Scattering Theory of Carrier Transport in Semiconductor Devices

Mark Lundstrom, Carl Huster, Kausar Banoo, and Ramesh Venugopal

Purdue University
School of Electrical and Computer Engineering
West Lafayette, Indiana 47907

Abstract

This paper reviews the scattering theory of semiclassical charge carrier transport in semiconductors. The derivation of the underlying equations from the Boltzmann equation, numerical solution to solve the Boltzmann equation in devices, and the application of simple versions of scattering theory which provide insight into devices are reviewed.

1. Introduction

Scattering theory provides an alternative to the more common descriptions of carrier transport. At a simple level, it provides insights that are complementary to traditional approaches. At a numerical level, it provides new methods for simulating carrier transport. At a different level, it describes quantum transport in mesoscopic devices [1]. Because of this generality, it may provide a convenient method for easily moving between different levels of the device simulation hierarchy and for interpreting detailed simulations. Our objective in this presentation is to survey the scattering theory of transport and its application to semiconductors.

2. Multi-Flux Formulation of the Boltzmann Equation

The Boltzmann equation is typically formulated in terms of the carrier distribution function, $f(\mathbf{r}, \mathbf{p}, t)$, but it can also be expressed in terms of the flux distribution, $\mathbf{j} = \upsilon f$ as,

$$\frac{\partial j_x}{\partial x} - q\mathcal{E}_x \frac{\partial (j_x/\upsilon_x)}{\partial p_x} = \hat{C} j_x, \tag{1}$$

where $\hat{C}$ is the collision operator and for simplicity we have assumed steady-state, nondegenerate conditions and spatial variations in one dimension. Scattering moves

carriers between momentum states. The electric field also moves carriers in momentum space, so the field and collision operators can be combined [2]. If we then discretize the Boltzmann equation into 2M bins in momentum space (M with velocities along the positive x-axis and M along the negative x-axis), then eq. (1) can be expressed as

$$\frac{d}{dx}|j_x(x)\rangle = [\Gamma_x]|j_x(x)\rangle, \tag{2}$$

where $|j_x(x)\rangle$ is a 2M x 1 vector in momentum space representing the flux carried by each bin. The elements of $[\Gamma_X]$ are inverse mean-free paths for scattering. The diagonal elements represent the probability per unit distance that carriers will out-scatter to other bins, and the off-diagonal elements describe in-scattering. Equation (1) is similar to the form commonly used in neutron transport [3]. The difference is that for semiconductors, the differential backscattering matrix, $[\Gamma_X]$, includes the effects of the electric field as well as the scattering processes. As discussed in Sec. 4, numerical solution procedures used in neutron transport can be generalized to solve eq. (2) for semiconductors.

Equation (2) is readily generalized for spatial variations in two or three dimensions [2]. In the general case, the flux vector in momentum space, $|j_x(x)\rangle$, becomes $|\mathbf{j}(\mathbf{r})\rangle$, where each element is a vector in real-space whose direction is determined by the local energy band structure. The spatial derivative is replaced by a diagonal directional derivative matrix representing the derivative in the direction that each of the 2M fluxes is traveling.

Equation (2) assumes a very simple form when the flux vector is represented by a single flux moving in the positive direction and another one moving in the negative direction, then

$$\frac{d}{dx}\begin{pmatrix} j^+ \\ j^- \end{pmatrix} = \begin{bmatrix} -\alpha & \beta \\ -\alpha & \beta \end{bmatrix}\begin{pmatrix} j^+ \\ j^- \end{pmatrix}, \tag{3}$$

where α and β are inverse mean-free-paths for backscattering. In the absence of an electric field, $\alpha = \beta$, but electric fields introduce asymmetry. The M=1 approach was introduced by McKelvey *et al.* in 1961 [4], and they showed that this "flux method" provided an alternative to the more conventional continuity and drift-diffusion formulation of carrier transport. An additional advantage is that ballistic transport can be treated easily. Equation (2) and (3) are valid in steady-state, but time dependence is readily included [5].

3. The Boltzmann Equation as a Drift-Diffusion Equation

By pairing each flux moving in one direction with one moving in the opposite direction, we can re-cast eq. (2) into a second order equation. It may come as a surprise that the result can be written in drift diffusion form as

$$|J_x(x)\rangle = q[\mu_{xx}]|n(x)\rangle\mathcal{E}_x + q[D_{xx}]\frac{d|n(x)\rangle}{dx} \tag{4a}$$

$$\frac{d|J_x(x)\rangle}{dx} = q[G_{xx}]|n(x)\rangle + q[\alpha_{xx}]|J_x(x)\rangle, \tag{4b}$$

where $|n(x)\rangle$ represents the particle density in each of the M bins and $|J_x(x)\rangle$ represents the net x-directed current carried by each bin. The M x M diffusion matrix, $[D_{xx}]$, describes particle scattering, the matrix $[\mu_{xx}]$ describes the influence of the electric field as well. The matrices $[G_{xx}]$ and $[\alpha_{xx}]$ describe the "generation" of particles in each bin due to scattering, the electric field, and recombination-generation processes.

The connection between the one-flux equations and the drift-diffusion equations was first noted by Shockley in 1962 [6]. Since the one-flux equations describe both collision-dominated and ballistic transport, we conclude that, at least under some conditions, the drift-diffusion equation may be used for ballistic transport. This fact was recently noted by Hansen in a study of diffusion across a thin base [7]. Equations (4a) and (4b) may also prove to be a useful way to formulate the Boltzmann equation for numerical solution. In the general case of spatial variations in two or three dimensions, the transport matrices become three by three tensors with each element an M by M matrix, and the spatial derivative becomes a directional derivative operator [2]. The multi-mode drift-diffusion equation also has pedagogical value; it indicates that solving the Boltzmann equation is equivalent to solving M coupled drift-diffusion equations. The increase in computational effort is easy to appreciate.

4. Numerical Solutions

The one-dimensional multi-flux equations have been solved by two different methods. One simply involves integrating eq. (2) across discrete elements in a nonuniform grid. Upwinding is essential to maintain positive fluxes, and careful discretization is necessary to

prevent unreasonably small spatial elements. Since the electric field acts like a scattering mechanism, strong electric fields result in very short effective mean-free-paths. A simple finite difference approximation to eq. (2) is restricted to spatial elements that are thinner than one mean-free-path, so higher order discretizations must be used where the electric field is large.

The scattering matrix approach is an alternative method to solve the first order equations [8-10]. Rather than working with differential elements as in Fig. 1a, we use slabs (in 1D) of finite thickness as illustrated in Fig. 1b. Equation (2) is integrated across a slab of finite thickness. In practice this is done by Monte Carlo simulation. One simply "shoots" electrons at a slab containing a given electric field and set of scattering processes. Electrons are tracked until they leave the slab. By taking the ratio of the number of electrons exiting in a given bin to those injected, the emerging fluxes can be related to the incident fluxes. The final result can be expressed as

$$\begin{bmatrix} |j^+(x+dx)\rangle \\ |j^-(x)\rangle \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} |j^+(x)\rangle \\ |j^-(x+dx)\rangle \end{bmatrix}, \tag{5}$$

where the scattering matrix, [S], relates the fluxes emerging from the two faces of the slab to the incident fluxes. These scattering matrices are pre-computed and stored in a library. Devices are then simulated by cascading pre-computed scattering matrices. (In the neutron transport community, this approach is known as the response matrix method [3]).

The use of pre-computed scattering matrices has a number of advantages, and some limitations. Monte Carlo simulation provides an easy way to integrate across a slab several mean-free-paths thick (but some of this advantage is lost because the field and collision operators are typically split). Pre-computing the matrices and storing them provides some computational efficiency. On the other hand, the memory requirements can be quite large and nonlinear processes, such as electron-electron scattering, are difficult to handle. Nevertheless, 1D solutions have provided a good deal of insight into important issues for transport in devices [11-13]. In addition to electronic devices, scattering matrix simulations have also been applied to optoelectronics where carrier dynamics are coupled to the phonon and photon populations [14].

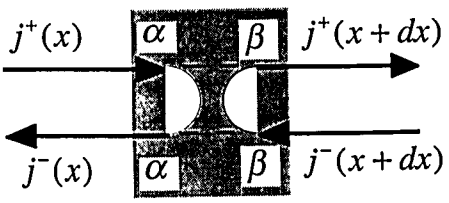


Fig. 1a The differential formulation of the 1-flux equations.

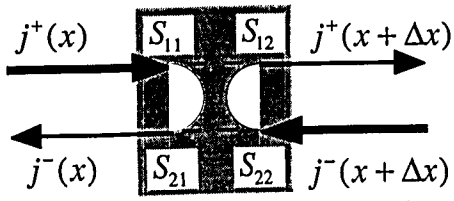
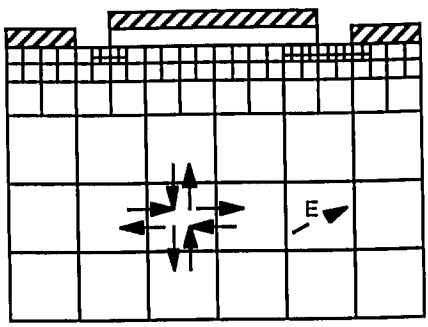


Fig. 1b The discrete formulation of the flux equations. Incident fluxes (heavy arrows) are related to emerging fluxes by [S]. The slab may thick compared to a mean-free-path.

The scattering matrix approach can be applied to two-dimensional transport as well. As illustrated in Fig. 2, a device is discretized into square elements, and each element has fluxes incident from the top, bottom, left and right. The emerging fluxes are, again, related to the incident fluxes by a scattering matrix,

$$\begin{pmatrix} a_L^- \\ a_R^+ \\ a_T^- \\ a_B^+ \end{pmatrix} = \begin{bmatrix} t_{LL} & t_{LR} & t_{LT} & t_{LB} \\ t_{RL} & t_{RR} & t_{RT} & t_{RB} \\ t_{TL} & t_{TR} & t_{TT} & t_{TB} \\ t_{BL} & t_{BR} & t_{BT} & t_{BB} \end{bmatrix} \begin{pmatrix} a_L^+ \\ a_R^- \\ a_T^+ \\ a_B^- \end{pmatrix}. \tag{6}$$

Each element of the 4 by 4 scattering matrix is an M by M matrix. Techniques for evaluating scattering matrices by Monte Carlo simulation and for solving for the flux distributions within a device are analogous to those employed for 1D analysis, but the size of the problem expands substantially.



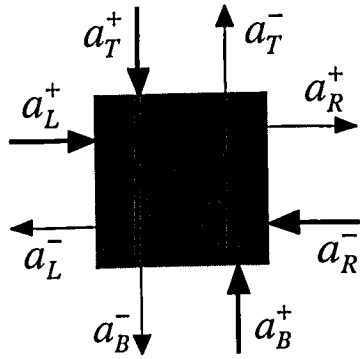


Fig. 2 Illustration of how the scattering matrix approach is applied to two dimensional devices. At the left we show how a device is discretized into square elements and at the right, how the emerging fluxes are related to the incident fluxes.

5. 1-Flux Scattering Theory

One flux (M=1) scattering theory proves to be a useful way to view ultra-small bipolar transistors [15, 16] and MOSFETs [17, 18]. For example, the saturated drain current of a MOSFET can be expressed as [17]

$$I_{Dsat} = C_{ox} W \upsilon_T \left(\frac{1 - R_c}{1 + R_c} \right) (V_{GS} - V_T), \tag{7}$$

where R_C is the channel reflection coefficient and υ_T the thermal velocity of electrons injected from the source. As shown in Fig. 3, thermal carriers are injected over the source-to-channel potential barrier (whose height is modulated by the gate voltage) into the channel, and a fraction, R_C, backscatters. For long channel devices, eq. (7) reduces to the conventional expression, but it also provides a clear prediction for the ballistic limit. If the channel is ballistic, the maximum drain current is set by the thermal injection velocity from the source (about 10^7 cm/s for nondegenerate electrons in silicon at room temperature). The channel reflection coefficient is determined by a region of the channel very close to the source [17]. Velocity overshoot, which is strongest near the drain, enters indirectly through the self-consistent electric field. Because the electric field is low near the source where the backscattering that controls R_C occurs, electrons are near thermal equilibrium, and R_C can be easily estimated from the near-equilibrium mobility. Scattering theory provides a simple, physical explanation for why the near-equilibrium electron mobility continues to be a physically meaningful parameter in a very small MOSFET.

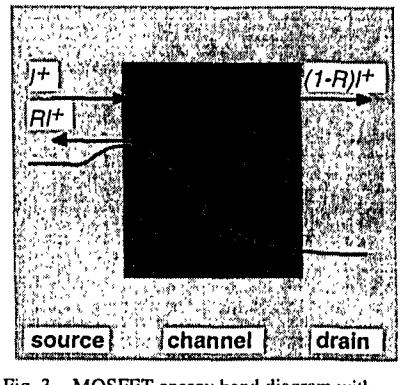


Fig. 3 MOSFET energy band diagram with injected and scattered fluxes

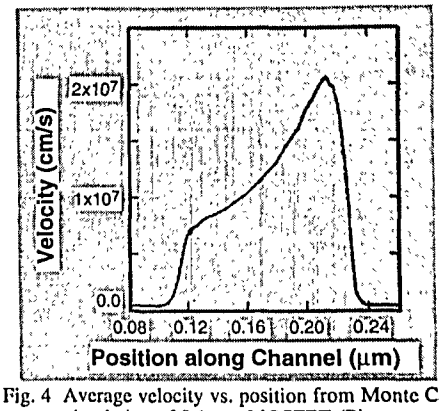


Fig. 4 Average velocity vs. position from Monte Carlo simulation of 0.1 μm MOSFET (Pinto et al, *Elect. Dev. Lett.*, 14, 375, 1993)

In the linear regime, I_D (for a nondegenerate channel) can be written as [18],

$$I_D = W C_{ox}\left(\frac{\upsilon_T}{k_B T/q}\right)(1-R_C)(V_{GS}-V_T)V_{DS}\,, \tag{8}$$

which shows that in the ballistic limit, $R_C = 0$, there is still a finite channel resistance. This result is analogous to the e^2/h contact resistance well-known for mesoscopic devices [1])

One flux theory also provides a useful way to interpret detailed simulations. For example, Fig. 4 shows the average velocity vs. position along the channel of a MOSFET as computed by Monte Carlo simulation. Strong velocity overshoot occurs, but the critical velocity is at the beginning of the channel. The ratio, $\langle\upsilon(0)\rangle/\upsilon_T$, is a drive current figure of merit for the device. According to scattering theory, thermal electrons are injected into the channel, and those that backscatter have only experienced a potential drop of about k_BT/q, so the backscattered electrons are a near-thermal population too. The result is that the critical velocity at the beginning of the channel can be related to R_C by

$$\mathcal{B} = \frac{\langle\upsilon(0)\rangle}{\upsilon_T} = \frac{1-R_C}{1+R_C}. \tag{9}$$

If there were no backscattering from the channel, then R_C would be zero, and the average velocity would be υ_T, the thermal injection velocity ($\approx 10^7$ cm/s for a thermal equilibrium hemi-Maxwellian). The fact that the velocity at the beginning of the channel in Fig. 2 is below 10^7 cm/s indicates that backscattering is occurring. Various device designs should be compared in terms of R_C if drive current is the parameter of interest.

6. Summary

Scattering theory provides a useful way to think about carrier transport in semiconductors. It has the ability to treat transport from an analytical (compact model) level to a full Boltzmann level. It may provide useful, new numerical methods for simulating carrier transport. It certainly provides useful new insights into carrier transport and device physics.

Acknowledgment- this work was supported by the Semiconductor Research Corporation.

References

[1] S. Datta, *Electronic Transport in Mesoscopic Structures*, Cambridge Univ. Press, Cambridge, UK, 1995.

[2] K. Banoo and M. Lundstrom, "Multi-Flux Formulation of the Boltzmann Equation for Carrier Transport in Semiconductors," technical report, TR-ECE 98-7, School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana, USA, April, 1998.

[3] E. Lewis and J.W.F. Miller, *Computational Methods of Neutron Transport*, Am. Nuc. Soc., Inc. LaGrange Park, IL, 1993.

[4] J.P. McKelvey, R.L. Longini, and T.P. Brody, "Alternative approach to the solution of added carrier transport problems in semiconductors, " *Phys. Rev.*, **123**, pp. 51-57, 1961.

[5] M.A. Alam, S.-I. Tanaka, and M.S. Lundstrom, "A small-signal, one-flux analysis of short base transport," *Solid-State Electron.*, **38**, pp. 177-182, 1993.

[6] W. Shockley, "Diffusion and drift of minority carrier in semiconductors for comparable capture and scattering mean free paths," *Phys. Rev.*, **125**, pp. 1570-1576, 1962.

[7] O. Hansen, "Diffusion in a thin base," *Solid-State Electron.*, **37**, pp. 1663-1669, 1994.

[8] A. Das, M.S. Lundstrom, "A Scattering Matrix Approach to Device Simulation," *Solid-State Electron.*, **33**, 1299-1307, 1990

[9] M.A. Alam, M.A. Stettler, and M.S. Lundstrom, "Formulation of the Boltzmann Equation in Terms of Scattering Matrices," *Solid-State Electron.*, **36**, 263-271, 1993.

[10] Stettler, M.A. and Lundstrom, M.S., "Self-consistent scattering matrix calculation of the distribution function in semiconductor devices," *Appl. Phys. Lett.*, **60**, pp. 2908-2910, 1992.

[11] M.A. Stettler, M.A. Alam, and M.S. Lundstrom, M.S., "A critical examination of the assumptions underlying macroscopic transport equations for silicon devices," *IEEE Trans. Electron Dev.*, **40**, pp. 733-740, 1993.

[12] M.A. Stettler and M.S. Lundstrom, "A detailed investigation of heterojunction transport using a rigorous solution of the Boltzmann equation," *IEEE Trans. Electron Dev.*, **41**, pp. 592-600, 1994.

[13] M.A. Stettler, and M.S. Lundstrom, "A microscopic study of transport in thin base silicon bipolar transistors," *IEEE Trans. Electron Dev.*, **41**, pp. 1027-1033, 1994.

[14] M.A. Alam and M.S. Lundstrom, "Effects of carrier heating on laser dynamics," IEEE J. Quantum Electron., **33**, pp. 2209-2220, 1997.

[15] S.I. Tanaka and M.S. Lundstrom, "A compact model HBT device model based on a one-flux treatment of carrier transport," Solid-*State Electron.*, **37**, pp. 401-410, 1994.

[16] S.I. Tanaka and M.S. Lundstrom, "A flux-based study of carrier transport in thin-base diodes and transistors," *IEEE Trans. Electron Dev.*, **42**, pp. 1806-1815, 1995.

[17] M.S. Lundstrom, "Elementary Scattering Theory of the Si MOSFET," *Electron Dev. Lett.*, **18**, 361-363, 1997.

[18] S. Datta, F. Assad, and M.S. Lundstrom, "The silicon MOSFET from a transmission viewpoint," *Superlattices and Microstructures*, **23**, 1998.