Mathematical modelling of charge transport in a semiconductor

The dynamics of charges in a semiconductor (or conductor) crystal is the result of three basic processes:

1) acceleration by an applied electric field;
2) Coulomb interaction with the crystal ions;
3) collision-type interactions with crystal vibrations (phonons) or crystal impurities.

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 energy *E* and wave vector *k* (also known as the semiconductor *band diagram)*, which turns out to be *multi-valued* and *periodic* (Figure 1).

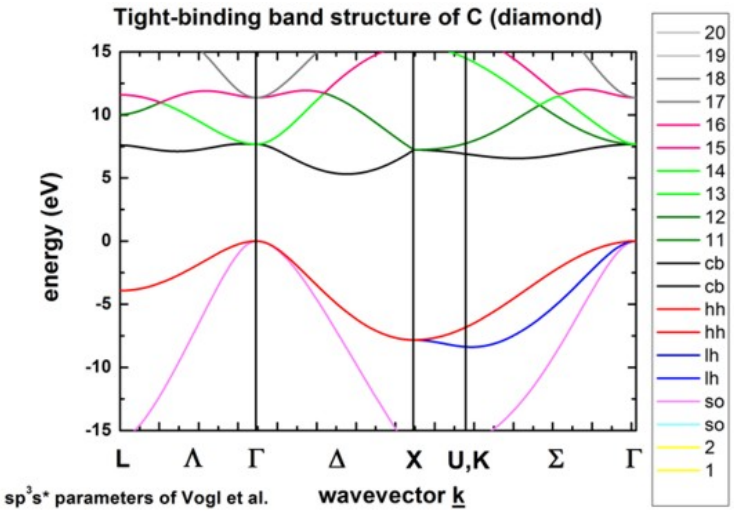

Figure 1. Band diagram of diamond (from NextNano.com)

This implies that mechanisms 1 and 2, alone, would produce a periodic motion, causing electrons to go back and forth, with zero average displacement. These are the so-called *Bloch oscillations* (Figure 2).

So, why a charge current is observed in semiconductors? The answer is that what allows the electrons to advance is the combination of the mechanisms 1 and 2 with mechanism 3. Thus, surprisingly, are the *collisions* that allow a current to flow.

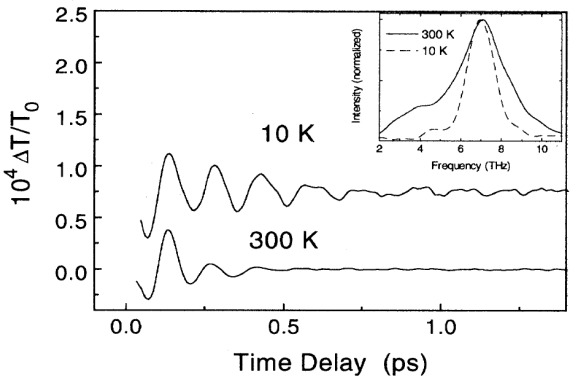

Figure 2. Experimental observation of Bloch oscillations (from T. Dekorsy et al., Phys. Rev. B, 1995)

Describing such dynamics in full details would require complicated models of charge transport, taking into account the full semiconductor band structure and several collisional processes.
The aim of the proposed work is to construct and numerically test a reasonably simple mathematical model, based on few macroscopic variables (such as density, current and temperature), that combines the basic features of the three mechanisms and describes the current flow.

The model should be based on some simplifying assumptions such as:

1) one-dimensional crystal lattice;
2) single-band;
3) simple (e.g. sinusoidal) dispersion relation;
4) relaxation-time collisional mechanism.

The goal is to provide a relatively simple mathematical model that is able to show the interplay between the various mechanisms and the role of the relevant physical parameters of the system (applied voltage, collisional frequency, lattice constant, etc).

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Requirement: Basic mechanics, mathematical physics, ODEs and PDEs. Basic experience with of Matlab.