Energy Conservation in Collisional Broadening

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1 Introduction

Electron-phonon coupling is central to semiconductor transport simulation. It is often treated in the simple Fermi's Golden Rule formulation, but even at modest fields, such as those commonly present in modern semiconductor devices, finite state lifetime effects become important. Such effects are treated formally by including self-energy in the scattering formulation [1, 2]. In order to make the problem more tractable, especially for efficient Monte Carlo simulation, various simplifying assumptions are made. The most common form is to assume a Lorentzian distribution. This assumption is well justified by perturbation theory, and is simple to calculate and implement. In the limit of infinite state life-time, it collapses to the energy-conserving delta function of the Fermi's Golden Rule. On the other hand, when non-zero broadening is present, energy is no longer conserved, and this has been noted in some cases to lead to accumulated broadening [3]. Such accumulation of energy can lead to non-physical results and push the electron energy distribution into the hot electron regime. Our goal is to explore the reasons for this accumulation of energy and propose remedies which can be implemented in standard simulation tools.

Problem Formulation

We will focus on optical phonon scattering and approximate the optical phonon energy to be a constant ω_o. Under this assumption, the Lorentzian distribution for the final energy after scattering takes the form of (1). The amount of broadening, represented by Γ, can be related by the Optical theorem [4] to the total electron scattering rate **R**, and the lifetime τ, as in (2).

$$P(E_f) = \frac{1}{\pi} \frac{\Gamma}{(E_f - E_i \pm \omega_o)^2 + \Gamma^2} \tag{1}$$

$$\Gamma(E_f) = \frac{\hbar}{2} R(E_i + \omega_o) = \frac{\hbar}{2\tau(E_f)} \tag{2}$$

Therefore, the value of final energy can be considered as a random variable, and a standard rejection technique can be employed to select the final energy according to the Lorentzian distribution. Under this view, we can also compute the expectation of the final energy for any initial energy level, and verify if the expected value matches the optical phonon energy; in other words, we can compute how much the final energy deviates from energy conservation in the average over many scatterings. This can be

expressed in the standard form, as in (3). At first glance, it seems like the expectation will be energy conserving, since the distribution is symmetric in energy, but due to the complex bandstructure, levels are distributed uniformly in momentum space, and non-uniformly in energy. Therefore we must convert the integral into an integral over momentum space (4), which is equivalent to an energy integral weighted by the density-of-states (DOS), as in (5).

$$< E_f >= \int d\vec{k} \frac{1}{\pi} \frac{\Gamma}{(E(\vec{k}) - E_i \pm \omega_o)^2 + \Gamma^2} \tag{3}$$

$$< E_f >= \frac{1}{\pi} \int \frac{E dE}{\mid \nabla_{\vec{k}} E(\vec{k}) \mid} \frac{\Gamma}{(E(\vec{k}) - E_i \pm \omega_o)^2 + \Gamma^2} \tag{4}$$

$$< E_f >= \frac{1}{\pi} \int \frac{E\, g(E) \Gamma(E)}{(E - E_i \pm \omega_o)^2 + \Gamma(E)^2} dE \tag{5}$$

This formulation allows us to compute the difference between the expected value of the final energy and the energy conserving value, which is equal to initial plus phonon energy $\tilde{E}_f = E_i \pm \omega_o$.

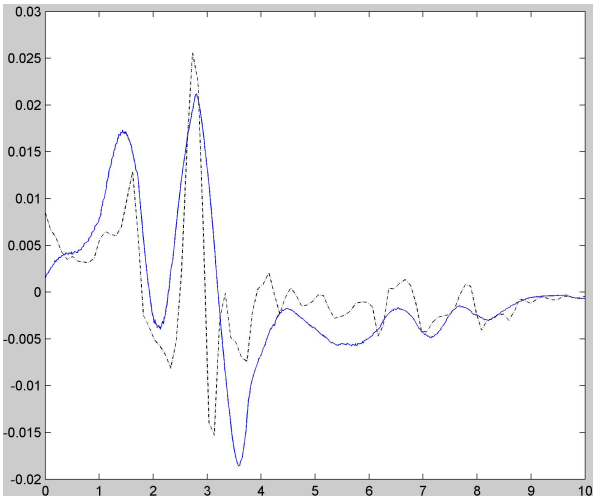

Figure 1: Numerically computed expected value of departure from energy conservation, shown by solid line, and derivative of the DOS, dashed line. Values are in meV. Note that, especially at higher electron energies, several meV of energy can be accumulated at each scattering event. This can lead to large unphysical energies in the simulation because energy conservation is not upheld. The striking similarity of the curves demonstrates that the departure from energy conservation at each scattering is due to non-uniform spacing of energy levels and large slopes of the DOS curve, especially at higher energies.

2 Discussion

The relevant parameters, such as the DOS can be computed numerically from realistic energy band-structure for most semiconductors of interest. The integration over energy can then be performed by quadrature to plot the expected, or average, value of departure from energy conservation as a function of initial energy, shown in Fig. 1. The resulting plot can be compared to the gradient of the DOS in order to explain the effect of loss of energy conservation. The plots are very similar because a slope in the DOS will cause a net difference of the effect of broadening for different energies, causing the average departure from energy conservation to be non-zero. In order to correct this problem, various solutions have been proposed, such as storing the amount of broadening at each scattering event in the simulation, and subtracting away this broadening at the following scattering event. This was termed Non-Accumulated Broadening (NAB) [5]. This procedure removes unphysical drift toward high energies, but also prevents the full impact of quasi-particle states to be explored. A better solution is to correct the Lorentzian distribution and divide it by the DOS curve, Fig. 3, in order to arrive at an energy distribution which is energy conserving in the average over many particles/scattering events. This idea can be termed a Corrected Distribution (CD) approach. Both of these techniques have been implemented into a Monte Carlo (MC) simulation and their impact on the electron distribution as well as overall energy conservation explored.

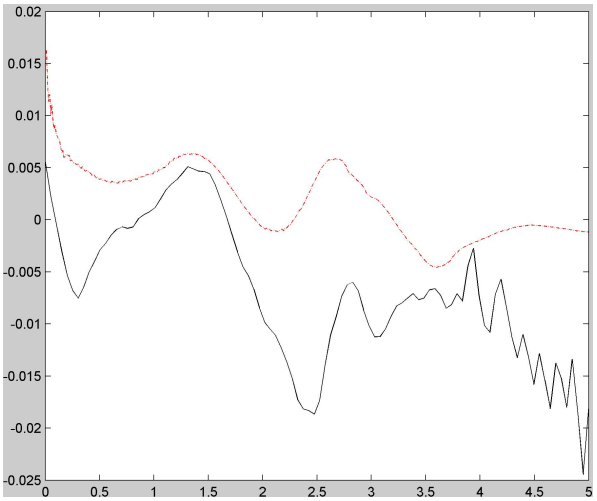

Figure 2: Plot of energy broadening extracted from a full-band Monte Carlo simulation (solid line). The deviation from energy conservation follows the same trends as the numerically computed expected value of final energy (dashed line). This demonstrates that final energies in Monte Carlo simulation including collisional broadening obey the expected trend and need to be corrected by the DOS.

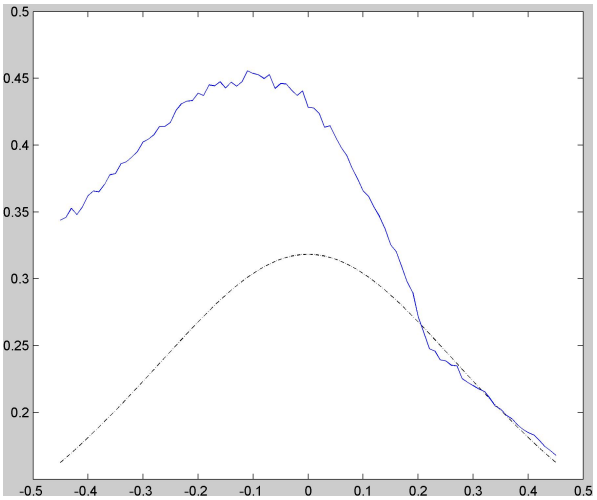

Figure 3: Plot of corrected (solid line) and original (dashed line) lorentzian broadening distribution. The corrected distribution is scaled by the DOS in order to offset the effect of non-uniform level spacing, or degeneracy, and produce a distrubution that will conserve energy on the average over many scattering events.

3 Acknowledgment

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