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Semiclassical Equations for Electron Transport in High-Field Semiconductor Devices

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ABSTRACT

The starting point in modeling electron and hole transport in semiconductors is the Boltzmann equations. In these equations, separate terms account for electron drift and scattering. The drift terms model the x - k motion of free (ballistic) electrons in a crystal lattice, with coefficients describing the electron velocity and applied force given by the semiclassical equations. The semiclassical equations, in turn, are the leading order reduction of the Schrödinger equations for a given crystal lattice, where the field is assumed to be slowly varying. As semiconductor devices become smaller, however, next-order corrections to the semiclassical equations must be taken into account in the Boltzmann equations. We derive these corrections and show their effects on the transport of electrons in semiconductors. In particular, we show that the Einstein relations are no longer valid in the high field limit, which may resolve the discrepancy between previous theory and experimental evidence.

Introduction

Understanding the quantum transport of carriers in crystals under spatially- and time-varying electromagnetic fields is necessary to accurately model the characteristics of modern and future micron and submicron semiconductor devices.[1,2] Here we describe our analysis of collisionless electron transport in the high-field regime. In particular, we derive the corrections to the semiclassical equations where the applied fields are no longer weak and show how it affects the transport of carriers when effects of scattering are not ignored.

Drift of carriers (electrons or holes) in semiconductors are driven by two different fields. One is due to the periodic potential arising from the atoms which make up the crystal lattice. The other is due to applied external fields and spatial distributions of dopants, electrons and holes, and may be spatially inhomogeneous and time varying. Where the latter inhomogeneous fields are small, one may derive the well-known semiclassical equations of motion for electrons[3] (for notational simplicity, we refer to electrons only; however, analogous expressions may be written for holes for all expressions which appear in this text),

$$\frac{d}{dt}\mathbf{x} \equiv \mathbf{v} = \frac{1}{\hbar}\nabla_k \mathcal{E}_n^\circ(\mathbf{k}), \tag{1a}$$

$$\frac{d}{dt}\mathbf{k} \equiv \mathbf{F} = -e\left(\mathbf{E}(\mathbf{x},t) + \frac{1}{c}\mathbf{v}\times\mathbf{H}(\mathbf{x},t)\right). \tag{1b}$$

Here, the applied force on the electron $\mathbf{F}$ is the classical Lorentz force. Quantum effects in the electron motion are expressed soley by the group-velocity of the electron $\mathbf{v}$ being dependent upon the n-th band energy $\mathcal{E}_n^\circ$ of the homogeneous semiconductor material. The band energies are the eigenvalues of the Bloch electron eigensolutions $\{u_n, \mathcal{E}_n^\circ\}_{n\in Z}$ of the Schrödinger equation for the spatially-periodic crystal potential. The velocity of the electron here is in fact not directly dependent on the applied force.

These semiclassical equations describe the trajectory of an electron in the position-momentum $(\mathbf{x},\mathbf{k})$ space, and are the leading-order asymptotic results from the Schrödinger equation when the external fields are sufficiently weak (Note that the position and momentum variables have been appropriately scaled such that Heisenberg's uncertainty principle is not violated). Since the scattering of electrons by collisions with other electrons, holes, impurities, and phonons have been neglected, no jumping of electrons is allowed in (1) between different bands or between two separated points of the same band. Thus, the semiclassical equations accurately describe electrons traveling a distance short enough such that no such scattering effects are encountered.

The effects of electron scattering are taken into account by the Boltzmann equation,

$$\frac{\partial}{\partial t}g + \mathbf{v}\cdot\nabla_x g + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_k g = \mathcal{L}g, \tag{2}$$

where $g = g(t,\mathbf{x},\mathbf{k})$ is the electron density. The left side of this equation describes the drift or streaming of the electrons as given by the semiclassical model. The scattering operator, $\mathcal{L}$, on the right side, accounts for intraband and interband tunneling caused by collision events.

Where the mean free path for $\mathcal{L}$ is short and the force F is weak (and excluding the magnetic field), an asymptotic expansion (the Hilbert expansion) may be used to reduce the

Boltzmann equation to the Basic Semiconductor (or van Roosbroeck) Equations,

$$\frac{\partial}{\partial t}n = \nabla_x \cdot (D\nabla_x n - \mu \mathbf{F} n), \tag{3}$$

where $n = \int g\, d^3k$ is the spatial distribution of the electrons. Electron diffusivity D and mobility μ are determined by the scattering operator and satisfy Einstein's relation,

$$\mu = \frac{D}{k_B T}. \tag{4}$$

Furthermore, Hagan, Cox and Wagner[4] have derived asymptotic reductions of the Boltzmann equation where the force $\mathbf{F}$ is no longer taken small. In their high field semiconductor equations, the electron diffusivity and mobility become nonlinear functions of $\mathbf{F}$. Even in this limit, Einstein's relation is still satisfied.

There is, however, a discrepancy between Einstein's relation and experimental observations[2] at high fields. Such discrepancy may arise from the field dependence of the scattering operator $\mathcal{L}$. We have shown[5] that such discrepancy may also arise from the neglect of higher-order terms in the semiclassical equations (1). To illustrate, the small parameter used, in asymptotically reducing the Boltzmann equation to the Basic Semiconductor Equation, is given by the ratio of the mean free path to the typical device size. For micron-sized devices, this ratio is on the order of $\tilde{\epsilon} \sim 10^{-2}$. In asymptotically reducing the Schrödinger equation to the semiclassical equation, the small parameter used is the ratio of the crystal lattice constant (the typical distance between atoms which make up the crystal) and the typical (macroscopic) device size, which is on the order of $\epsilon \sim 10^{-4}$. Since the Basic Semiconductor Equation (3) is valid to $O(\tilde{\epsilon}^2)$,[4] the next-order corrections to the semiclassical equations do arise as next-order corrections to Einstein's relations. In fact, since such corrections depends upon the Lorentz force, the neglected terms are expected to become more significant as the field strength in a semiconductor increases.

In our work,[5] we use a multi-scaling asymptotic method in order to derive the next-order terms of the semiclassical equations. The external field is not taken to be weak; however, it is defined to be slowly-varying in both time and space. These corrected semiclassical equations show that intraband scattering driven by the Lorentz force leads to a correction in the Einstein's relation. We also show that our asymptotic solutions are valid as long as any two different band energies, $\mathcal{E}_n^\circ(\mathbf{k})$ and $\mathcal{E}_m^\circ(\mathbf{k})$ for $m \neq n$, are sufficiently separated for a given $\mathbf{k}$. A brief overview of our work follows.

Derivation of the Semiclassical Equations

We now describe the asymptotic reduction of the Schrödinger equation to the semiclassical equation. The Schrödinger equation for an electron in a periodic crystal lattice with applied external fields is given as

$$i\hbar\frac{\partial}{\partial t'}\psi = \frac{1}{2m_e}\left(-i\hbar\nabla_r + \frac{e}{c}\mathbf{A}\right)^2\psi + (V - e\Phi)\psi, \tag{5}$$

where ψ is the electron wave function, V is the potential due to the crystal lattice, and $\mathbf{A}$ and Φ are the vector and scalar potential due to the external field.

Since the crystal lattice is spatially periodic, $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$ for any vector $\mathbf{R}$ which defines the primitive cell. We take the external field to be slowly-varying and introduce slow scales $t = \epsilon t'$ and $\mathbf{x} = \epsilon \mathbf{r}$, where $0 < \epsilon \ll 1$. The small parameter ϵ is the ratio of the crystal lattice constant (5.431 Å for Si) to the typical device size ($\sim 0.1 - 1.0$ micron). Thus, the potentials are written as $\mathbf{A} = \mathbf{A}(\mathbf{x}, t)$ and $\Phi = \Phi(\mathbf{x}, t)$, and the relations

$$\mathbf{E} = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{A} - \nabla_x \Phi, \tag{6a}$$

$$\mathbf{H} = \nabla_x \times \mathbf{A}, \tag{6b}$$

give the slowly-varying electric $\mathbf{E}$ and magnetic $\mathbf{H}$ fields.

We carry out the multi-scale expansion as described by Whitham[6] and express the electron wave function in the WKB-type form

$$\psi = \phi(\mathbf{r}, \mathbf{x}, t) e^{\frac{i}{\epsilon}\theta(\mathbf{x},t)}, \tag{7}$$

and define the band energy as

$$\mathcal{E}(\mathbf{x}, t) \equiv -\hbar \frac{\partial}{\partial t}\theta + e\Phi$$

and the "crystal" momentum as

$$\mathbf{k}(\mathbf{x}, t) \equiv \nabla_x \theta + \frac{e}{c\hbar}\mathbf{A}.$$

Since the external field is not constant, both the band energy and momentum are now functions of $\mathbf{x}$ and t.

With the scaling as given for (5), however, both are essentially constant on the crystal lattice scale. This obviates the need to impose restrictive boundary conditions on $\mathbf{k}$, which pose the main difficulty in deriving the "accelerated Bloch electrons".[1,7] Furthermore, the typical width of the electron wave-packet spread is taken to be intermediate to the crystal and external field lengthscales. This allows the electron to be described by trajectories in the position-momentum $(\mathbf{x}, \mathbf{k})$ space without violating the uncertainty principle. The drawback is that the asymptotic expansion may break down near semiconductor-semiconductor junctions or device boundaries, since large field gradients may be present at those locations.

To leading order, the Bloch electron eigensolutions are obtained,

$$\left\{\frac{1}{2m_e}(-i\hbar\nabla_r + \hbar\mathbf{k})^2 + V(\mathbf{r}) - \mathcal{E}_n^\circ(\mathbf{k})\right\} u_n(\mathbf{r}, \mathbf{k}) = 0, \tag{8}$$

where $\{u_n(\mathbf{r}, \mathbf{k}), \mathcal{E}_n^\circ(\mathbf{k})\}_{n\in\mathbb{Z}}$ constitutes a complete and orthonormal basis for the spatially-periodic crystal lattice. Solutions to (8) can be found numerically using the pseudopotential method.[8] To derive the next-order results, we expand both the Bloch eigenvalue and eigenfunction in ϵ,

$$\mathcal{E} = \mathcal{E}_n^\circ + \epsilon \mathcal{E}_n^1 + \cdots, \tag{9a}$$

$$\phi = \phi_n^\circ + \epsilon \phi_n^1 + \cdots, \tag{9b}$$

and define the inner product $\langle \alpha, \beta \rangle \equiv \int \alpha^* \beta \, d^3r$, where the integral is over one primitive cell.

Leading order gives $\mathcal{E}_n^\circ = \mathcal{E}_n^\circ(\mathbf{k})$ and $\phi_n^\circ = a_n(\mathbf{x}, t)\, u_n(\mathbf{r}, \mathbf{k})$, where a_n is the slowly-varying coefficient to be found at next order. Since we are neglecting the effects of interband transitions for now, each band n may be treated independently. The validity of this assumption will be discussed later.

With the independent band assumption, $\langle \psi, \psi \rangle = a_n^2 + O(\epsilon^2)$ gives the distribution of an electron in a given band n up to next-order corrections. Deriving the next-order terms in the expansions (9), we obtain the expression

$$\frac{\partial}{\partial t} a_n^2 + \nabla_x \cdot \left(\mathbf{v} a_n^2 \right) = 0, \tag{10}$$

where $\mathbf{v}$ is the group velocity of the electron (including the $O(\epsilon)$ correction term).

Expression for the electron drift (10) may be rewritten in terms of characteristic coordinates in the position-momentum space. These characteristic equations, then, are the semiclassical equations of motion. With a change of variables $(\mathbf{x}, \mathbf{k}) \to (\mathbf{q}, \mathbf{p})$,

$$\begin{aligned} \mathbf{q} &\equiv \mathbf{x} - i\epsilon \langle u_n, \nabla_k u_n \rangle, \\ \mathbf{p} &\equiv \hbar \mathbf{k} - \frac{e}{c} \mathbf{A}, \end{aligned}$$

the Hamiltonian for the electron motion is derived,

$$\frac{d}{dt}\mathbf{q} = \frac{\delta}{\delta \mathbf{p}} H, \qquad \frac{d}{dt}\mathbf{p} = -\frac{\delta}{\delta \mathbf{q}} H,$$

where the Hamiltonian H is given by

$$H(\mathbf{q}, \mathbf{p}) \equiv \mathcal{E}\left(\mathbf{q}, \frac{1}{\hbar}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{q}, t) \right), t \right) + e\Phi(\mathbf{q}, t), \tag{11}$$

and where the band energy now includes the $O(\epsilon)$ term, $\mathcal{E}(\mathbf{x}, \mathbf{k}, t) = \mathcal{E}_n^\circ(\mathbf{k}) + \epsilon \mathcal{E}_n^1(\mathbf{x}, \mathbf{k}, t)$. We have computed the correction term $\mathcal{E}_n^1$ and present it elsewhere.[5]

Thus, the next-order terms of the semiclassical equations as given by the Hamiltonian above arises from the corrections to the band energy. At this order, the band energy becomes dependent on the applied Lorentz force. In essence, the Lorentz force drives intraband transitions, denoted by $\langle u_n, \nabla_k u_n \rangle$, which slightly alter (from leading order) the characteristic lines on which the electron travel. The above also shows that, even with the corrections to the velocity $\mathbf{v}$ and applied force $\mathbf{F}$, the electron motion still retains its Hamiltonian form.

Since the electron motion may be described by the Hamiltonian (11), the Boltzmann equation still retains the form given in (2) but with $O(\epsilon)$ correction to the $\mathbf{v}$ and $\mathbf{F}$ now included. This expression thus includes the lowest-order field-dependent intraband scattering terms on the left side (rather than including it in the scattering operator $\mathcal{L}$ on the right side). Neglecting the magnetic field and scaling for the Hilbert expansion, the corrections to the semiclassical equations leads to a correction in the electron mobility of the Basic Semiconductor Equations (3). Einstein's relation, to this order, is now expressed as

$$\mu = \frac{D}{k_B T} + \epsilon^2 \mu_1.$$

The term μ_1, which we have derived, is presented elsewhere.[5] In taking the high field limit of the Boltzmann equation, we expect this correction term to become more significant since the intraband transitions driven by the Lorentz force would increase.

Discussion and Future Work

In deriving the semiclassical equation of motion, we have assumed that there were no scattering between the different bands as given by the Bloch electron solutions. Here we discuss briefly the validity of this independent band assumption.

Correction to the leading order Bloch electron solution $u_n(\mathbf{r}, \mathbf{k})$ is given in (9) as $\phi_n^1(\mathbf{r}, \mathbf{x}, t)$. This function is obtained in the course of deriving the asymptotic results above.[5] Since the set of Bloch electron eigensolutions represent a complete and orthonormal basis for $\mathbf{R}$-periodic functions, we may expand ϕ_n^1 in terms of $\{u_n, \mathcal{E}_n^\circ\}_{n\in\mathbf{Z}}$. When such an expansion is done,[5] we observe that a condition for the validity of the expansion (9) is given as

$$\left|\frac{\langle u_m, \nabla_k u_n\rangle \cdot \mathbf{F}}{\mathcal{E}_m^\circ(\mathbf{k}) - \mathcal{E}_n^\circ(\mathbf{k})}\right| = O(1) \tag{12}$$

for all $m \neq n$. This condition (12) indicates that interband (Zener) tunneling effects between two bands are significant where two Bloch eigenvalues become nearly degenerate, i.e. $\mathcal{E}_m^\circ \approx \mathcal{E}_n^\circ$ and the Lorentz force $\mathbf{F}$ is strong enough. Such conditions do arise in semiconductor devices, especially near junctions, barriers and device boundaries, where appreciable fields strengths may occur.

Given two conduction bands, such effects are significant especially near the local minimas (in $\mathbf{k}$-space) of the higher-energy band (local maximas of a lower-energy band for valence bands). The results of our asymptotic analysis presented in the previous section would then be valid away from such regions. Near the local minimas of $\mathcal{E}_n^\circ(\mathbf{k})$, the asymptotic expansion of (5) must be rescaled.

The semiclassical equations suggests that the passage of an electron through a region in $\mathbf{k}$-space where the interaction between two bands is $O(1)$ is rapid for high fields (see (1)). Thus, deriving uniformly consistent asymptotic results in the entire position-momentum space would require solving a *passage through resonance*[9] problem. We are currently carrying out this analysis. Note that the semiclassical equations with corrections which we have derived would then represent the outer solution for this problem.

Furthermore, scattering of electrons by interactions with phonons have not been taken into account here. These interactions would cause intraband and interband transitions between points in the bands separated in $\mathbf{k}$-space. Involved in this process is the absorption or emission of phonons with momentum $\mathbf{K} = \pm(\mathbf{k}_m - \mathbf{k}_n)$ (where $\mathbf{K}$ is mapped back into the first Brillouin zone of the periodic $\mathbf{k}$-domain). These and other scattering events must be taken into account if one is to derive an asymptotically accurate quantum Boltzmann equation. We intend to carry out this derivation in the future.

References

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Konstantin Efetov, Max-Planck Inst., quantum dots

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Ben Luce, Clarkson Univ., turbulence in the complex Ginzburg-Landau equation

Peter Prelovsek, J. Stefan Inst., pairing and blustering t-J and Hubbard models

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Jan Wehr, Univ. of Arizona., chaos and complexity in simple dynamical systems

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Title	Dates	Location	Technical Host
Low Dimensional Behavior in Nonlinear PDEs	8/3-31	CNLS	D. Holm
Fluctuations and Order: The New Synthesis	9/9-12	Los Alamos	M. Millonas

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- From a UNIX machine, use the xmosaic utility and open the document "http://cnls-www.lanl.gov/"
- If you have a CNLS computer account, you can alternatively rlogin to goshawk, set your DISPLAY variable, and type "xmosaic" -- your default home page will be the CNLS welcome page.

You can obtain "xmosaic" by anonymous ftp from the machine ftp.ncsa.uiuc.edu in directory Mosaic/xmosaic-binaries. There are also browsers available on the net for other machines (such as Macintoshes, PCs and NeXTs). We also have a "line-mode" browser installed at CNLS called "www" - this allows you to web over a phone line. ENJOY!

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