Treating Non-Equilibrium Green's Functions with a Monte Carlo Method

D. K. Ferry
School of Electrical, Computer, and Energy Engineering, Arizona State University,
Tempe, AZ 25287-6206 USA
e-mail: ferry@asu.edu

ABSTRACT SUBMISSION

The use of ensemble Monte Carlo (EMC) methods for the simulation of transport in semiconductor devices has become extensive over the past few decades. This method allows for simulation utilizing particles while addressing the full physics within the device, leaving the computational difficulties to the computer. Here, a particle EMC approach to NEGF is discussed, and preliminary results are obtained for quantum transport in Si at 300 K.

INTRODUCTION

From the beginning, there has been a rich history for the use of particles in quantum mechanics, ranging from Kennard to Feynman. The use of particles in the EMC approach has become standard in studying the operation and performance of semiconductor devices. However, today one of the most popular approaches to quantum transport and quantum distributions, especially in devices, is thought to be non-equilibrium Green's functions (NEGF). But, these functions bring considerable computational difficulty to any transport problem. Here, the Airy transform is used to formulate the important "less-than" Green's function in a manner that is amenable to solution via EMC techniques.

MODEL

In this work, a continuous *Airy transform* is used. The Airy transform of a function $f(\boldsymbol{r}, z)$ is given as

$$F(\boldsymbol{k}, s) = \int d^2\boldsymbol{r} \int \frac{dz}{2\pi L} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} Ai\left(\frac{z-s}{L}\right) f(\boldsymbol{r}, z)\,.$$

Use of this transform allows us to rewrite the less-than function in the generalized Kadanoff-Baym manner as [1]

$$G^{<}(\boldsymbol{k}, s, \omega) = A(\boldsymbol{k}, s, \omega) f(s, \omega)$$

with

$$f(s, \omega) = \frac{\Sigma^{<}(\boldsymbol{s},, \omega)}{2Im\{\Sigma_r(s, \omega)\}}\,.$$

THE SILICON PROPERTIES

To illustrate this new EMC approach to solving for NEGF, the case of Si will be considered. While the situation for electrons in the conduction band is complicated by the multi-valley nature of this band, the scattering processes themselves are very local and do not require some of the more complicated higher-order corrections. Scattering by acoustic and *f*- and *g*-intervalley phonons are considered. Non-parabolic bands are considered.

The imaginary parts of the retarded self-energy is shown in Fig. 1 for an applied electric field of 50 kV/cm. In Fig. 2, the spectral density is shown for this same field. An important aspect of the present EMC approach is that drift time is replaced by drift distance [2]. This drift distance is then used to determine the drift time needed to evaluate the change in particle momentum. In Fig. 3, the average drift distance is shown as a function of the electric field. Figure 4 shows the drift velocity as a function of electric field, and the distribution function at 50 kV/cm is shown in Fig. 5.

CONCLUSION

The use of the ensemble Monte Carlo process has been shown to be effective in evaluating non-equilibrium Green's functions in a fast and effective approach. Methods to extend this to both inhomogeneous material, such as devices, and to polar optical phonons are under consideration and represent future work on this topic.

REFERENCES

[1] R. Bertoncini, A. M. Kriman, and D. K. Ferry, *Airy Coordinate Approach for Nonequilibrium Green's Functions in High Field Quantum Transport,* Phys. Rev. B 41, 1390 (1990).
[2] D. K. Ferry, *Using Ensemble Monte Carlo Methods to Evaluate Nonequilibrium Green's Functions, submitted for publication.*

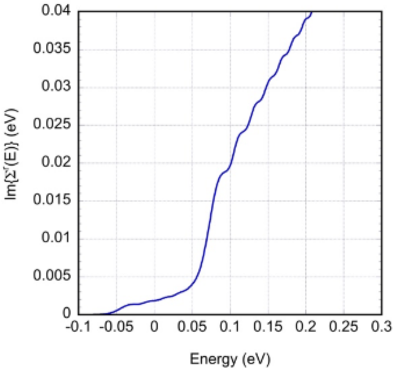

Fig. **1**. Imaginary part of the self-energy in Si at 50 kV/cm and 300K.

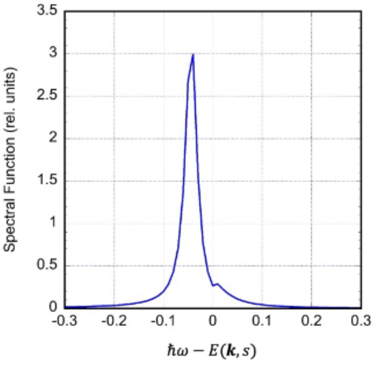

Fig. 2. The spectral density for a field of 50 kV/cm and 300 K.

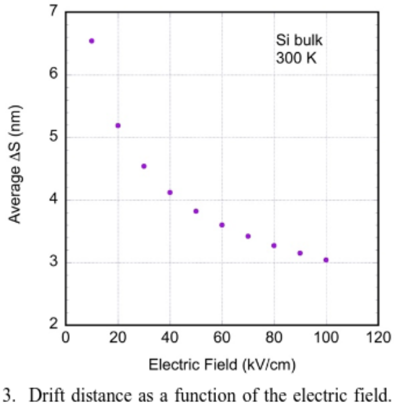

Fig. 3. Drift distance as a function of the electric field. This distance is averaged over 10^5 particles and 200 iterations.

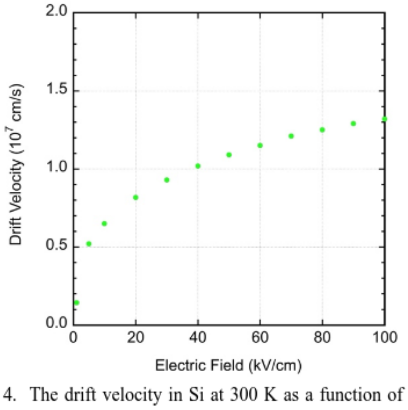

Fig. 4. The drift velocity in Si at 300 K as a function of the applied electric field.

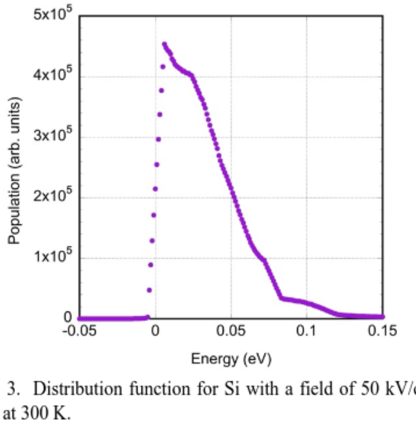

Fig. 3. Distribution function for Si with a field of 50 kV/cm and at 300 K.