^2} e^{-\frac{\varepsilon \rho}{\frac{F}{n}}},
\]

(47)

(where, of course, \( J_{\text{diff}} \) and \( \rho_c \) indicate the corresponding dimensional variables).

Equation (45) indicates that a current can actually flow in our device. On the other hand, it also reflects the fact that, on the diffusive time scale, our system shows a completely classical behavior, where every trace of the quantum dynamics, in particular the BO, is lost. Therefore, in order to observe the Bloch oscillations we have now to shift back our attention to the shorter time scale, which will be done in next section.
4. Averaging over space

Let us consider the space averages of the hydrodynamic variables $\rho, j$ and $\kappa$ introduced in the last section:

\[
N(t) = \int_0^1 \rho(x, t) \, dx, \quad J(t) = \int_0^1 j(x, t) \, dx, \quad K(t) = \int_0^1 \kappa(x, t) \, dx
\] (48)

(we recall that the non-dimensional space variable $x$ varies in the interval $[0, 1]$, while its dimensional counterpart varies in $[0, L]$). Let us make the reasonable assumption that the total flux of $\rho$ through the device boundaries is zero, so that there is no charge accumulation nor depletion in the device. Then, by integrating both sides of Equation (35) with respect to $x \in [0, 1]$, we obtain

\[
\frac{dN}{dt} = 0,
\] (49)

which obviously means that the total number of electrons (and, therefore, the total charge) is conserved. By also assuming that the total fluxes of $j$ and $\kappa$ through the boundaries is zero, the integration of (36) and (37), with respect to $x \in [0, 1]$ yields the system of ODEs

\[
\begin{align*}
\frac{dJ}{dt} - K &= -\frac{1}{\tau} J, \\
\frac{dK}{dt} + J &= -\frac{1}{\tau} K + \frac{\varepsilon N_0}{\tau},
\end{align*}
\] (50)

where $N_0$ is the total number of particles, which is constant, according to Equation (49). Hence we see that the averaged hydrodynamic variables $J(t)$ and $K(t)$ behave as a damped harmonic oscillator with a forcing term. System (50) can be readily recast into the following second-order equation for $J$

\[
\frac{d^2J}{dt^2} + \frac{2}{\tau} \frac{dJ}{dt} + \left(1 + \frac{1}{\tau^2}\right) J = \frac{\varepsilon N_0}{\tau}.
\] (51)

Solving this equation is a standard exercise in ODEs, and the solution is

\[
J(t) = e^{-t/\tau} \left[ a \cos(t) + b \sin(t) \right] + \frac{\tau \varepsilon N_0}{1 + \tau^2},
\] (52)

with $a$ and $b$ to be determined from the initial conditions $J_0$ and $K_0$. By writing this formula in physical variables and substituting $a$ and $b$ with their expressions in terms of the initial conditions we obtain

\[
J(t) = e^{-t/\tau_0} \left[ (J_0 - J_\infty) \cos(\omega t) + \left( K_0 - \frac{1}{\omega \tau_0} J_\infty \right) \sin(\omega t) \right] + J_\infty,
\] (53)

where
\[
\omega = \frac{1}{t_0} = \frac{F}{p_0}
\]  

(54)
is the BO frequency,

\[
J_\infty = \frac{F\tau_0E_0N_0}{p_0^2 + (F\tau_0)^2} e^{-\frac{\mu r}{\Delta_0}}
\]  

(55)
is the asymptotic value of the current and

\[
J_0 = \int_0^L \int_{-\pi p_0}^{\pi p_0} \frac{E_0}{p_0} \sin\left(\frac{p}{p_0}\right) f_{\text{in}}(x, p) \, dp \, dx,
\]

\[
K_0 = \int_0^L \int_{-\pi p_0}^{\pi p_0} \frac{E_0}{p_0} \cos\left(\frac{p}{p_0}\right) f_{\text{in}}(x, p) \, dp \, dx,
\]

(56)
are the initial values of \(J\) and \(K\) (in physical variables) obtained from the initial phase-space distribution \(f_{\text{in}}\). We see from (53) that, after a transient which is dominated by Bloch oscillations, the current reaches the stationary value \(J_\infty\).

It is worth to remark that the difference between \(J_\infty\) and the stationary diffusive current \(J_{\text{diff}}\) (see (47)) is due to the fact that the diffusive limit is not a limit for large times, but it is a time-scale asymptotics for \(\tau \ll 1\) (that is \(\tau_0 \ll p_0/F\)), which is not necessarily the case in general.

We can observe that in both limits \(\tau \to \infty\) and \(\tau \to 0\) the current vanishes. The behavior when \(\tau\) approaches 0 (which means that there are many collisions in the time it takes \(p\) to span the band period) is close to the classical ohmic regime (and indeed \(J_\infty \approx J_{\text{diff}}\) becomes a linear function of \(F\)). So, the limit \(\tau \to 0\) corresponds to the resistivity becoming infinite. The behavior for large \(\tau\), instead, corresponds to the opposite regime in which the collisions are rarefied, compared to the band-spanning time, and electrons tend to remain trapped in the periodic trajectories. The limit \(\tau \to \infty\) is therefore a clear illustration of the Bloch paradox: without collisions no current can flow.

5. Comparison with experiments and discussion

In order to discuss the possibility of comparing formula (53) with experimental measurements, we first have to make some considerations about the band parameter \(p_0\). Assume that the periodic structure has a period \(d\). Then the period of the reciprocal lattice (i.e., the wave number) is \(k_0 = 2\pi/d\). Now, the De Broglie identity implies that the corresponding momentum period \((2\pi p_0)\) is given by \(2\pi p_0 = \hbar k_0\), where \(\hbar = h/2\pi\) is the reduced Planck constant. Then, we have a simple relation between the lattice period and \(p_0\):
As a consequence, the BO frequency as a function of the applied voltage is given by

$$\omega = \frac{F}{2\pi p_0} = \frac{qVd}{hL},$$  \hspace{1cm} (58)$$

and the non-dimensional parameter $\tau$, that is the ratio between the collision time and the band-spanning time, is given by

$$\tau = \frac{\tau_0 F}{p_0} = \frac{\tau_0 qVd}{Lh}.$$  \hspace{1cm} (59)$$

In natural crystals this number is very small, which means that Bloch oscillations are extremely difficult to observe. Indeed, all experimental results are aimed at observing Bloch oscillations in semiconductor superlattices (SL), which are artificial periodic structures made by repetitions of layers of different semiconductors (Dekorsy et al. 1995; Leo et al. 1992). Here, the periodicity $d$ is several tenths of the bulk crystal periodicity, resulting in a smaller $p_0$ and a larger $\tau$. Unfortunately, our simple model is inadequate to describe such a device, since its modelisation would involve different time and space scales and more complicated collisional interactions.

The major weakness of our model is that the ohmic behavior ($\tau < 1$) and a damping time large enough for the BO to be observed ($\tau > 1$) are mutually excluded (see Figure 2). In the SL experiments, actually, the two conditions are met at the same time. This limitation of our model can be fixed “by hands” with the substitution of the asymptotic current $J_\infty$ (55) with the diffusive current $J_{\text{diff}}$ (47). This modification leads to a surprisingly good agreement with the experimental results, as it is shown below.
According to the experimental device described in Dekorsy et al. (1995), we choose the following values of the physical parameters:

- device length: \( L = 1.0 \times 10^{-6} \, \text{m} \);
- lattice period: \( d = 8.4 \times 10^{-9} \, \text{m} \);
- band width: \( E_0 = 3.6 \times 10^{-2} \, \text{eV} \);
- mean collision time at \( T = 10 \, \text{K} \): \( \tau_0 = 3.7 \times 10^{-13} \, \text{sec} \);
- mean collision time at \( T = 300 \, \text{K} \): \( \tau_0 = 1.3 \times 10^{-13} \, \text{sec} \);
- cross-sectional electronic density: \( n = 2.0 \times 10^9 \, \text{cm}^{-2} \).

The value \( p_0 = 0.13 \times 10^{-25} \, \text{Kg m/sec} \) is calculated by means of (57). These values are used in formula (53) (with \( J_{\text{diff}} \) in place of \( J_{\infty} \)) to compute \( J(t) \) for different values of voltage and temperature. In Figure 3, \( J(t) \) is plotted for several values of the applied potential \( V \) and compared with the analogous experimental figure, shown in the inset. In Figure 4, \( J(t) \) is plotted for two different values of the temperature and again compared with the corresponding experimental figure. In both case we can observe a good qualitative agreement of our (modified) model with the real data.

In conclusion, we have proposed a reasonably simple mathematical model with the aim of illustrating the “paradox” of Bloch oscillations. In spite of its simplicity, the model is able to give qualitatively good results.
when comparing its predictions with experimental data. Of course, in order to have an accurate description of a real device, a more refined model is needed, especially with regards to the description of collisions. There are many available kinetic model of electron-phonon interaction (see e.g., Camiola, Mascali, and Romano 2020) that could be used to improve the transport Equation (13) and possibly reproduce the experimental results without any ad hoc assumptions.

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ORCID

Luigi Barletti http://orcid.org/0000-0003-2111-2813

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