Team report on the problem

Modelling Charge Transport in a Semiconductor

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Abstract

A model of charge transport in a one-dimensional semiconductor crystal is considered, where each electron follows the Hamiltonian characteristics, determined by the semiconductor band structure, and undergoes non-elastic collisions with a phonon bath. Starting from a detailed kinetic (Boltzmann-like) model, a closed system of ODEs is obtained for phase-space averaged quantities. Such a simplified model is nevertheless capable of describing the damping of Bloch oscillations, due to collisions, and the consequent onset of a steady current flow, which is in very good agreement with the available experimental data.

I. INTRODUCTION

It is known that semiconductors have crystalline structure. What that means is that the electrons can flow throughout the material, and the ions of the atoms remain in a fixed position forming what it's called a crystalline *lattice*. In this work we make the assumption that the crystal has no impurities, so that this lattice is perfectly periodic.

We can take into account several factors in order to model the dynamics of the electrons:

- From basic quantum mechanics it is known that the interaction of an electron with the Coulomb potential generated by the ions of the crystal lattice results into a dispersion relation, i.e., the relation between kinetic energy \mathcal{K} and momentum p (also known as the semiconductor band diagram), which turns out to be multi-valued and periodic.
- An external force can be applied to the electrons in the semiconductor. Typically this will be done by means of an external electric field.
- Electrons can scatter with the vibrations of the crystal lattice (phonons). In this process electrons can transfer momentum to the phonons, changing their velocity.
- Coulomb interaction between different electrons. This force is proportional to r^{-2} , where r is the distance between electrons. If the electron density is low, we can make the assumption that the electrons are always far away, so that this term is negligible.

If we just take into account the lattice potential and the external force, the electrons just follow what it is known as the *Bloch Oscillations*. The average displacement that this oscillations have is 0, so even if we apply a strong electric field the average current that will flow through the semiconductor is null. From the experience we know that this is false.

The aim of this work is to include the electron-phonon interactions in the model, so that it is shown that they are responsible for the current flow in semiconductors.

II. MODEL FOR THE ELECTRON DYNAMICS

The first approximation we make is that the semiconductor only has *one conduction band* and the crystal has only one spatial dimension. The kinetic energy of the electrons in this band is derived from Quantum Mechanics and takes the form:

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

which is known as Kronig-Penney dispersion relation [1]. This energy has a period of $2\pi p_0$, and an amplitude of E_0 . On the other hand, the potential energy of the electric field is supposed to be linear:

$$\mathcal{U}(x) = -Fx \tag{2}$$

and corresponds to a constant force 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 system's Hamiltonian can be written as

$$\mathcal{H}(x,p) = E_0 \left(1 - \cos \left(\frac{p}{p_0} \right) \right) - Fx \tag{3}$$

so that the Hamilton equations are

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p} = \frac{E_0}{p_0} \sin\left(\frac{p}{p_0}\right) \tag{4}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial x} = F \tag{5}$$

Let f(x, p, t) be the phase space density function. As the crystal has only one spatial dimension, the spatial electron density ρ can be expressed as

$$\rho(x,t) = \int_{-\pi p_0}^{\pi p_0} f(x, p', t) dp'. \tag{6}$$

In virtue of Liouville's theorem, the phase-space distribution function is constant along the trajectories of the system. This can be expressed as

$$\frac{d}{dt}f(x,p,t) = 0\tag{7}$$

or

$$\frac{\partial f}{\partial t} + \dot{x}\frac{\partial f}{\partial x} + \dot{p}\frac{\partial f}{\partial p} = \frac{\partial f}{\partial t} + \frac{E_0}{p_0}\sin\left(\frac{p}{p_0}\right)\frac{\partial f}{\partial x} + F\frac{\partial f}{\partial p} = 0.$$
 (8)

Equation (8) is known as Liouville's equation, and it describes the behavior of our system without taking into account the interactions between phonons and electrons.

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These interactions will have two parts: out-scattering and in-scattering. The first one takes into account the electrons that had momentum p and loose it because of a collision with a phonon. This type of event will happen with a frequency of $1/\tau_0$ so that the following term is added to equation (8):

$$\left. \frac{\partial f(x, p, t)}{\partial t} \right|_{o.s.} = -\frac{f(x, p, t)}{\tau_0} \tag{9}$$

The second type of interactions is derived from statistical physics considerations, and it takes the form:

$$\left. \frac{\partial f(x, p, t)}{\partial t} \right|_{i.s.} = \frac{1}{\tau_0} M(p) \rho(x, t) \tag{10}$$

where

$$M(p) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{p^2}{2\sigma^2}}, \quad \sigma^2 = m_e^* \kappa_B T$$
 (11)

In the last expression m_e^* is the effective electron mass, κ_B is Boltzmann's constant and T is the temperature. Is it possible now to include the scattering terms into equation 8, which results in

$$\left| \frac{\partial f(x,p,t)}{\partial t} + \frac{E_0}{p_0} \sin\left(\frac{p}{p_0}\right) \frac{\partial f(x,p,t)}{\partial x} + F \frac{\partial f(x,p,t)}{\partial p} = \frac{1}{\tau_0} \left[M(p) \cdot \rho(x,t) - f(x,p,t) \right] \right|$$
(12)

Note that the collisions term described by the right-hand side, can be interpreted as follows: electrons collide with a typical frequency $1/\tau_0$ and and the effect of collisions is to redistribute the electron momenta according to a Maxwellian (thermal) distribution at the temperature of the phonon bath.

Equation (12) is semiclassical Boltzmann-type equation [2], and it describes the system that we propose in this work. An important remark to be made is that this equation has an integral term, because of (6), and that will complicate its resolution.

III. NON-DIMENSIONALISATION

We shall non-dimension (12) by changing $x \mapsto x_0 x$, $p \mapsto p_0 p$, $t \mapsto t_0 t$ and $f \mapsto N_0 f$, where x_0 , p_0 , t_0 and N_0 are reference length, momentum, time and density, respectively, and

the new variables x, p, t and f are non-dimensional. Making these substitutions into (12) and multiplying by t_0 yields

$$N_0 \frac{\partial f}{\partial t} + \frac{N_0 E_0 t_0}{P_0 x_0} \sin(p) \frac{\partial f}{\partial x} + \frac{N_0 t_0 F}{P_0} \frac{\partial f}{\partial p} = \frac{t_0 N_0}{\tau_0} \left(p_0 M(p_0 p) \int_{-\pi}^{\pi} f dp - f \right). \tag{13}$$

It is natural to set $x_0 = L$ and it is clear than N_0 is arbitrary as it multiplies every term. We choose that $t_0 = \frac{p_0}{F}$ and and define the new parameters

$$A = \frac{E_0}{FL} \qquad \tau = \frac{F\tau_0}{p_0} \tag{14}$$

to yield the non-dimensionalised equation

$$\frac{\partial f}{\partial t} + A\sin(p)\frac{\partial f}{\partial x} + \frac{\partial f}{\partial p} = \frac{1}{\tau} \left(m(p) \int_{-\pi}^{\pi} f \, dp - f \right), \tag{15}$$

where

$$m(p) = p_0 M(p_0 p) = \frac{1}{\sqrt{2\pi\epsilon^2}} e^{-\frac{p^2}{2\epsilon^2}}, \qquad \epsilon = \sigma/p_0.$$

IV. AVERAGING OVER MOMENTA p

In order to arrive at a macroscopic description, we start by averaging the non-dimensional equation over the momenta p. In other words, we calculate

$$\int_{-\pi}^{\pi} \frac{\partial f}{\partial t} + A \sin(p) \frac{\partial f}{\partial x} + \frac{\partial f}{\partial p} dp = \int_{-\pi}^{\pi} \frac{1}{\tau} \left(m(p) \int_{-\pi}^{\pi} f \, dp - f \right) dp. \tag{16}$$

By defining

$$\rho(x,t) := \int_{-\pi}^{\pi} f dp,\tag{17}$$

which is the density of electrons at any particular spatial point x and time t, the left hand side of (16) simplifies to

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \int_{-\pi}^{\pi} A \sin(p) f dp + f(x, \pi, t) - f(x, -\pi, t), \tag{18}$$

by using the Fundamental Theorem of Calculus. However, as f is periodic in p the final term is zero. Hence, the left hand side of (16) is in fact given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x},\tag{19}$$

where $j(x,t) = \int_{-\pi}^{\pi} A \sin(p) f dp$, which has the interpretation of current.

The right hand side of (16) is zero. To see this, note that the Gaussian m(p), if assumed to be sufficiently tightly distributed around zero will normalise to one. In other words, we have

$$\int_{-\pi}^{\pi} m(p)\rho - f dp = \rho - \rho = 0, \tag{20}$$

noting the definition (17). Hence, by equating (19) and (20), (16) simplifies to

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0. \tag{21}$$

To understand how j varies with t we multiply the origin non-dimensional equation by $A\sin(p)$ and average over p once more. In particular, we compute

$$\int_{-\pi}^{\pi} A \sin(p) \left(\frac{\partial f}{\partial t} + A \sin(p) \frac{\partial f}{\partial x} + \frac{\partial f}{\partial p} \right) dp = \int_{-\pi}^{\pi} \frac{A \sin(p)}{\tau} \left(m(p) \int_{-\pi}^{\pi} f \, dp - f \right) dp. \quad (22)$$

The left hand side of this expression simplifies to

$$\frac{\partial j}{\partial t} + \frac{\partial}{\partial x} \left(\int_{-\pi}^{\pi} A^2 \sin^2(p) f(x, p) dp \right) + \int_{-\pi}^{\pi} \frac{\partial f}{\partial p} dp.$$
 (23)

By using integration by parts, the last term reduces to

$$A\cos(p) (f(x,\pi,t) - f(x,-\pi,t)) - \int_{-\pi}^{\pi} A\cos(p) f dp.$$
 (24)

Recalling the periodicity of f in p and defining $k := \int_{-\pi}^{\pi} A \cos(p) f dp$ (which is related to kinetic energy) we then find that (23) becomes

$$\frac{\partial j}{\partial t} + \frac{\partial}{\partial x} \left(\int_{-\pi}^{\pi} A^2 \sin^2(p) f(x, p, t) dp \right) - k. \tag{25}$$

We now focus attention on the right hand side of (22). As the density ρ does not depend on p we can pull it out of the first integral so that we have

$$\int_{-\pi}^{\pi} \frac{A\sin(p)}{\tau} \left(m(p) \int_{-\pi}^{\pi} f \, dp - f \right) dp = \frac{1}{\tau} \left(\rho \int_{-\pi}^{\pi} A\sin(p) m(p) dp - \int_{-\pi}^{\pi} A\sin(p) f dp \right). \tag{26}$$

As $\sin(p)$ is an odd function and m(p) is even, the first integral on the right hand side reduces to zero. The second term is how we define j. Hence we have

$$\int_{-\pi}^{\pi} \frac{A\sin(p)}{\tau} \left(m(p) \int_{-\pi}^{\pi} f \, dp - f \right) dp = -\frac{j}{\tau}. \tag{27}$$

By equating this expression with (25), we arrive at the following simplification of (22):

$$\frac{\partial j}{\partial t} + \frac{\partial}{\partial x} \left(\int_{-\pi}^{\pi} A^2 \sin^2(p) f(x, p, t) dp \right) - k = -\frac{j}{\tau}$$
 (28)

Similar calculations, but instead by first multiplying the original non-dimensional equation by $A\cos(p)$ we arrive at an equation describing the time evolution of k:

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x} \left(\int_{-\pi}^{\pi} A^2 \sin(p) \cos(p) f(x, p, t) dp \right) + j = \frac{1}{\tau} (\delta \rho - k), \qquad (29)$$

where δ is a constant given by

$$\delta = \int_{-\pi}^{\pi} A \, m(p) \cos(p) \, dp. \tag{30}$$

V. AVERAGING OVER SPACE x

Coupled with initial conditions, the system of equations (21), (28) and (29) form a closed system. However, to deal with the unwieldly integral terms in (28) and (29) we also average over x. We can get rid of the boundary terms by assuming that the spatial boundaries of the device are very far with respect to the initial location of electrons. In other words, we may substitute (at least up to some maximum time) the space interval $x \in [0, L]$ with $x \in (-\infty, +\infty)$. If we define

$$H(t) := \int_{-\infty}^{\infty} \rho(x, t) dx \tag{31}$$

$$J(t) := \int_{-\infty}^{\infty} j(x, t) dx \tag{32}$$

$$K(t) := \int_{-\infty}^{\infty} k(x, t) dx \tag{33}$$

then averaging (21) we get

$$\frac{dH}{dt} + \lim_{x \to \infty} J(x) - \lim_{x \to -\infty} J(x) = 0, \tag{34}$$

However, we suppose that the current at both limits drops to zero. Hence we have

$$\frac{dH}{dt} = 0. (35)$$

Similarly, if we average (28) over x we obtain

$$\frac{dJ}{dt} + \left(\lim_{x \to \infty} \int_{-\pi}^{\pi} A^2 \sin^2(p) f(x, p, t) dp - \lim_{x \to -\infty} \int_{-\pi}^{\pi} A^2 \sin^2(p) f(x, p, t) dp\right) - K = -\frac{J}{\tau}, (36)$$

where for the term involving limits we have used the Fundamental Theorem of Calculus. As the limits are with respect to x, and not p, we can pull them inside the integrals. Then, as before, we assume that as x gets very large the electron density function f(x, p, t) decays. Thus, we find

$$\frac{dJ}{dt} - K = -\frac{J}{\tau} \tag{37}$$

Using the same decay assumptions, we find the spatially averaged equivalent of (29) to be:

$$\frac{dK}{dt} + J = \frac{1}{\tau} \left(\delta H - K \right). \tag{38}$$

From (35), it is clear that H is a constant. We relabel this constant N. Thus, (35), (37) and (38) form a closed system (the first equation being trivial), with initial conditions

$$N = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} f_0(x, p) \, dp \, dx$$

$$J_0 = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} A \sin(p) \, f_0(x, p) \, dp \, dx$$

$$K_0 = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} A \cos(p) \, f_0(x, p) \, dp \, dx,$$

where $f_0(x, p)$ is the initial density distribution.

An idea of the charge movement inside the semiconductor can be given in term of the average position

$$\mathcal{X}(t) = \int_{-\infty}^{\infty} x \rho(x, t) dx.$$

From (19) the equation for $\mathcal{X}(t)$ is readily found to be

$$\frac{\mathcal{X}}{dt} = J,$$

and so

$$\mathcal{X}(t) = \mathcal{X}(0) + \int_0^t J(s)ds. \tag{39}$$

VI. SOLVING THE SYSTEM

We have already seen that the previous differential equation corresponds to a macroscopic description of our problem, so now we are going to give an explicit solution of the unknowns J and K.

We remind that the differential equation is

$$\begin{cases} \dot{J}(t) = -\frac{1}{\tau}J(t) + K(t) \\ \dot{K}(t) = -J(t) - \frac{1}{\tau}K(t) + \frac{R}{\tau} \end{cases}$$

where $R = Ne^{\epsilon^2/2}$ and the initial conditions are

$$J(0) \equiv J_0 = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} A \sin(p) f_0(x, p) dp dx$$
$$K(0) \equiv K_0 = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} A \cos(p) f_0(x, p) dp dx.$$

Firstly, to solve the system, we compute the second derivative of J, which is

$$\ddot{J}(t) = -\frac{1}{\tau}\dot{J}(t) + \dot{K}(t) = -\frac{1}{\tau}\dot{J}(t) - J(t) - \frac{1}{\tau}K(t) + \frac{R}{\tau} = -\frac{1}{\tau}\dot{J}(t) - J(t) - \frac{1}{\tau}\dot{J}(t) + \frac{1}{\tau}J(t)$$

$$= \ddot{J} + \frac{2}{\tau}\dot{J} + \left(1 + \frac{1}{\tau^2}\right)J = \frac{R}{\tau}$$

Typically, these kind of problems are solved by finding a particular solution of the differential equation, and then, we just have to solve the homogeneous solution.

Is easily check that

$$S_p = \left(1 + \frac{1}{\tau^2}\right) \frac{\tau}{R} = \frac{(\tau^2 + 1) e^{-\epsilon^2/2}}{\tau N}$$

verifies the differential equation, so is a particular solution. Now, to solve the homogeneous solution

$$\ddot{J} + \frac{2}{\tau}\dot{J} + \left(1 + \frac{1}{\tau^2}\right)J = 0$$

we are going to consider, as usual, that the solution has this expression:

$$S_h(t) = \mathcal{A}^{\lambda t},$$

where A, $\lambda \in \mathbb{C}$. So, in this case, we get

$$S_h(t) = \mathcal{A}e^{\lambda t}$$
$$\dot{S}_h(t) = \lambda \mathcal{A}e^{\lambda t}$$
$$\ddot{S}_h(t) = \lambda^2 \mathcal{A}e^{\lambda t}$$

and if we want to impose that S_h is the solution of the homogeneous case, it must verify the differential equation, namely

$$\mathcal{A}e^{\lambda t}\left[\lambda^2 + 2\frac{2}{\tau}\lambda + \left(1 + \frac{1}{\tau^2}\right)\right] = 0,$$

and this is true if and only if

$$\lambda = -\frac{1}{\tau} \pm i.$$

Hence,

$$S_h(t) = e^{-t/\tau} [\alpha \cos t + \beta \cos t],$$

and

$$J(t) = e^{-t/\tau} [\alpha \cos t + \beta \cos t] + J_a, \tag{40}$$

where

$$J_a = \frac{(\tau^2 + 1) e^{-\epsilon^2/2}}{\tau N} \tag{41}$$

is the asymptotic current.

The constants α and β depend on the initial conditions J_0 and K_0 , namely:

$$\alpha = J_0 - J_a, \qquad \beta = K_0 - \frac{1}{\tau} J_a.$$

We can notice that in both limits $\tau \to \infty$ (no collisions) and $\tau \to 0$ (infinite collision frequency), the current is zero. In fact, in the first case, the dynamics reduces to Bloch oscillations while, in the second one, the collisions are "too many" and electrons remain stuck.

Finally, the expression (40) can be integrated to obtain an explicit expression for the mean position (39):

$$\mathcal{X}(t) = \mathcal{X}(0) = \underbrace{\frac{J_a t}{N}}_{Drift} + \underbrace{\frac{(J_0 - J_a)\tau^2}{N(1 + \tau^2)} \left(e^{-t/\tau} (\sin(t) - \frac{1}{\tau} \cos(t)) + \frac{1}{\tau} \right)}_{Damped Bloch Oscillation} + \underbrace{\frac{(K_0 - K_a)\tau^2}{N(1 + \tau^2)} \left(1 - e^{-t/\tau} (\cos(t) + \frac{1}{\tau} \sin(t)) \right)}_{Damped Bloch Oscillation}, \tag{42}$$

where the asymptotic current J_a is given by (41).

VII. NUMERICAL SOLUTION AND COMPARISON WITH THE EXPERIMENTS

Now we are going to plot the results that we have obtained and to compare them with the experimental results reported in Ref. [3]. In order to do that it is first of all necessary to return to the dimensional variables and parameters

We remember that, in non-dimensional variables, we have obtained for the averaged current this expression:

$$J(t) = e^{-t/\tau} \left[\alpha \cos t + \beta \sin t \right] + \frac{AN\tau e^{-\epsilon^2/2}}{1 + \tau^2}.$$

Then, we make the inverse changes with respect to the ones that we used to perform the non-dimensionalisation, i.e.:

$$\tau = \frac{F\tau_0}{p_0}, \qquad \omega = \frac{F}{p_0}, \qquad t = \frac{Ft}{p_0}$$

$$\hat{\alpha} = \frac{\alpha p_0}{E_0 N}, \qquad \hat{\beta} = \frac{\beta p_0}{E_0 N}$$

$$m_e^* = \frac{p_0^2}{E_0}, \qquad \sigma^2 = m_e^* K_B T, \qquad \epsilon^2 = \frac{\sigma^2}{p_0^2} = \frac{k_B T}{E_0}.$$

The dimensional expression of the current reads as follows:

$$J(t) = \frac{E_0 N}{p_0} \left[e^{-t/\tau_0} \left(\hat{\alpha} \cos(\omega t) + \hat{\beta} \sin(\omega t) \right) + \frac{\tau_0 \omega e^{-k_B T/2E_0}}{1 + (\omega \tau_0)^2} \right],$$

or

$$J(t) = \frac{E_0 N}{p_0} \left[e^{-t/\tau_0} \left(\hat{\alpha} \cos(\omega t) + \hat{\beta} \sin(\omega t) \right) + J_a \right],$$

where $\omega = \frac{F}{p_0}$ is the frequency of Bloch oscillations, and

$$J_a = \frac{\tau_0 \omega e^{-K_B T / 2E_0}}{1 + (\omega \tau_0)^2}$$

is the asymptotic current expressed in dimensional variables.

In our plots we use the following values, which are taken from Ref. [3]:

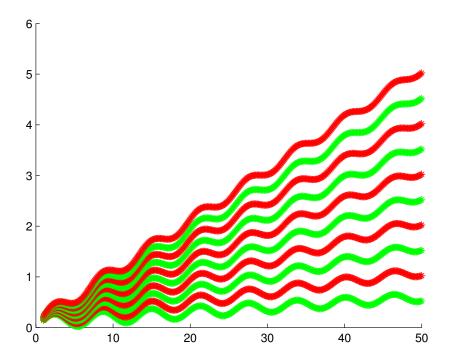
• Device length: $L = 0.147 \cdot 10^{-6} m$

• Band period: $p_0 = 7.89 \cdot 10^{-26} \, Kg \cdot m/s$

• Band width: $E_0 = 5.76 \cdot 10^{-21} J$

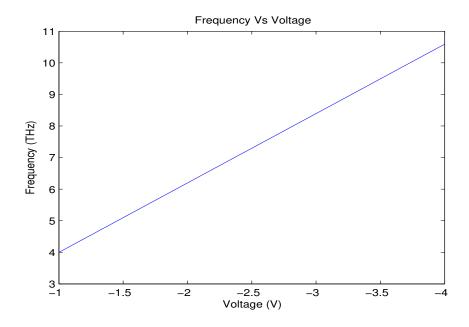
The first thing we do is to represent the graph of the mean position $\mathcal{X}(t)$ for different values of the voltage

$$V = \frac{VL}{q}.$$



We see that, as V increases, the slope (that is the asymptotic current J_a) also increases. Also, as expected, as time increases, the amplitude of oscillations decrease.

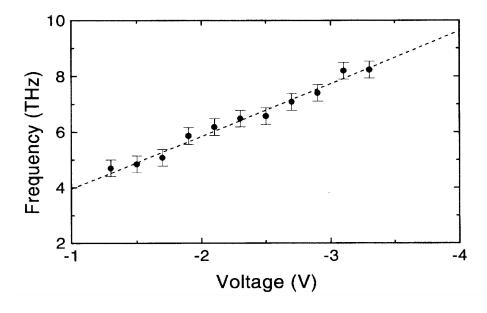
In the following image, we will represent the relation between the voltage and the frequency.



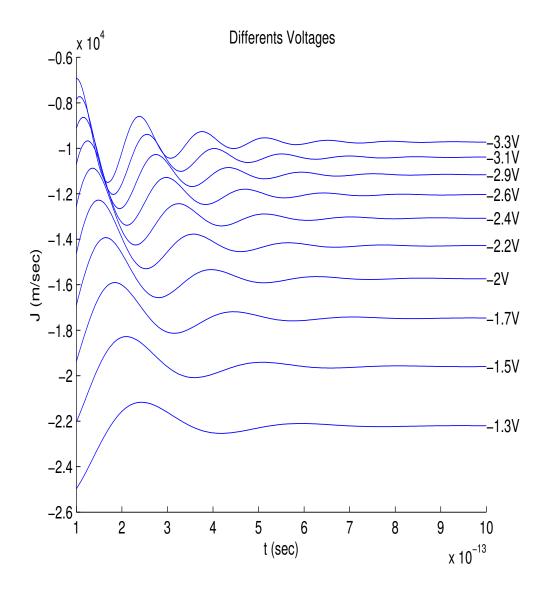
We can see that frequency increases linearly with voltage, because they are proportional:

$$\omega = \frac{F}{P_0} = \frac{qV}{P_0 L} \tag{43}$$

Now we compare our image with the one taken from experiments, and we see that they are very similar, both having a slope close to 2.1:

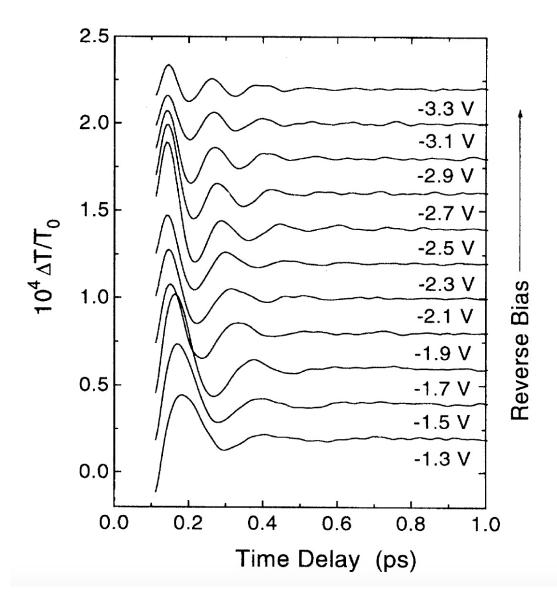


Next figure show the the current versus time for different voltages:



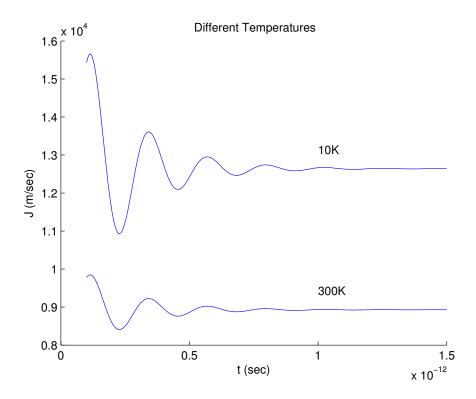
Note that the current, at first, has some oscillations (which are exactly the Bloch oscillations) and, after a time of order τ_0 , it reaches the asymptotic value J_a , due to the effect of collisions. The asymptotic value of the current increases with the absolute value of the applied voltage.

The comparison with the analogous figure obtained experimentally shows a very good agreement:

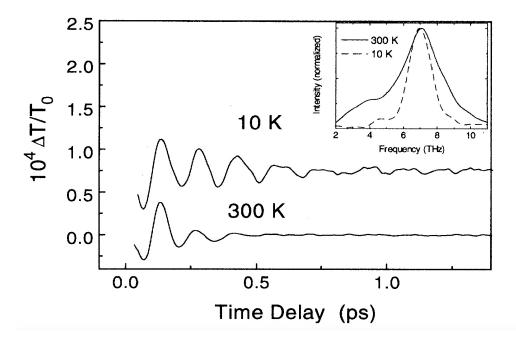


Note that in the experimental figure the current axis is measured in units that depends on the way the current is experimentally measured, and so the comparison with our values is possible only up to an overall scale factor.

Finally, we are going to check how the temperature T affects the current. To this aim we represent, just like in the previous image, the value of the current as a function of time, but now we will vary the value of the temperature. For example, we take the same representative values also considered in Ref. [3], i.e. 10K (Kelvin) and 300K (room temperature):



Once again, our simulations are very good agreement with the values from experiments:



We can see in the picture that if the temperature is higher the current decreases, this makes sense since, if the temperature increases, the mean energy of the phonons increases, which makes the Bloch oscillations more damped and, at the same time, the asymptotic current smaller.

VIII. CONCLUSIONS

In conclusion, the team was able to achieve the assigned target, i.e. to provide a simple mathematical model that is able to describe the onset of a current flow in a semiconductor, as determined by the concurrent action of the Hamiltonian dynamics and of the collisions.

The model is derived from a detailed kinetic (Boltzmann-like) description and consist of a system of ODEs for the phase-space averaged velocity and energy.

The model depend on all relevant physical parameters, namely the applied voltage V, the collisional frequency $1/\tau_0$, the band-energy period p_0 and width E_0 (that depend on the lattice structure), and the crystal temperature T.

A comparison with the available experimental data shows a very good agreement.

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