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Introducing Energy Broadening in Semiclassical Monte Carlo Simulations

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In the past, several attempts have been made to introduce collisional broadening in semiclassical electron transport Monte Carlo (MC) simulations [1, 2]. The inclusion of energy non-conservation at each scattering event has produced non-physical instabilities. In this work we propose an algorithm which overcomes the difficulties encountered in previous approaches. Moreover, it is suitable for a direct implementation in device modelling, since it can be easily introduced in existing MC simulators. The scaling of device architecture will shortly require this effect to be taken into account in simulations.

In order to include energy broadening without losing long term energy conservation, one must consider the following:

1. That the overall energy in transport is conserved because the Hamiltonian for the total system of the electron(s) and phonons is time independent.
2. In an electron-phonon interaction the crystal-momentum conservation, in a homogeneous system, is guaranteed by the matrix elements.
3. An electron can be scattered to a state with an energy not given by the simple balance between the energy before scattering and the energy of the involved phonon. This is due to the fact that the final state, considered in transition, is an eigenstate of the unperturbed Hamiltonian, which is not a state of well defined energy in the total interacting system.

Therefore we may assume that the energy is conserved at each scattering event. In fact, in the two-time Wigner-function approach a frequency contribution is transferred to the electron equal to the frequency of the phonon [3]. But, we have to distinguish the true "frequency energy" of the electron E from the "momentum energy" E':

$$E' = \frac{p^2}{2m} \tag{1}$$

Because of collisions, the energy-momentum relation is no longer given by equation (1), but it broadens.

In this type of MC simulation, it is necessary to keep track of both E and E'. The energy exchanged at each scattering event is determined by the phonon frequency ω_{ph}, and the momentum exchanged is determined by the phonon wave-vector q. But, the final electron energy and electron momentum are not necessarily related by (1).

The energy spreading is related to the time between collisions via the Heisenberg uncertainty relation:

$$\sigma_{Ei} \approx \frac{\hbar}{t_i - t_{(i-1)}} \tag{2}$$

Where t_i is the time at which the i-th scattering event takes place.

The MC algorithm will then proceed as follows.

Initial state:

The semiclassical simulation starts at time $t = t_0$; the initial momentum p_0 is generated according to the thermal distribution, the initial energy E_0 is calculated according to (1).

Flights:

The duration $(t_i - t_{(i-1)})$ of the flights is determined, in a traditional way, according to the scattering probabilities, including self-scattering. The value of the momentum at the end of the flights is p_{ib} (where b stands for "before" the scattering event) and is determined classically. Starting from the value $p_{(i-1)a}$ "after" the previous scattering, the variation in the momentum can be calculated classically:

$$\Delta p_i = eF(t_i - t_{(i-1)}) \tag{3}$$

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Where F is the field (assumed to be constant and uniform within the flight) acting on the system. Under the action of the electric field, the variation $\Delta_f E_i$ of the energy during the i-th flight is determined by the distance Δz covered by the electron:

$$\Delta z_i = \frac{p_{(i-1)a}}{m}(t_i - t_{(i-1)}) + \frac{1}{2}\frac{eF}{m}(t_i - t_{(i-1)})^2 \quad (4)$$

The energy variation is therefore:

$$\Delta_f E_i = eF\Delta z_i \quad (5)$$

The energies at the end of each flight can be easily calculated from the above equation:

$$E_{ib} = E_{(i-1)a} + \Delta_f E_i \quad (6)$$

Scattering events:

Firstly, for simplicity, we limit ourselves to the case of scattering from non-polar optical and acoustic phonons, within the elastic approximation, and with deformation potential interaction.

At the time t_i a scattering event occurs. Before each scattering event the position can be calculated from equation (4), allowing a relatively simple implementation of this algorithm in a device simulation. At the scattering time t_i, a new energy E'_{ib} is defined, taking into account the energy broadening δE_i. This is chosen from a distribution determined using the standard deviation given by equation (2):

$$E'_{ib} = E_{ib} + \delta E_i \quad (7)$$

The new value of E'_{ib} is calculated based on the value of the true electron energy E_{ib}. The type of scattering is determined using the probabilities $P(E'_{ib})$. Applying this approach, the energy non conservation due to the flight duration is taken into account, affecting the type of process chosen as scattering. If self scattering is chosen, then the flight continues. If true scattering is chosen, the new values for the electron energy and momentum are determined as follows:

$$E_{ia} = E_{ib} \pm \hbar\omega_0 \quad (8)$$

$$E'_{ia} = E'_{ib} \pm \hbar\omega_0 \quad (9)$$

$$p_{ia} = \sqrt{\frac{E'_{ia}}{2m}} \quad (10)$$

The orientation of the momentum is chosen from an isotropic distribution; once p_{ia} is calculated then the q of the phonon is determined. The sign $\pm$ corresponds to an absorption or emission process.

The new energy E'_{ib} is calculated based on the value of the true electron energy E_{ib}, not on the previous E'_{ib}, so that the energy broadening is not propagated from one scattering event to the following ones. Moreover, no memory of the energy broadening that occurred in the previous scattering event is retained. The energy spreading given by equation (2) is calculated according to the time interval $(t_i - t_{(i-1)})$. With this approach, a physical collisional broadening is accounted for. This influences threshold processes, such as impact ionisation or oxide penetration. The overall energy conservation is, however, guaranteed and the stability of the system is achieved.

Initially this algorithm has been tested on bulk semiconductors, in order to understand the effect on threshold processes, before application to realistic device models.

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