A CONSISTENCY TEST OF ENERGY TRANSPORT AND HYDRODYNAMIC MODELS

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Abstract

This paper proposes a scheme to test the consistency of various hydrodynamic models which have been developed so far. The basis of this test is that we can perform a self-consistent full Monte Carlo simulation on some test devices and therefore accurately evaluate each term in energy transport or hydrodynamic equations using ensemble averages. We have compared a few models for their consistency and also demonstrated the effect of different transport parameters on predicting macroscopic quantities of interest.

Testing Procedure

Although this test can be performed with any device, the the following results are based on the Monte Carlo (MC) simulation of an abrupt junction $n^+ - n^- - n^+$ silicon diode with an applied bias of 2 volts. This test device consists of an n^--region ($0.1\mu m < x < 0.5\mu m$) doped with $N_d = 2\times 10^{15} cm^{-3}$ which is sandwiched between two n^+ regions ($0 \leq x \leq 0.1\mu m, 0.5 \leq x \leq 0.6\mu m$) doped with $N_d = 5 \times 10^{17} cm^{-3}$.

The MC method has been used to accurately evaluate the $\phi(\vec{k})$-moments of the distribution function, $\int \phi(\vec{k}) f d\vec{k}$. A novel scheme developed by Lee and Tang [1],[2] has also been used to evaluate the moments of the collision term in the Boltzmann Transport equation (BTE), $\int \phi(\vec{k}) \left[\frac{\delta f}{\delta t}\right]_{coll} d\vec{k}$. The first-order moment of the BTE yields the momentum conservation equation,

$$\frac{1}{n}\nabla_{\vec{r}} \cdot (n\hat{U}) - \vec{F} = \vec{C_p} \tag{1}$$

where $\hat{U} \triangleq \langle \vec{v}\hbar\vec{k} \rangle$ and $\vec{C_p} \triangleq \int \hbar\vec{k} \left[\frac{\delta f}{\delta t}\right]_{coll} d\vec{k}/n$. In this equation, the energy tensor $\hat{U}$ can be evaluated at each point in the device by a time ensemble averaging scheme. The self-consistent MC simulation ensures that Poisson's equation is satisfied along with the BTE. Hence the electric field obtained through these simulations can be used to calculate $\vec{F}$. We perform the $\nabla_{\vec{r}}$ operation using a three point interpolation technique. We then compute each side of the Eq.(1) separately for the device and compare the two to see if the consistency exists without any modeling for $\hat{U}$ or $\vec{C_p}$. This is the first step in the procedure for the consistency test.

Testing of Charge Transport Models

All the models being compared here are for non-parabolic energy band structures, with the nonparabolicity factor $\alpha = 0.5eV^{-1}$. The same homogeneous mobility model μ^*, obtained from our own bulk MC simulations has been used in all the other models. The following empirical expression was used to model the mobility:

$$\frac{1}{\mu^*} = \frac{1}{1.34}\left[\sqrt{1 + \frac{N_d\left(0.73\left(\frac{W_o}{W}\right)^{32} + \frac{W_o}{W}\right)}{10^{17} + 0.05N_d}}\right.$$
$$\left. +25.8W - 0.9525 + \frac{[-1 + 6.5(W - W_o)]\,(W - W_o)^4}{0.005 + (W - W_o)^4}\right] \tag{2}$$

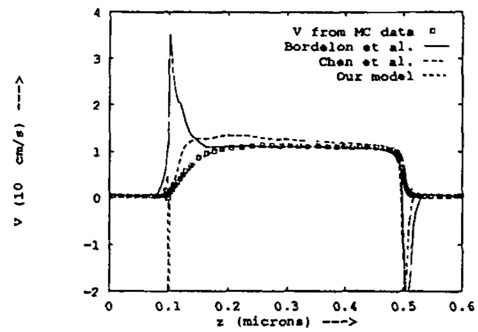

Figure 1: Comparison of $\vec{V}$ obtained from MC data with some of the models developed.

where N_d is the doping concentration in cm^{-3}, $W_o = \frac{3}{2}k_B T_o$ is the equilibrium lattice energy in eV and μ^* is expressed in $\frac{cm^2}{mV-sec}$. The empirical formula for μ^* given above is accurate for N_d ranging from $1 \times 10^{15} cm^{-3}$ to $3 \times 10^{18} cm^{-3}$ and for $W \geq 0.04eV$.

The following models were tested for consistency:

- Bordelon et al. [3]:

$$\vec{V} = \frac{\mu^*}{q}\left[\vec{F} - \frac{2}{3}WG(W)\frac{\nabla n}{n} - \frac{2}{3}H(W)\nabla W\right] \tag{3}$$

  where $G(W)$ and $H(W)$ are given by:

$$G(W) = \frac{1 + 2\alpha(1 + \alpha W)}{(1 + 2\alpha W)^2} \quad , \quad H(W) = \frac{1 + \alpha W}{1 + 2\alpha W} \tag{4}$$

- Chen et al. [4]:

$$\vec{V} = \frac{\mu^*}{q}\left[\vec{F} - k_B T_m \frac{\nabla n}{n} - \alpha_T \nabla(k_B T_m)\right] \tag{5}$$

  where $\alpha_T = \left[1 + \frac{T_m}{\mu^*}\frac{\partial \mu^*}{\partial T_m}\right]$, and T_m is given by

$$k_B T_m = \frac{1}{5\alpha}\left(-1 + \sqrt{1 + \frac{20}{3}\alpha W}\right) \tag{6}$$

- Our new model [5],[6]:

$$\vec{V} = \frac{\mu^*}{q}\left[\vec{F} - \hat{U} \cdot \frac{\nabla n}{n} - (1 - \lambda_p)\nabla \cdot \hat{U}\right] \tag{7}$$

  where $\hat{U} = \vec{V}\vec{P} + u(W)\hat{I}$, $\vec{P} = \langle \hbar\vec{k} \rangle = m_c\vec{V} + 2\alpha m_c\vec{S}$, $u(W) = -0.006 + 0.85W - 2.5W^2 + 13.43W^3 - 38.61W^4 + 42.81W^5$ and $\lambda_p = -0.2\frac{\nabla W}{|\nabla W|}e^{3.5\left(1 - \frac{W}{W_o}\right)} + 0.15$. The parameter λ_p represents the effect of the collision moment $\vec{C}_p$ deviating from homogeneous bulk data [6].

Comparison of the three results obtained from substituting the MC data in the right hand side of each model with the average velocity obtained directly from the MC method is shown in Fig.1.

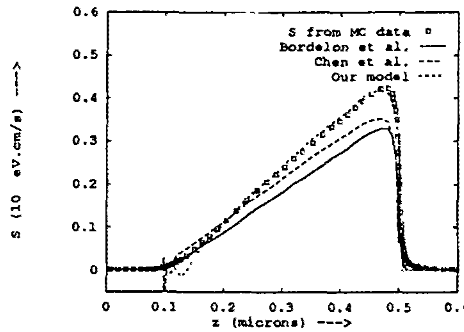

Figure 2: Comparison of $\vec{S}$ obtained from MC data with some of the models developed.

Testing of Energy Transport Models

The following models for the average energy flow $\vec{S} \triangleq \langle \varepsilon \vec{v} \rangle$ have been tested.

- Bordelon et al. [3]:

$$\vec{S} = \vec{V} W \tag{8}$$

- Chen et al. [4]:

$$\vec{S} = C_e \left[k_B T_m \vec{V} - \frac{k_B^2}{q} \mu^* T_m \nabla T_m \right] \tag{9}$$

where, according to its definition, $C_e = 1.95$ has been obtained from our bulk MC simulations.

- Our new model [5],[6]:

$$\vec{S} = -\frac{0.79\mu^*}{q} \left[(W\hat{I} + \hat{U}) \cdot q\vec{E} + \hat{R}\frac{\nabla n}{n} + (1 - \lambda_{ep}) \nabla \cdot \hat{R} \right] \tag{10}$$

where $\hat{R} \triangleq \langle \vec{v} \hbar \vec{k} \varepsilon \rangle = \vec{S}\vec{P} - 3.8W\hat{U} + r(W)\hat{I}$, $r(W) = -0.008 + 0.22W + 3.31W^2 - 5.53W^3 + 18.08W^4 - 22.37W^5$ and $\lambda_{ep} = -0.4\frac{\nabla W}{|\nabla W|} e^{3.5\left(1 - \frac{W}{W_o}\right)} + 0.2$. The parameter λ_{ep} represents the effect due to a difference between homogeneous and inhomogeneous third-moment collision terms of the BTE [6].

Fig.2 compares the three results obtained from substituting the MC data in the right hand side of each model with the average energy flow obtained directly from the MC method.

Effect of Different Transport Parameters

The consistency test can be used to determine the effect of different transport parameters on macroscopic quantities such as the average velocity and energy flow. For example, by using this method we can show that the modeling of the parameter λ_p is critical in predicting the average velocity profile in the device. Neglecting λ_p entirely causes an overestimation of $\vec{V}$ on the decreasing side of the velocity profile. However, as λ_p is increased, there is a distinct overestimation of the velocity on the increasing side of the velocity profile as seen in Fig.3.

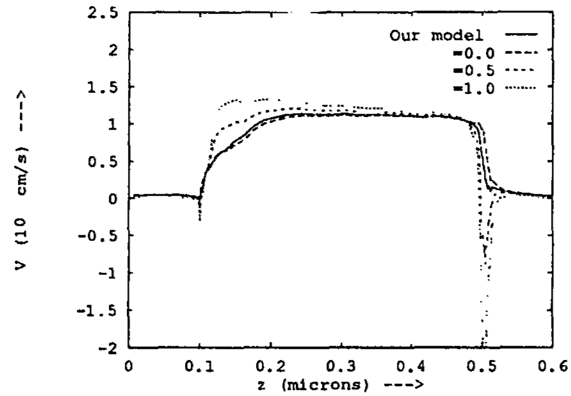

Figure 3: Average velocity using four different models for λ_p

In addition, this testing procedure can also be used to identify the approximations and errors introduced at each level of modeling. For example, by replacing the MC data for $\hat{U}$ on the left hand side of Eq.(1) by modeled data for $\hat{U}$, this test can tell us how the model affects the consistency of this equation.

Conclusion

We have developed a novel scheme to perform consistency checks on various hydrodynamic models. These tests can be used to predict the relative accuracy of each transport model. However, it must be remembered that the final solution of a coupled set of transport equations may be better than what the consistency tests indicate. This is because the solution of macroscopic equations is always a smooth function of position and sometimes errors introduced in different places might cancel each other.

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