

# Implementation of a two-particle Monte Carlo method for the treatment of electron-electron scattering in semiconductors

by

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Submitted to the Department of Microelectronics  
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## Abstract

In this thesis a Monte Carlo (MC) simulator is implemented in Python that focuses on electron-electron scattering (EES). Simulating the EES events is an exciting challenge because two electrons are affected simultaneously. In case of EES the Boltzmann transport equation (BTE), which is the mathematical model that describes the time evolution of the momentum and real space distribution of electrons in a semiconductor becomes non linear. Therefore the two-particle kinetic equation is used instead of the BTE. It is linear for the two-particle distribution function. Earlier attempts were made to solve the non-linear BTE where only one particle was simulated and the partner electron's momentum distribution was assumed. Contrary to this approach in this thesis the trajectory of both involved electrons are sampled and no assumptions about the distribution function need to be made. The derivation of the phonon scattering rates and the EES rates used in the algorithm is shown. It is based on quantum mechanics and its entry point is Fermi's golden rule. The MC algorithm with its adoptions for including EES is explained. Sampling and selection of scatter mechanisms is discussed. The algorithm is used to do stationary and transient simulations in bulk silicon. The stationary ones show the velocity and energy distributions as well as the mean velocity and energy as a function of the electric field. Regardless of whether EES is taken into account or not, stationary simulations bring identical results. In the transient case step response functions and relaxation processes are simulated. The relaxation process is the only simulation case where the consideration of EES shows an significant effect. Due to EES hot electrons entering a cold domain relax much faster.

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## Kurzfassung

In dieser Diplomarbeit wird ein Monte Carlo (MC) Simulator in Python implementiert, der speziell zur Untersuchung von Elektron-Elektron-Streuung (EES) konzipiert worden ist. Es ist eine Herausforderung EES zu simulieren, da immer zwei Elektronen gleichzeitig von der Streuung betroffen sind. Die zeitliche Entwicklung der Orts- und Impulsverteilung der Elektronen in einem Halbleiter wird mittels der Boltzmann-Transportgleichung (BTE) beschrieben. Durch die Berücksichtigung von EES in der Gleichung, wird die BTE nichtlinear. Daher wird anstelle der BTE die kinetische Zwei-Teilchen-Gleichung verwendet. Diese ist linear in der Zweiteilchen-Verteilungsfunktion. Es gab bereits Versuche, die nichtlineare BTE zu lösen, indem nur ein Teilchen simuliert und die Impulsverteilung des Partnerelektrons angenommen wurde. Im Gegensatz dazu wird in dieser Arbeit die Flugbahn beider beteiligter Elektronen abgetastet, und es müssen keine Annahmen über die Verteilungsfunktion getroffen werden. Die Herleitung der Phononenstreuraten und EES-Raten basiert auf der Quantenmechanik. Ausgangspunkt dafür ist die goldenen Regel von Fermi. Die einzelnen Teilschritte des Algorithmus, wie die Wahl der Abtastpunkte oder die Wahl des Streumechanismus werden dargelegt. Auch die Erweiterungen vom Einteilchen-MC-Algorithmus zum Zweiteilchen-MC-Algorithmus, die nötig sind um EES zu simulieren, werden erklärt. Anschließend wird der Algorithmus verwendet, um stationäre und transiente Simulationen in Bulk-Silizium durchzuführen. Die Ergebnisse der stationären Simulationen zeigen die Geschwindigkeits- und Energieverteilungen sowie die mittlere Geschwindigkeit und Energie als Funktion des elektrischen Feldes. In den Ergebnissen der stationären Simulationen ist kein Einfluss durch EES zu erkennen. Im transienten Fall wurden Sprungantwortfunktionen und Relaxationsvorgänge simuliert. Der Relaxationsprozess ist der einzige Simulationsfall, bei dem die Berücksichtigung von EES einen signifikanten Effekt zeigt. Durch EES relaxieren Elektronen, die von einem heißeren in ein kälteres Gebiet kommen, deutlich schneller.

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# Chapter 1

## Introduction

MC methods solve complex problems with the help of statistics. In semiconductor physics they are used to simulate the movement of charge carriers. A physical model that describes the carrier transport is the BTE. It is remarkable that an algorithm based on statistics leads to a solution for the BTE, a integro-differential equation [4][5].

### 1.1 Motivation

Most of the MC algorithms have been designed to study the interactions of an electron ensemble with the environment such as crystal vibrations, dopants and impurity atoms. They neglect interactions between the individual carriers. The interaction between two electrons results in physical phenomena like EES. In order to study these phenomena, modifications to the standard one-particle MC algorithm have to be made. This thesis focuses on charge transport in the presence of EES. Since this type of scattering involves two electrons, the approach used calculates a pair of two electron trajectories simultaneously instead of just one. Also the probability of scattering depends on the momenta of two electrons.

## 1.2 Transport model

The path of the electron is calculated by solving the classical equations of motion

$$\frac{\partial \mathbf{r}}{\partial t} = \mathbf{v}, \quad \frac{\partial \mathbf{v}}{\partial t} = \frac{\mathbf{F}}{m}, \quad \mathbf{F}(t) = \mathbf{E}(t)e \quad (1.1)$$

and gets interrupted by scattering events. Those scattering events happen at random times and instantaneously. The probability of scattering is calculated quantum mechanically. The transport model is termed semi-classical [3].

## 1.3 Algorithms

MC algorithms for the solution of the BTE can be divided into stationary and transient ones.

Stationary algorithms are useful to predict physical quantities of an electron ensemble under time-independent conditions. An example would be an ensemble in a bulk material accelerated by a constant electric field. It is sufficient to calculate only the trajectory of one electron of the ensemble, since the time mean values of one electron are equal to the ensemble mean values. The difference between sample mean and time mean can be seen in Figure 1-1. Trajectory calculation continues until the desired precision is achieved. Finally, the sample values will be averaged, to determine the mean values.

In order to investigate the time dependence of the physical quantities of an electron ensemble, transient algorithms are used. The trajectories of many ensemble electrons will be sampled during a given simulation time with equidistant time steps. Then at each sampling point in time the physical quantities of the ensemble electrons will be averaged. In this way the time evolution of the ensemble's physical quantities can be found. An example would be to study the behavior of an electron ensemble responding to an electric field step in time.

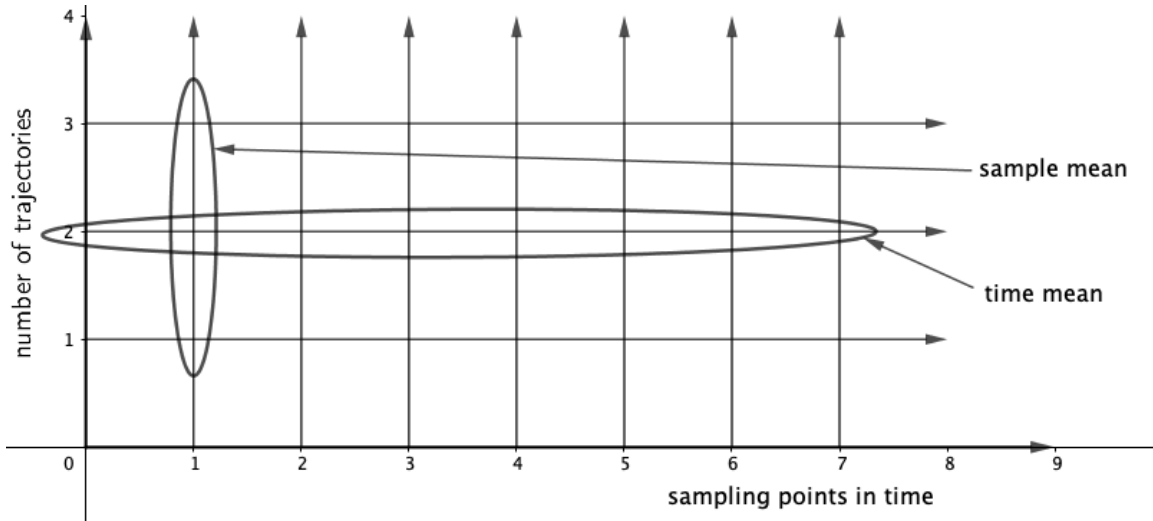


Figure 1-1: Sample mean versus time mean

## Approximations

In this thesis two approximations will be considered. The parabolic band approximation,  $E(\mathbf{k}) = \hbar^2|\mathbf{k}|^2/(2m)$  approximates the full band dispersion relation at its minimum by a parabola. The second assumption concerns the distribution function  $f(\mathbf{k})$ , which is the probability that an electron occupies a state with a certain wave vector  $\mathbf{k}$ . The Pauli blocking factor  $(1 - f(\mathbf{k}))$  will be neglected,  $(1 - f(\mathbf{k})) \approx 1$  since the occupation of the conduction band states is small enough if the electron density is not too high. For a energy range close to the conduction band edge and moderate electron density both approximations are valid.

## 1.4 Outline

In Chapter 2 the transport equations will be discussed. The BTE is the fundamental equation that describes the time evolution of the particle distribution in momentum and real space. In the case of EES the equation becomes nonlinear. To avoid this nonlinearity the two particle kinetic equation will be introduced, which is linear in the two particle distribution.

In Chapter 3 the scattering rates used in the MC algorithm will be derived. The calculation of the electron state after scattering as well as the used parameter values

are given.

Chapter 4 describes the implementation of the MC algorithm. Different topics like the flight time evaluation, calculation of state after the flight, sampling techniques and scattering type selection will be explained. Also the adaptations needed to include EES are described.

Chapter 5 shows some results from the simulator implemented in this work.

# Chapter 2

## Transport equations

### 2.1 Boltzmann transport equation

The Boltzmann equation (2.1) is an integro-differential equation which describes the carrier distribution in semiconductors [5, chapter 3], [7, chapter 1], [3, chapter 1], [10, chapter 4]. If a function  $f(\mathbf{k}, \mathbf{r}, t)$  can be found that solves the equation, one knows how many gas particles are at a certain place with a certain momentum at a certain time. Electrons in semiconductor materials can also be modeled as gases (electron-gases). By knowing the distribution function and how it evolves in time, many physical quantities can be found and studied, such as electron density, current density, mean energy, mean velocities and the like.

$$\left( \frac{\partial}{\partial t} + \sum_{n=1}^3 \left( v_n \frac{\partial}{\partial r_n} + \frac{F_n}{\hbar} \frac{\partial}{\partial k_n} \right) \right) f(\mathbf{r}, \mathbf{k}, t) = \hat{Q}f(\mathbf{r}, \mathbf{k}, t) \quad (2.1)$$

Newton's law  $\mathbf{F} = \dot{\mathbf{p}}$  and the relation  $\mathbf{p} = \hbar\mathbf{k}$  lead to  $d\mathbf{k}/dt = \mathbf{F}/\hbar$ , whereas  $d\mathbf{r}/dt = \mathbf{v}$  is the particle velocity. The left hand side of the equation (2.1) represents the total derivative of  $f$  with respect to time. In this case every variable is time dependent and therefore the derivative is also called a convective derivative.

$$\frac{\partial f(\mathbf{k}(t), \mathbf{r}(t), t)}{\partial t} = \sum_{n=1}^3 \left( \frac{\partial f}{\partial k_n} \frac{\partial k_n}{\partial t} + \frac{\partial f}{\partial r_n} \frac{\partial r_n}{\partial t} \right) + \frac{\partial f}{\partial t} \quad (2.2)$$

If the right hand side of the BTE is set to zero, Liouville's equation is obtained. It describes a collisionless system of particles. In the BTE the scattering operator  $\hat{Q}$  describes collisions and is responsible for discontinuities in time of the electron momentum  $\mathbf{p}(t)$ .

### 2.1.1 Scattering operator

An operator  $\hat{O}$  is a mathematical object similar to a function. Unlike functions that transfer input values into output values, operators transform functions. If the operator  $\hat{O}$  acts on a certain function  $f_1$ , another function is received:  $f_2 = \hat{O}f_1$ .

The scattering operator  $\hat{Q}$  is an integral operator  $\hat{O}$  of the form

$$\hat{O}[f](\xi) = \int K(\xi, \xi')f(\xi')d\xi' \quad (2.3)$$

The function  $K(\xi, \xi')$  is called the kernel of the integral operator. The operator (2.3) is linear:  $\hat{O}[\alpha f + \beta g] = \alpha\hat{O}[f] + \beta\hat{O}[g]$ . In case of the BTE the scattering operator acts on the momentum distribution function  $f(\mathbf{r}, \mathbf{k}, t)$ , and its kernel is the transition rate. The operator can be split in a gain and a loss term:

- The gain term increases the occupation of a given electron state,
- The loss term decreases the occupation of an electron state.

$$\hat{Q}[f](\mathbf{k}_i) = \hat{Q}_{gain} - \hat{Q}_{loss} = \int P(\mathbf{k}_i, \mathbf{k}_f)f(\mathbf{k}_f)d\mathbf{k}_f - \int P(\mathbf{k}_f, \mathbf{k}_i)f(\mathbf{k}_i)d\mathbf{k}_f \quad (2.4)$$

Since  $f(\mathbf{k}_i)$  is a constant regarding the integration over  $\mathbf{k}_f$ , the loss term can be written as  $\Gamma(\mathbf{k}_i)f(\mathbf{k}_i)$  with  $\Gamma(\mathbf{k}_i) = \int P(\mathbf{k}_i, \mathbf{k}_f)d\mathbf{k}_f$  being the total scattering rate.

The Boltzmann equation then becomes

$$\frac{df(\mathbf{k}_i(t))}{dt} + \Gamma(\mathbf{k}_i(t))f(\mathbf{k}_i(t)) = Q_{gain}[f](\mathbf{k}_i(t)) \quad (2.5)$$

A formal way to solve this equation is recursive integration.



## Scattering Operator for EES

In contrast to an electron-phonon scattering event, where only one electron changes its state, in an EES event two electrons change their states simultaneously. The initial and final  $\mathbf{k}$ -vectors of electron 1 and electron 2 will be denoted by  $\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2$ . In this case gain and loss terms become

$$\begin{aligned}\hat{Q}_{gain}[f](\mathbf{k}_i^1) &= \int \underbrace{\left( \int \int P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2) f(\mathbf{k}_f^2) d\mathbf{k}_i^2 d\mathbf{k}_f^2 \right)}_{K(\mathbf{k}_i^1, \mathbf{k}_f^1)} f(\mathbf{k}_f^1) d\mathbf{k}_f^1 \\ \hat{Q}_{loss}[f](\mathbf{k}_i^1) &= \int \underbrace{\left( \int \int P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2) f(\mathbf{k}_i^2) d\mathbf{k}_i^2 d\mathbf{k}_f^2 \right)}_{K(\mathbf{k}_i^1, \mathbf{k}_f^1)} f(\mathbf{k}_i^1) d\mathbf{k}_f^1\end{aligned}\quad (2.6)$$

The kernel is no longer constant, but depends on the solution  $f$ . Therefore, the scattering operator is nonlinear which complicates the numerical solution of the BTE.

## 2.2 Two particle kinetic equation

In order to receive a linear operator for EES, both single electron momentum distributions need to be combined  $f(\mathbf{k}_1)f_2(\mathbf{k}_2) \rightarrow g(\mathbf{k}_1, \mathbf{k}_2)$  [2].

$$\hat{Q}_{ee}[g](\mathbf{k}_i^1, \mathbf{k}_i^2) = \int \int P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2) [g(\mathbf{k}_f^1, \mathbf{k}_f^2) - g(\mathbf{k}_i^1, \mathbf{k}_i^2)] d\mathbf{k}_f^1 d\mathbf{k}_f^2 \quad (2.7)$$

A kinetic equation for the two electron distribution can be derived as

$$\left( \frac{\partial}{\partial t} + \sum_{n=1}^3 F_n \left( \frac{\partial}{\partial k_n^1} + \frac{\partial}{\partial k_n^2} \right) \right) g(\mathbf{k}^1, \mathbf{k}^2, t) = \left( \hat{Q}_{ph} + \hat{Q}_{ee} \right) [g](\mathbf{k}^1, \mathbf{k}^2, t) \quad (2.8)$$



# Chapter 3

## Scattering

In a semiconductor crystal, electrons experience different scattering mechanisms. In this work the focus is put on electron-phonon scattering, which is most dominant, and the interaction between two electrons (EES).

The likelihood that an electron changes its state from an initial state  $|\mathbf{k}_i\rangle$  to a final state  $|\mathbf{k}_f\rangle$  is described by Fermi's golden rule.

$$P(\mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} |\langle \mathbf{k}_f | V | \mathbf{k}_i \rangle|^2 \delta(\epsilon_{\mathbf{k}_f} - \epsilon_{\mathbf{k}_i} \pm \hbar\omega_0) \quad (3.1)$$

The matrix-element  $\langle \mathbf{k}_f | V | \mathbf{k}_i \rangle$  quantifies how similar an initial state  $|\mathbf{k}_i\rangle$  on which the potential  $V$  acts is compared to a specific final state  $|\mathbf{k}_f\rangle$ . It gets evaluated by the scalar product, which becomes one for parallel state vectors and zero for orthogonal state vectors. If the scattering potential is time-dependent, there will be an energy transfer of the magnitude  $\hbar\omega_0$ , where  $\omega_0$  is the oscillation frequency of the potential. For stationary potentials there is no energy transfer. The rate that one electron leaves its state is given by the sum over all transition rates to other states,  $\Gamma(\mathbf{k}_i) = \sum_{\mathbf{k}_f} P(\mathbf{k}_i, \mathbf{k}_f)(1 - f(\mathbf{k}_f))$ . By using the density of states this can be written as an integral.

$$\Gamma(\mathbf{k}_i) = \frac{\Omega}{(2\pi)^3} \int P(\mathbf{k}_i, \mathbf{k}_f)(1 - f(\mathbf{k}_f)) d\mathbf{k}_f \quad (3.2)$$

## Normalization volume and density of states

The volume of the crystal is arbitrary and denoted by  $\Omega$ . The probability of finding an electron or phonon inside the crystal is given by the integral over the probability density  $|\Psi(\mathbf{r})|^2$  and is set to one  $\int_{\Omega} |\Psi(\mathbf{r})|^2 d\mathbf{r} = 1$ . To achieve this the plane wave functions  $\exp(\mathbf{k} \cdot \mathbf{r})$  representing the particles need to be scaled by the square root of the volume  $\Psi(\mathbf{r}) = \exp(\mathbf{k} \cdot \mathbf{r})/\sqrt{\Omega}$ .

The density of states  $g$  is an expression for the available states in an infinitesimal energy or wave number range around a specific energy or wave number. It is used to calculate how many states  $n$  are in an certain energy or wave number range

$$n = \int_{k_{start}}^{k_{end}} g(k) dk = \int_{\epsilon_{start}}^{\epsilon_{end}} g(\epsilon) d\epsilon. \quad (3.3)$$

To fulfill Schrödinger's equation with its boundary conditions in a finite crystal only discrete  $k$  values are allowed. In a three dimensional crystal wave numbers are equally spaced. One state takes up the volume  $(2\pi)^3/\Omega$ . The density of states  $g$  therefore writes as

$$g(k) = \Omega/(2\pi)^3 \quad (3.4)$$

To find the density of states as a function of energy, one starts by calculating how many states can fit in a sphere with the radius  $k$  and the volume  $4\pi k^3/3$ .

$$n = \frac{4\pi k^3}{3} \frac{\Omega}{(2\pi)^3} \quad (3.5)$$

Then one needs to insert the dispersion relation  $k = \sqrt{2m\epsilon}/\hbar$  to make the expression depending on the energy instead of the wave number.

$$n = \frac{\Omega(2m\epsilon)^{3/2}}{6\hbar^3 \pi^2} \quad (3.6)$$

The derivative  $\partial n/\partial \epsilon$  then gives the density of states

$$g(\epsilon) = \frac{(2m^*)^{3/2} \sqrt{\epsilon}}{4\pi^2 \hbar^3} \quad (3.7)$$

## 3.1 Electron-phonon scattering

Phonons are quantized lattice vibrations. There exist acoustic and optical phonon modes. They differ in their dispersion relation. In order to calculate the allowed oscillations, the connections of the atoms in the crystal are modeled as linear springs. The balance of forces is expressed by a difference equation, which has plane wave solutions of the form  $e^{j\mathbf{k}\cdot\mathbf{r}}$ . It turns out that only plane waves with certain  $\mathbf{k}$ -values can exist in the crystal [1].

The displacement  $\mathbf{R}$  of an atom at place  $\mathbf{r}$  in the crystal is expressed by the sum over all eigenmodes.

$$\mathbf{R}(\mathbf{r}, t) = \sum_{\mathbf{q}} \sqrt{\frac{\hbar}{2\rho\Omega\omega_{\mathbf{q}}}} (\hat{a}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}^{\dagger}) e^{j\mathbf{q}\cdot\mathbf{r}} \quad (3.8)$$

In this equation the quantum mechanical operators of creation and annihilation of a phonon are denoted by  $\hat{a}^{\dagger}$  and  $\hat{a}$ . The mass density of the crystal is denoted by  $\rho$  and the phonon frequency by  $\omega_{\mathbf{q}}$ .

### Acoustic phonon scattering

The Hamiltonian  $\hat{H}$  is proportional to lattice strain  $\nabla \cdot \mathbf{R}(\mathbf{r}, t)$  and the phenomenological deformation potential  $D_A$ .

$$\hat{H} = D_A \nabla \cdot \mathbf{R}(\mathbf{r}, t), \quad \hat{H} = \sum_{\mathbf{q}} j\mathbf{q} D_A \sqrt{\frac{\hbar}{2\rho\Omega\omega_{\mathbf{q}}}} (a_{\mathbf{q}} + a_{-\mathbf{q}}^{\dagger}) e^{j\mathbf{q}\cdot\mathbf{r}} \quad (3.9)$$

The matrix element of the combined system [9] considers the change of the phonon state as well as the electron state. The initial, the final and the momentum transfer wave vectors are denoted by  $\mathbf{k}_i$ ,  $\mathbf{k}_f$  and  $\mathbf{q}$  respectively.

$$\langle \mathbf{k}_f, n_{\mathbf{q}} \pm 1 | \hat{H} | \mathbf{k}_i, n_{\mathbf{q}} \rangle = j\mathbf{q} D_A \sqrt{\frac{\hbar}{2\rho\Omega\omega_{\mathbf{q}}}} \sqrt{n_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2}} \delta(\mathbf{k}_f - \mathbf{k}_i \pm \mathbf{q}) \quad (3.10)$$

Inserting the matrix element (3.10) into the golden rule (3.1) gives

$$P(\mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} q^2 D_A^2 \frac{\hbar}{2\rho\Omega\omega_{\mathbf{q}}} \left( n_{\mathbf{q}} + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\mathbf{k}_f - \mathbf{k}_i \pm \mathbf{q}) \delta(\epsilon_{\mathbf{k}_f} - \epsilon_{\mathbf{k}_i} \mp \hbar\omega_{\mathbf{q}}) \quad (3.11)$$

The average number  $n_{\mathbf{q}}$  of phonons with a certain energy  $\hbar\omega_{\mathbf{q}}$  is given by the Bose-Einstein statistics

$$n_{\mathbf{q}} = \frac{1}{\exp\left\{\frac{\hbar\omega_{\mathbf{q}}}{k_B T} - 1\right\}} \quad (3.12)$$

The delta functions represent momentum and energy conservation.

$$\mathbf{k}_f = \mathbf{k}_i \pm \mathbf{q}, \quad \epsilon_{\mathbf{k}_f} = \epsilon_{\mathbf{k}_i} \mp \hbar\omega_{\mathbf{q}} \quad (3.13)$$

The two cases of phonon emission and absorption are considered by the upper and lower sign respectively. The delta functions can be substituted into one equation by using the dispersion relation  $E(\mathbf{k}) = \mathbf{k}^2 \hbar^2 / 2m$

$$\frac{\mathbf{k}_f^2 \hbar^2}{2m} = \frac{(\mathbf{q}^2 \pm 2\mathbf{q} \cdot \mathbf{k}_i + \mathbf{k}_i^2) \hbar^2}{2m}, \quad \frac{\mathbf{k}_f^2 \hbar^2}{2m} = \frac{\mathbf{k}_i^2 \hbar^2}{2m} \pm \hbar\omega_{\mathbf{q}}, \quad (3.14)$$

$$\delta\left(\frac{\hbar^2 q^2}{2m} \pm \frac{\hbar^2 q k_i \cos \vartheta}{m} \pm \hbar\omega_{\mathbf{q}}\right) \quad (3.15)$$

At this point two approximations are made:

- $\hbar\omega_{\mathbf{q}} \ll k_B T$  makes the transition an elastic one, which means  $\hbar\omega_{\mathbf{q}}$  can be neglected in (3.14).
- $n_{\mathbf{q}} \gg 1$  hence  $n_{\mathbf{q}} \approx n_{\mathbf{q}} + 1$  this allows to express  $(n_{\mathbf{q}} + 1/2 \pm 1/2) \approx k_B T / \hbar\omega_{\mathbf{q}}$  in (3.14).  $n_{\mathbf{q}} \approx k_B T / \hbar\omega_{\mathbf{q}}$  follows from the linearization of (3.12)

With these approximations the delta functions in (3.15) can be written as

$$\frac{k_i}{qE(k_i)} \delta\left(\frac{q}{2k_i} \pm \cos \vartheta\right) \quad (3.16)$$

The transition rate (3.1) becomes then

$$P(\mathbf{k}_i, \mathbf{k}_f) = \frac{\pi D_A^2 q^2 k_B T}{\rho \Omega \omega_{\mathbf{q}}} \frac{k}{\hbar \omega_{\mathbf{q}}} \frac{1}{q E(k_i)} \delta \left( \frac{q}{2k_i} \pm \cos \vartheta \right) \quad (3.17)$$

The scattering rate is found according to (3.2), with the speed of sound  $u_L = \omega_{\mathbf{q}}/q$ .

The integration is done in spherical coordinates.

$$\Gamma(\mathbf{k}_i) = \frac{\pi D_A^2 k_B T}{\hbar \Omega u_L^2 \rho} \frac{k}{E(k)} \frac{\Omega}{(2\pi)^3} \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{q} \delta \left( \frac{q}{2k} \pm \cos \vartheta \right) d\varphi d\vartheta dq \quad (3.18)$$

The scattering rate is finally attained by

$$\Gamma(\mathbf{k}_i) = \frac{2\pi D_A^2 k_B T}{\hbar u_L^2 \rho} \frac{(2m^*)^{3/2} \sqrt{\epsilon_{\mathbf{k}_i}}}{4\pi^2 \hbar^3} \quad (3.19)$$

The scattering rate contains the expression for the density of states (3.7) and is proportional to it

$$\Gamma(\mathbf{k}_i) = \frac{2\pi D_A^2 k_B T}{\hbar u_L^2 \rho} g(\epsilon) \quad (3.20)$$

## Intervalley phonon scattering

Electrons that scatter into other valleys involve phonons with wavenumbers close to the edge of the Brillouin zone, where the dispersion relation  $\omega_{\mathbf{q}}$  is independent of  $q$ . The scattering potential is proportional to the lattice displacement  $\hat{H} = \mathbf{D} \cdot \mathbf{R}(\mathbf{r}, t)$ . This scattering type is called non-polar optical phonon scattering [9].

$$\hat{H} = \sum_{\mathbf{q}} (D_t K) \sqrt{\frac{\hbar}{2\rho\Omega\omega_{\mathbf{q}}}} (\hat{a}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}^\dagger) e^{j\mathbf{q} \cdot \mathbf{r}} \quad (3.21)$$

By performing similar operations as done for the acoustic phonons the golden rule evaluates as

$$P(\mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} (D_t K)^2 \frac{\hbar}{2\rho\Omega\omega_0} \left( n_0 + \frac{1}{2} \pm \frac{1}{2} \right) \delta \left( \frac{\hbar^2}{2m} \pm \frac{\hbar^2 q k \cos \vartheta}{m} \pm \hbar\omega_0 \right) \quad (3.22)$$

In contrast to the acoustic phonons, in this case  $\hbar\omega_{\mathbf{q}}$  can not be neglected. The parameters  $n_{\mathbf{q}}$  and  $\omega_{\mathbf{q}}$  are assumed to be independent of  $\mathbf{q}$  and therefore will be denoted as  $n_0$  and  $\omega_0$ . The scattering rate is found according to (3.2). The integration is done in spherical coordinates

$$\Gamma(\mathbf{k}_i) = \frac{(D_t K)^2}{8\pi^2 \rho \omega_0} \int_0^\infty \int_0^\pi \int_0^{2\pi} \delta\left(\frac{\hbar^2}{2m} \pm \frac{\hbar^2 q k \cos \vartheta}{m} \pm \hbar\omega_0\right) d\varphi d\vartheta dq \quad (3.23)$$

The scattering rate is finally attained by

$$\Gamma(\mathbf{k}_i) = \frac{\pi(D_t K)^2}{\rho \omega_0} \left(n_0 + \frac{1}{2} \pm \frac{1}{2}\right) \frac{(2m^*)^{3/2} \sqrt{\epsilon_{\mathbf{k}_i} \pm \hbar\omega_0}}{4\pi^2 \hbar^3} \quad (3.24)$$

The scattering rate contains the expression for the density of states (3.7) and is proportional to it

$$\Gamma(\mathbf{k}_i) = \frac{\pi(D_t K)^2}{\rho \omega_0} \left(n_0 + \frac{1}{2} \pm \frac{1}{2}\right) g(\epsilon_{\mathbf{k}_i} \pm \hbar\omega_0). \quad (3.25)$$



## Implemented equations and parameters

Equation (3.26) shows the implemented scattering rate for electron-acoustic phonon scattering and equation (3.27) for electron-intervalley scattering. The parameters in Table 3.1 are taken from [4].

$$\Gamma_{e,ac} = \frac{2^{1/2} m^{3/2} K_B T_0 D_A^2}{\pi \hbar^4 u_L^2 \rho} \sqrt{\epsilon} \quad (3.26)$$

The energy gained or lost by intervalley scattering is given by  $\hbar\omega_i$ , the related parameter is given by the temperature  $\theta_i$ . The number of phonons is given by the Bose-Einstein statistics  $N_i = (e^{\theta_i/T} - 1)^{-1}$ .

By looking at the conduction band energy as a function of the wave vector direction, one can identify three valleys, with different deformation potentials for g- and f-processes. Scattering processes which happen along the axis of motion are called g-processes, perpendicular to it, f-processes. For f-processes there exist four equivalent final valleys,  $Z_f = 4$ , for g-processes only one,  $Z_f = 1$ .

$$\begin{bmatrix} \Gamma_{e,abs} \\ \Gamma_{e,ems} \end{bmatrix} = \frac{(D_t K)_i^2 m^{3/2} Z_f}{2^{1/2} \pi \hbar^3 \rho \omega_i} \begin{bmatrix} N_i \\ N_i + 1 \end{bmatrix} \sqrt{\epsilon \pm \hbar\omega_i} \quad (3.27)$$

Parameter	value	Parameter	value
$(D_t K)_{g1}$	$0.5 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{g1}$	140 K
$(D_t K)_{g2}$	$0.8 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{g2}$	215 K
$(D_t K)_{g3}$	$11 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{g3}$	720 K
$(D_t K)_{f1}$	$0.3 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{f1}$	220 K
$(D_t K)_{f2}$	$2 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{f2}$	550 K
$(D_t K)_{f3}$	$2 \times 10^8 \text{ eV cm}^{-1}$	$\theta_{f3}$	685 K
$Z_f$ for g-process	1	$u_L$	$9 \times 10^5 \text{ cm s}^{-1}$
$Z_f$ for f-process	4	$D_A$	9 eV
$m$	$0.3 m_0$	$m_0$	$9.109\,383\,701\,5 \times 10^{-28} \text{ g}$
$\rho$	$2.33 \text{ g/cm}^3$		

Table 3.1: Parameter for silicon [4]

## State after scattering

For acoustic phonons, where the electron does not gain or lose energy during the scattering event, only the direction of the momentum changes. The new direction is the result of the uniformly distributed random numbers  $\varphi \in [0, 2\pi]$  and  $\cos \vartheta \in [-1, 1]$

$$k_x = |\mathbf{k}| \sin \vartheta \cos \varphi \quad (3.28a)$$

$$k_y = |\mathbf{k}| \sin \vartheta \sin \varphi \quad (3.28b)$$

$$k_z = |\mathbf{k}| \cos \vartheta \quad (3.28c)$$

For intervalley phonons, where the electron does gain or lose energy during the scattering event, first energy and the related wavenumber  $k$  after scattering need to be calculated. Afterwards the new direction of the  $\mathbf{k}$  vector is found again by (3.28).

## Plot of phonon scattering rates

In Figure 3-1 the rates of the different scattering mechanisms can be seen. In the last subplot the rates of all mechanisms are superimposed.

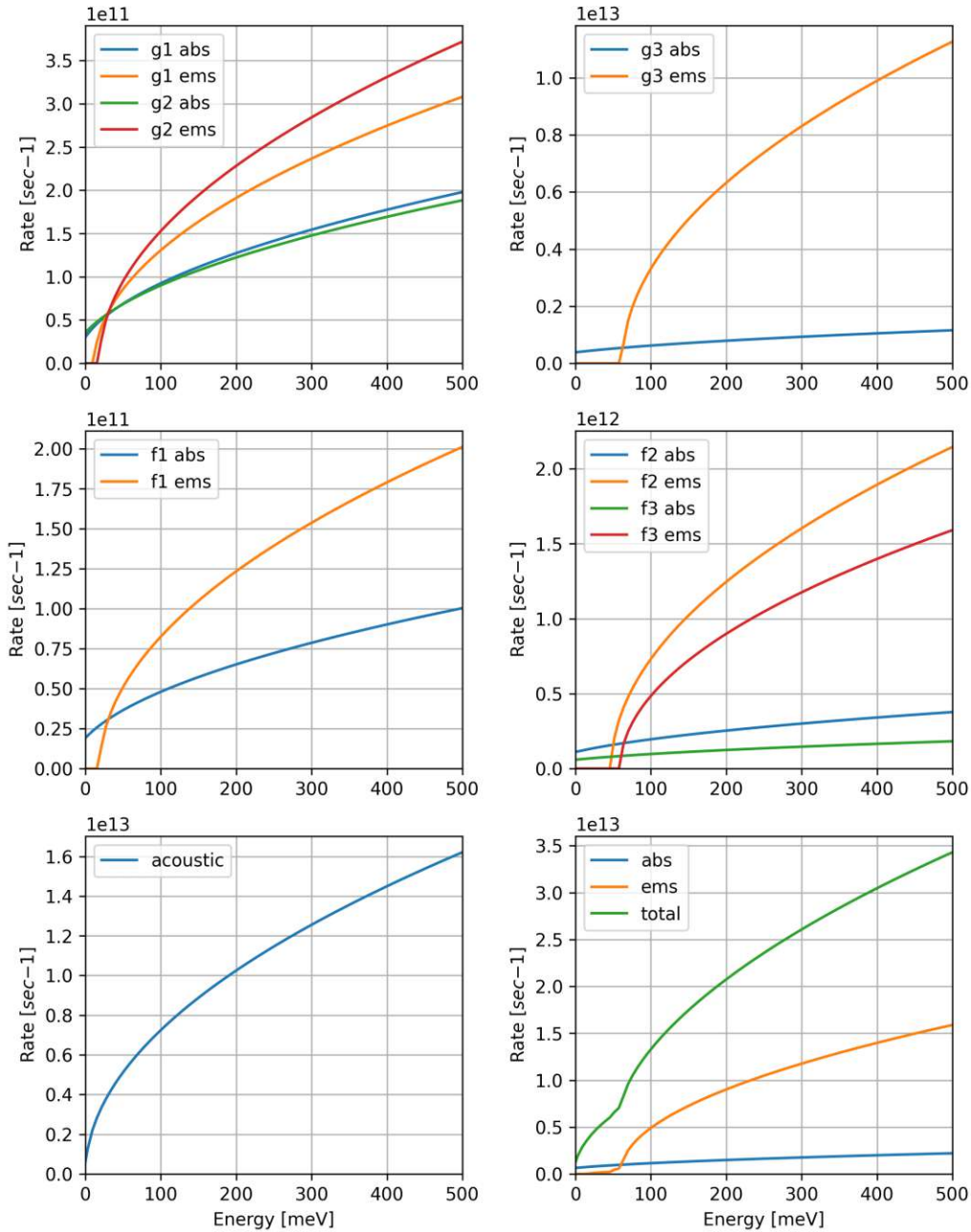


Figure 3-1: Electron-phonon scattering rates

## 3.2 Electron-electron scattering

The electrons repel each other according to Coulomb's law. Since the interaction takes place in the vicinity of many other electrons, a screened Coulomb potential  $U_s$  is used [6]. The distance between the electrons is denoted by  $u$ , the magnitude of  $\mathbf{u}$ .

$$U_S(u) = \frac{e}{4\pi\epsilon} \frac{\exp(-u/l_c)}{u}, \quad \mathbf{u} = \mathbf{r}_1 - \mathbf{r}_2, \quad l_c = \sqrt{\frac{\epsilon_s k_B T}{e^2 n}} \quad (3.29)$$

The characteristic length  $l_c$  is the Debye length. In order to calculate the scattering rate, the transition probability according to Fermi's golden rule must be evaluated first. Since two electrons are involved, it is a combined system and its states can be written as a product of plane waves. The initial and final wave vectors of electron 1 and 2 are denoted by  $\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2$ .

$$|\mathbf{k}_i\rangle = |\mathbf{k}_i^1\rangle |\mathbf{k}_i^2\rangle = \frac{1}{\Omega} e^{j(\mathbf{k}_i^1 \cdot \mathbf{r}_1 + \mathbf{k}_i^2 \cdot \mathbf{r}_2)}, \quad |\mathbf{k}_f\rangle = |\mathbf{k}_f^1\rangle |\mathbf{k}_f^2\rangle = \frac{1}{\Omega} e^{j(\mathbf{k}_f^1 \cdot \mathbf{r}_1 + \mathbf{k}_f^2 \cdot \mathbf{r}_2)} \quad (3.30)$$

### Transition rate

The matrix element needs to be calculated first.

$$\langle \mathbf{k}_f | U | \mathbf{k}_i \rangle = \frac{e^2}{\epsilon_s \Omega^2} \int_{\Omega} \int_{\Omega} e^{-j(\mathbf{k}_f^1 \cdot \mathbf{r}_1 + \mathbf{k}_f^2 \cdot \mathbf{r}_2)} \frac{\exp(-u/l_c)}{4\pi u} e^{j(\mathbf{k}_i^1 \cdot \mathbf{r}_1 + \mathbf{k}_i^2 \cdot \mathbf{r}_2)} d\mathbf{r}_2 d\mathbf{r}_1 \quad (3.31)$$

The exponential of the inner integral can be written as

$$e^{-j(\mathbf{k}_f^1 \cdot \mathbf{r}_1 + \mathbf{k}_f^2 \cdot \mathbf{r}_2) + j(\mathbf{k}_i^1 \cdot \mathbf{r}_1 + \mathbf{k}_i^2 \cdot \mathbf{r}_2)} = e^{j(\mathbf{k}_i^1 - \mathbf{k}_f^1) \cdot \mathbf{u}} e^{j(\mathbf{k}_i^2 + \mathbf{k}_i^1 - \mathbf{k}_f^1 - \mathbf{k}_f^2) \cdot \mathbf{r}_2} \quad (3.32)$$

By substituting  $\mathbf{u} = \mathbf{r}_1 - \mathbf{r}_2$  the functional determinant becomes  $\partial(x_1, y_1, z_1)/\partial(u_x, u_y, u_z) =$

1. The integral of (3.31) can be split in a product of two integrals

$$\begin{aligned}
& \int_{\Omega} \int_{\Omega} \frac{\exp(-u/l_c)}{4\pi u} e^{-j(\mathbf{k}_i^1 + \mathbf{k}_f^1) \cdot \mathbf{u}} e^{j(\mathbf{k}_i^1 + \mathbf{k}_i^2 - \mathbf{k}_f^1 - \mathbf{k}_f^2) \cdot \mathbf{r}_2} d\mathbf{r}_2 d\mathbf{u} \\
&= \int_{\Omega} \frac{\exp(-u/l_c)}{4\pi u} e^{-j(\mathbf{k}_i^1 + \mathbf{k}_f^1) \cdot \mathbf{u}} \int_{\Omega} e^{j(\mathbf{k}_i^1 + \mathbf{k}_i^2 - \mathbf{k}_f^1 - \mathbf{k}_f^2) \cdot \mathbf{r}_2} d\mathbf{r}_2 d\mathbf{u} \\
&= \int_{\Omega} e^{j(\mathbf{k}_i^1 + \mathbf{k}_i^2 - \mathbf{k}_f^1 - \mathbf{k}_f^2) \cdot \mathbf{r}_2} d\mathbf{r}_2 \int_{\Omega} \frac{\exp(-u/l_c)}{4\pi u} e^{-j(\mathbf{k}_i^1 + \mathbf{k}_f^1) \cdot \mathbf{u}} d\mathbf{u}
\end{aligned} \tag{3.33}$$

The first integral of (3.33) can be evaluated as

$$\int_{\Omega} e^{j(\mathbf{k}_i^1 + \mathbf{k}_i^2 - \mathbf{k}_f^1 - \mathbf{k}_f^2) \cdot \mathbf{r}_2} d\mathbf{r}_2 = \Omega \delta_{\mathbf{k}_i^1 + \mathbf{k}_i^2, \mathbf{k}_f^1 + \mathbf{k}_f^2} \tag{3.34}$$

The second one is the Fourier transform of the screened Coulomb potential [6].

$$\int_{\Omega} \frac{\exp(-u/l_c)}{4\pi u} e^{-j(\mathbf{k}_i^1 + \mathbf{k}_f^1) \cdot \mathbf{u}} d\mathbf{u} = \frac{1}{|\mathbf{k}_i^1 - \mathbf{k}_f^1|^2 + 1/l_c^2} \tag{3.35}$$

Substituting both integrals back in (3.33) gives the matrix element

$$\langle \mathbf{k}_f | U | \mathbf{k}_i \rangle = \frac{e^2}{\epsilon_S \Omega} \frac{\delta_{\mathbf{k}_i^1 + \mathbf{k}_i^2, \mathbf{k}_f^1 + \mathbf{k}_f^2}}{|\mathbf{k}_i^1 - \mathbf{k}_f^1|^2 + 1/l_c^2} \tag{3.36}$$

Fermi's golden rule (3.1) then writes as

$$P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{k}_f^1, \mathbf{k}_f^2) = \frac{2\pi}{\hbar} \left( \frac{e^2}{\epsilon_S \Omega} \right)^2 \frac{\delta_{\mathbf{k}_i^1 + \mathbf{k}_i^2, \mathbf{k}_f^1 + \mathbf{k}_f^2}}{(|\mathbf{k}_i^1 - \mathbf{k}_f^1|^2 + 1/l_c^2)^2} \delta[\epsilon(\mathbf{k}_f^1) + \epsilon(\mathbf{k}_f^2) - \epsilon(\mathbf{k}_i^1) - \epsilon(\mathbf{k}_i^2)] \tag{3.37}$$

The Kronecker- $\delta$  in this equation states momentum conservation. The rate is non-zero only when  $\mathbf{k}_i^1 + \mathbf{k}_i^2 = \mathbf{k}_f^1 + \mathbf{k}_f^2$  or  $\mathbf{k}_f^1 - \mathbf{k}_i^1 = \mathbf{k}_i^2 - \mathbf{k}_f^2$ . This difference denotes the momentum transfer vector  $\mathbf{q}$ , which we define as  $\mathbf{q} = \mathbf{k}_f^1 - \mathbf{k}_i^1$ . Inserting  $\mathbf{q}$  in (3.37) gives

$$P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{q}) = \frac{2\pi}{\hbar} \left( \frac{e^2}{\epsilon_S \Omega} \right)^2 \frac{\delta[\epsilon(\mathbf{k}_i^1 + \mathbf{q}) + \epsilon(\mathbf{k}_i^2 - \mathbf{q}) - \epsilon(\mathbf{k}_i^1) - \epsilon(\mathbf{k}_i^2)]}{(|\mathbf{q}|^2 + 1/l_c^2)^2} \tag{3.38}$$

## Scattering rate

The scattering rate is the probability per unit time that a transition from an initial state to any final state happens. The transferred momentum is between 0 and  $q_{max} = |\mathbf{k}_i^1 - \mathbf{k}_i^2|$ . By assuming that all final states are empty  $1 \approx (1 - f(k))$  this rate can be written as

$$\Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) = \sum_{\mathbf{q}} P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{q}). \quad (3.39)$$

By using the density of states the sum can be converted to an integral

$$\Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) = \left( \frac{\Omega}{(2\pi)^3} \right)^2 \int P(\mathbf{k}_i^1, \mathbf{k}_i^2, \mathbf{q}) d\mathbf{q}. \quad (3.40)$$

Inserting the transition rate from (3.38) in (3.40) gives

$$\Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) = \frac{2\pi}{\hbar} \left( \frac{e^2}{\epsilon_S \Omega} \right)^2 \left( \frac{\Omega}{(2\pi)^3} \right)^2 \int \frac{\delta[\epsilon(\mathbf{k}_i^1 + \mathbf{q}) + \epsilon(\mathbf{k}_i^2 - \mathbf{q}) - \epsilon(\mathbf{k}_i^1) - \epsilon(\mathbf{k}_i^2)]}{(q^2 + 1/l_c^2)^2} d\mathbf{q} \quad (3.41)$$

With the dispersion relation  $\epsilon(k) = \hbar^2 k^2 / 2m$  the delta function can be rewritten as

$$\delta \left( \frac{\hbar^2 q}{m} (q - q_{max} \cos \vartheta) \right) \quad (3.42)$$

where  $\vartheta$  denotes the angle between  $\mathbf{q}$  and  $\mathbf{q}_{max} = \mathbf{k}_i^1 - \mathbf{k}_i^2$ . The integral can be evaluated in spherical coordinates.

$$\Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) = \frac{e^4}{(2\pi)^4 \epsilon_s^2 \hbar} \int_0^\infty \int_0^{\pi/2} \frac{\delta(\frac{\hbar^2 q}{m} (q - q_{max} \cos \vartheta))}{(q^2 + 1/l_c^2)^2} \sin \vartheta d\vartheta q^2 dq \quad (3.43)$$

By substituting  $u = \cos \vartheta$ ,  $d\vartheta = du / \sin \vartheta$  the integral can be further simplified.

$$\begin{aligned} \Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) &= A \int_0^\infty \frac{q^2}{(q^2 + 1/l_c^2)^2} \int_0^1 \delta(q^2 - q_{max} q u) du dq \\ &= A \int_0^\infty \frac{q^2}{(q^2 + 1/l_c^2)^2} \frac{1}{q_{max} q} [\Theta(q_{max} - q) - \Theta(-q)] dq \\ &= \frac{A}{q_{max}} \int_0^{q_{max}} \frac{q}{(q^2 + 1/l_c^2)^2} dq \end{aligned} \quad (3.44)$$

Here the prefactor  $A$  is defined as  $A = e^4 m / ((2\pi)^4 \epsilon_s^2 \hbar^3)$  and  $\Theta$  denotes the unit step function. One finally attains the EES rate

$$\Gamma_{ee}(\mathbf{k}_i^1, \mathbf{k}_i^2) = B \frac{q_{max}}{q_{max}^2 + 1/l_c^2} \quad (3.45)$$

with

$$B = \frac{ne^4 m}{4\pi \hbar^3 \epsilon_s^2 1/l_c^2}, \quad 1/l_c^2 = \frac{e^2 n}{\epsilon_s k_B T} \quad (3.46)$$

### Momentum transfer, selection of the angle, state after scattering

If two electrons with a certain momentum collide, the transferred momentum will be  $q \in \{0, q_{max}\}$ . The momentum transfer vector  $\mathbf{q}$  is chosen randomly, its magnitude  $q$  is calculated by the inversion method [6]. A bijective mapping  $r \in \{0, 1\} \longleftrightarrow q \in \{0, q_{max}\}$  is needed. The mapping is found by the monotonically increasing function  $F(q)$  which gets normalized by  $F(q_{max})$ .

$$F(q) = \int_0^q P(\mathbf{k}_i^1, \mathbf{k}_i^2, q') dq' \quad (3.47)$$

The desired integral in (3.47) can be found in (3.44).

$$P(q) = \frac{F(q)}{F(q_{max})} = \frac{q^2}{q^2 + l_c^2} \frac{q_{max}^2 + l_c^2}{q_{max}^2} \quad (3.48)$$

A random number  $r_1$  will be set and the equation  $P(q) = r_1$  solved. Then  $q$  can be found by rearranging (3.48).

$$q^2 = \frac{r_1 q_{max}^2 1/l_c^2}{q_{max}^2 (1 - r_1) + 1/l_c^2} \quad (3.49)$$

The magnitude of  $\mathbf{q}$  is given by the square root of (3.49). According to (3.42) it holds  $q - q_{max} \cos \vartheta = 0$ . Therefore, the angle  $\vartheta$  between  $\mathbf{q}$  and  $\mathbf{q}_{max}$  is given by

$$\vartheta = \arccos \frac{q}{q_{max}}, \quad (3.50)$$

whereas  $\varphi$  is chosen uniformly distributed in  $[0, 2\pi]$ .

$$\varphi = 2\pi r_2 \quad (3.51)$$

In order to create a vector  $\mathbf{q}$  that fulfils the angle relations between  $\mathbf{q}$  and  $\mathbf{q}_{max}$ , a local spherical coordinate system  $(\mathbf{e}_k, \mathbf{e}_1, \mathbf{e}_2)$  with  $\mathbf{q}_{max}$  as polar axis needs to be created. The basis vectors are written in the basis of the Cartesian coordinate system. The direction of  $\mathbf{q}$  is therefore given as

$$\mathbf{e}_q = \cos \vartheta \mathbf{e}_k + \sin \vartheta \sin \varphi \mathbf{e}_1 + \sin \vartheta \cos \varphi \mathbf{e}_2 \quad (3.52)$$

The new wave vectors  $\mathbf{k}_f^1$  and  $\mathbf{k}_f^2$  can be written as

$$\mathbf{k}_f^1 = \mathbf{k}_i^1 + q\mathbf{e}_q, \quad \mathbf{k}_f^2 = \mathbf{k}_i^2 - q\mathbf{e}_q \quad (3.53)$$

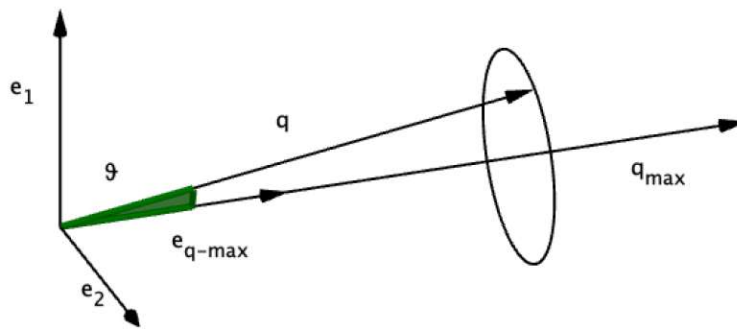


Figure 3-2: Momentum transfer



# Chapter 4

## Monte Carlo algorithm

The core of the algorithm is the MC loop (Figure 4-1). The number of the loop passes is typically in the range of  $10^4$  to  $10^8$ , which makes an effective implementation important. Every pass of the MC loop consists of a free flight followed by a scattering event. The flight procedure first generates the random flight-time. Then the trajectory will be calculated and sampled either at given time steps  $\Delta t$  or at the end of the flight. The scattering procedure starts by evaluating the scattering rates which depend on the energy of the electron. A scattering mechanism will then be chosen randomly and the new state is calculated.

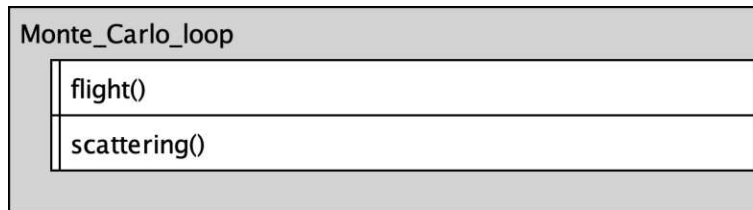


Figure 4-1: Structogram of MC loop

In the stationary algorithm the MC loop (Figure 4-1) is executed only once. An average of all sampling points will be calculated to produce the mean values of interest. Such simulations can be used, for example, to predict the mean velocity or mean energy of the ensemble as a function of the electric field.

In the transient algorithm the MC loop (Figure 4-1) is executed for a large number of electrons. In order to study the ensemble properties evolving in time, the trajectories

need to be sampled at equidistant time steps.

If EES is included, pairs of two trajectories instead of single trajectories need to be simulated. The algorithms using single trajectories and trajectory pairs are very similar, the differences are explained in Chapter 4.2

## 4.1 MC-algorithm without EES

### 4.1.1 Initial state

The initial state should be chosen in a way that its energy is close to the settled end value. This way the transient is short, and most sampling values are taken from the stationary solution.

In the case of the transient algorithm it is important that every electron starts with a different initial state. Each electron of the ensemble gets its initial momentum according to a Gaussian distribution  $\mathcal{N}(\mu, \sigma^2)$  with an expected value  $\mu = 0$  and a variance of  $\sigma^2 = mk_B T / \hbar^2$ .

### 4.1.2 Flight duration

In order to find out how long it will take till the next scattering event occurs, one needs to consider the scattering rates described in Chapter 3. The total rate  $\Gamma_{tot}$  is the sum of the rates  $\Gamma_i$  of all individual mechanisms. The rates depend on the electron energy  $\epsilon(t)$ , which in general is a function of time. In the equilibrium case no electric field is applied and the rates are constant throughout the free flight. In the non-equilibrium case an electric field is applied and the rates are changing during the free flight.

#### Equilibrium

The probability density  $p(t)$  describes how likely a scattering event takes place at a certain point in time. The time dependence can be written as  $dp/dt = -\Gamma p$ . This

differential equation is solved by

$$p(t) = \Gamma \exp(-\Gamma t) \quad (4.1)$$

The cumulative probability  $P(t)$  describes how likely a scattering event takes place till a certain point in time.

$$P(t) = \int_0^t p(t') dt' \quad (4.2)$$

After infinite time, it is certain that the electron had experienced an scattering event such that  $P(t \rightarrow \infty) = 1$ . This way  $P(t)$  acts as bijective mapping  $P \in \{0, 1\} \longleftrightarrow t_f \in \{0, \infty\}$ . For a uniform random number  $r$ ,  $t_f$  can be evaluated by rearranging (4.2). This approach is called inversion method [6].

$$r = P(t = t_f) = \int_0^{t_f} p(t) dt, \quad t_f = \frac{-1}{\Gamma} \ln(1 - r) \quad (4.3)$$

### Non-equilibrium / self scattering

In the presence of an electric field, the electron is accelerated and  $\Gamma$  becomes time dependent  $\Gamma(t)$ . Equation (4.2) would become a path integral, this would still work but results in a much higher computational effort. Thus the method described for equilibrium must be adapted. An additional self scattering rate  $\Gamma_{ss}$  is added such that the total rate  $\Gamma_{tot} = \Gamma_{ss} + \sum \Gamma_i$  becomes constant. This self scattering mechanism has no physical meaning and the electron state remains the same as before. The total rate  $\Gamma_{tot}$  is chosen at the begin of the simulation and is kept constant throughout the simulation. It must be chosen small enough to keep computational overhead small and big enough to avoid failures. In the course of a simulation it must always hold  $\sum \Gamma_i < \Gamma_{tot}$ . This way (4.3) for flight duration stays valid.

#### 4.1.3 State before scattering

If an electron is accelerated by an electric field  $\mathbf{E}$ , the electron gains energy. Therefore the electron's energy and momentum must be updated at the end of the flight. The

force due to the electric field is given by  $\mathbf{F} = e\mathbf{E}$ , where  $e$  denotes the charge of the electron. The change in the  $\mathbf{k}$ -vector is then given by  $\Delta\mathbf{k} = \Delta\mathbf{p}/\hbar$ , where, for a constant force during the flight the change in momentum is  $\Delta\mathbf{p} = \mathbf{F}t_f$ . The energy can then be calculated through the dispersion relation.

$$\mathbf{k}_b = \mathbf{k}_a + \frac{\mathbf{F}}{\hbar}t_f, \quad \epsilon_b = \frac{\hbar^2\mathbf{k}_b^2}{2m} \quad (4.4)$$

The subindices  $b$  and  $a$  refer to the state immediately before and after the scattering event.

#### 4.1.4 Selection of the scattering mechanism

After a flight the rates  $\Gamma_i$  of the single scattering mechanism  $i \in \{1, n\}$  are evaluated. Then one scattering mechanism is chosen by a uniform random number  $r$ . This can be implemented by storing the partial sums of the rates in an array, so that the array element  $S[i]$  with index  $i$  stores

$$S[0] = 0, \quad S[n] = \sum_{i=1}^n \Gamma_i \quad (4.5)$$

If there are  $n$  different mechanisms the array is of the size  $n + 1$  and the last element  $S[n]$  stores the total rate  $\Gamma_{tot}$ . Then scattering mechanism  $i$  will be selected if it fulfills  $S[i - 1] < \Gamma_{tot} \cdot r < S[i]$ .

#### 4.1.5 Sampling

There are two sampling approaches, the before scattering method, which has the advantage of a simple implementation, and the constant  $\Delta_t$  sampling method, which is required for transient simulations.

##### Before scattering sampling

The sampling of the physical quantities of interest happens at the end of a free flight, immediately before the scattering event. Since the flight time differs for every flight,

the values that will be saved need to be weighted. This statistical weight can either be the flight time or the reciprocal of the total scattering rate.

### Sampling at constant time steps

Sampling with a fixed time step  $\Delta_t$  is used in the transient algorithms, since the trajectories of many electrons need to be sampled at the same points in time to enable the calculation of ensemble averages.

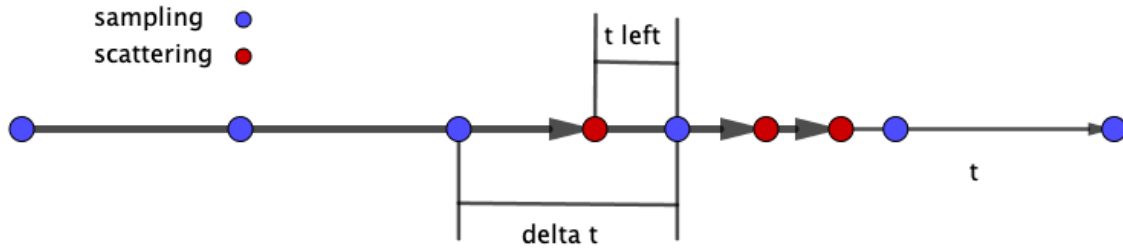


Figure 4-2: Constant  $\Delta_t$  sampling

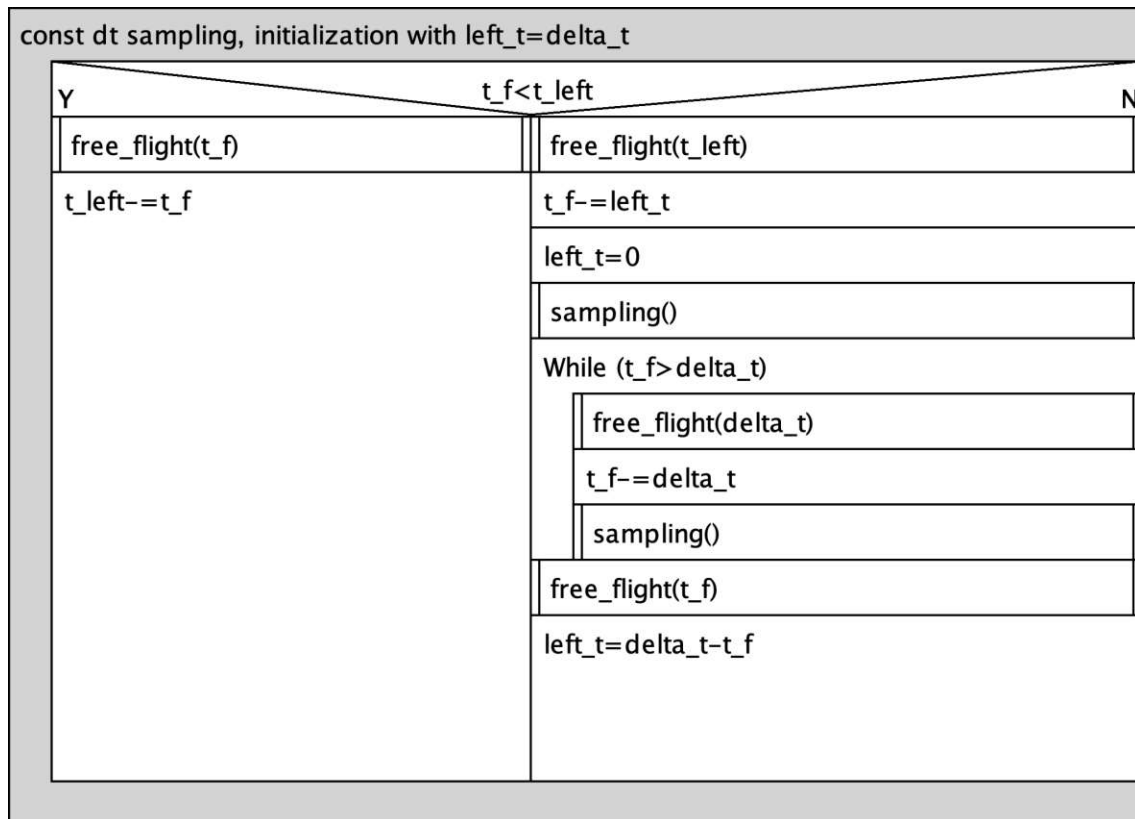


Figure 4-3: Structogram of sampling with constant  $\Delta_t$

## 4.2 Modifications for MC-algorithm to include EES

In order to simulate EES the trajectories of two individual electrons need to be considered simultaneously. The algorithm is very similar to the one particle MC algorithm. It differs in the calculation of the flight time and in the additional EES mechanism.

### Sampling

Sampling is performed as described in Section 4.1.2. Since two trajectories will be sampled it is possible to average the results of both trajectories to gain more sampling points. However, in some simulation cases the two electrons start with different initial energies, which result in two trajectories that can not be merged. The relaxation simulation where an ensemble of hot electrons interact with cold electrons would be such a case.

### Determination of flight duration and selection of scattering event

Selection of the scattering mechanism is a two step process. At first the affected electrons need to be determined. This can either be electron 1 or electron 2 in the case of phonon scattering, or both electrons in case of EES. This is done by evaluating the different scattering rates  $\Gamma_{Ph}^{(1)}$ ,  $\Gamma_{Ph}^{(2)}$  for both electrons and  $\Gamma_{ee}$ . Then the respective flight times can be calculated by  $t_f = -\ln(1 - r)/\Gamma$ . The shortest flight time will be used for the flight and the according scattering event is performed after the flight. The second step, which is only required for phonon scattering, is the selection of the phonon scattering mechanism. It is explained in Section 4.1.5.

# Chapter 5

## Results

In the following simulations we assumed the material parameters of bulk silicon. All results have been obtained with the constant  $\Delta t$  sampling method. The simulation code is implemented in Python according to Chapters 3, 4 and Appendix A

### 5.1 Stationary simulations

Figure 5-1 and Figure 5-2 show the mean values of energy and momentum as a function of the electric field. The simulation was done with the parameters from Table 5.1. The saturation in velocity is due to the high scattering rates that decelerate the electrons. Figure 5-3 shows the velocity distribution for different electric fields. The momentum distributions broaden for higher electric fields. Figure 5-4 shows the energy distribution for different electric fields. In the equilibrium case ( $\mathbf{E} = 0$ ), carriers are Maxwell distributed which can be observed in the exponential decrease of the distribution. An important finding is that EES does not affect the mean values.

sampling points	$\Delta t$	Temperature
$1 \times 10^6$	$10^{-14}$ s	300 K

Table 5.1: Parameters for the stationary algorithm

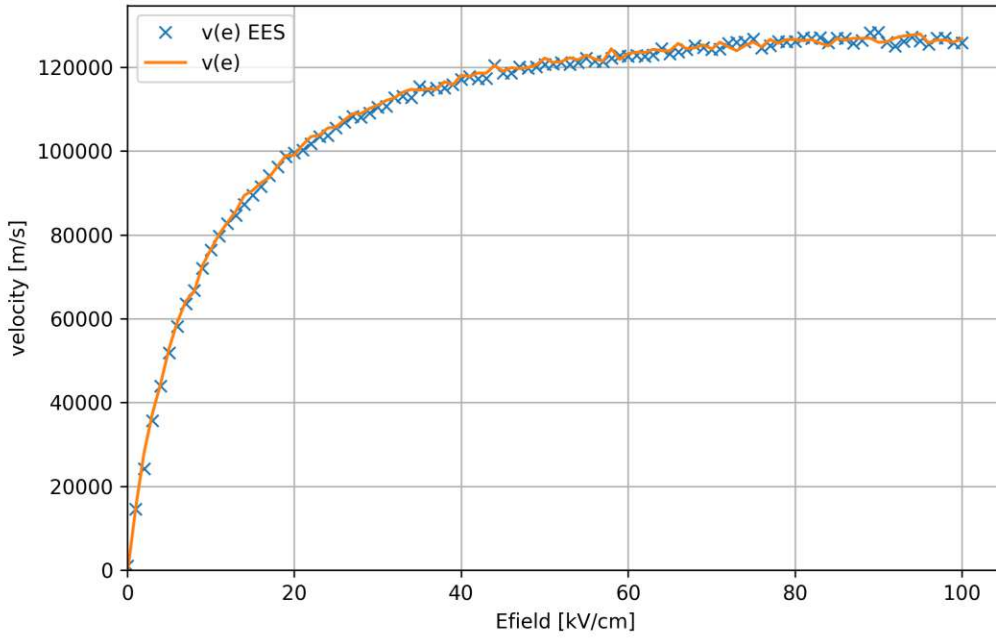


Figure 5-1: Mean velocity as a function of the electric field  
solid curve: phonon scattering only; Symbols: EES included

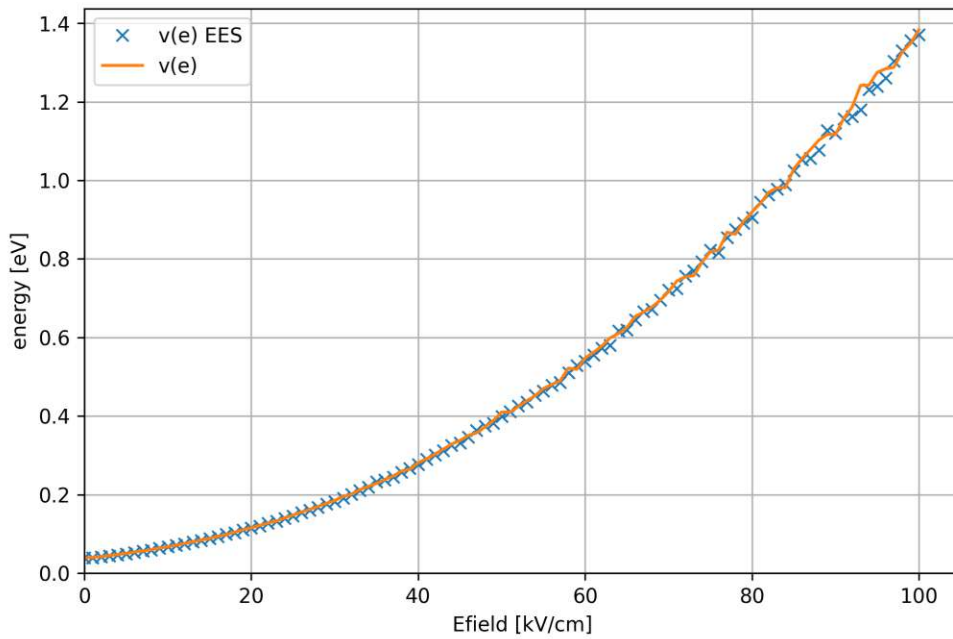


Figure 5-2: Mean energy as a function of the electric field  
solid curve: phonon scattering only; Symbols: EES included



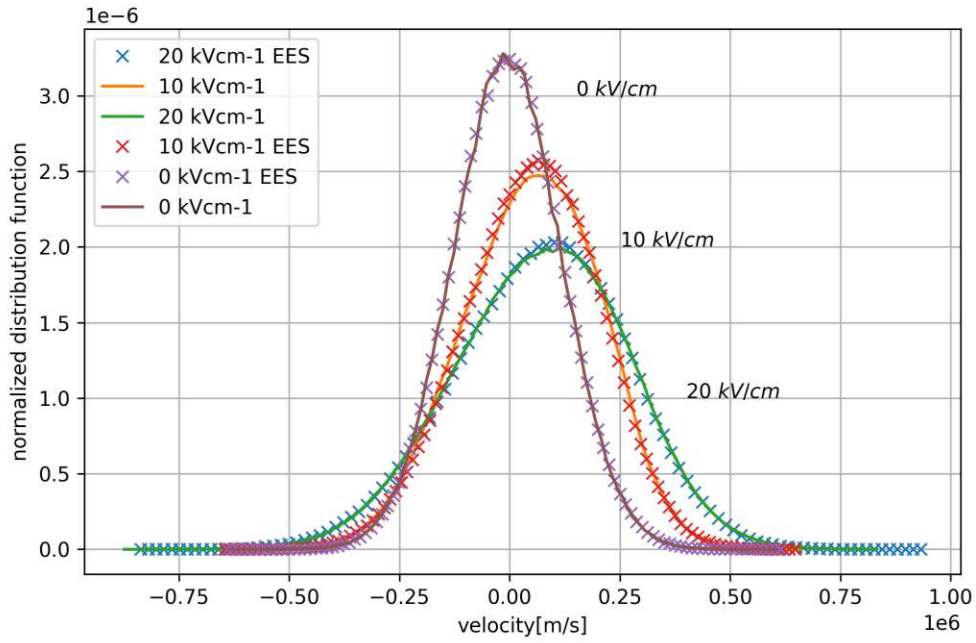


Figure 5-3: Velocity distribution function for different electric field strengths

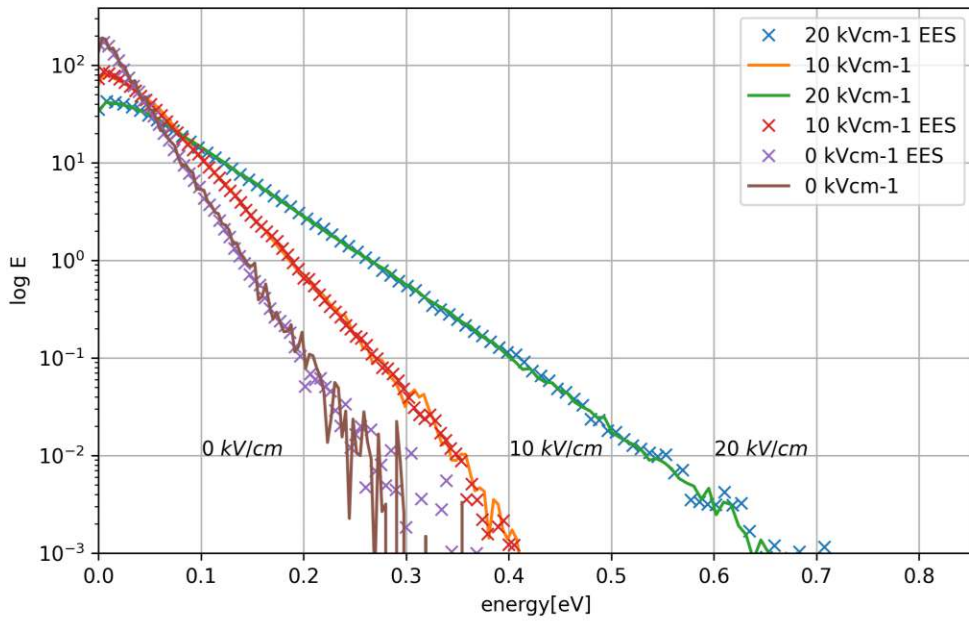


Figure 5-4: Energy distribution function for different electric field strengths

## 5.2 Transient simulations

The following results are time dependent and thus simulated by an ensemble of electrons or electron pairs. The results show the sample mean at the given time step.

### 5.2.1 Step response

Figure 5-5 shows how the mean velocity and the mean energy of the electron respond to a Heaviside step function in the electric field. After 1 ps the electric field changes from  $1 \text{ kV cm}^{-1}$  to  $50 \text{ kV cm}^{-1}$ . The simulation was done with the parameters from Table 5.2. The result shows a velocity overshoot.

ensemble size	sampling points	$\Delta_t$	Temperature
10000	300	$10^{-14} \text{ s}$	300 K

Table 5.2: Parameter for transient algorithm

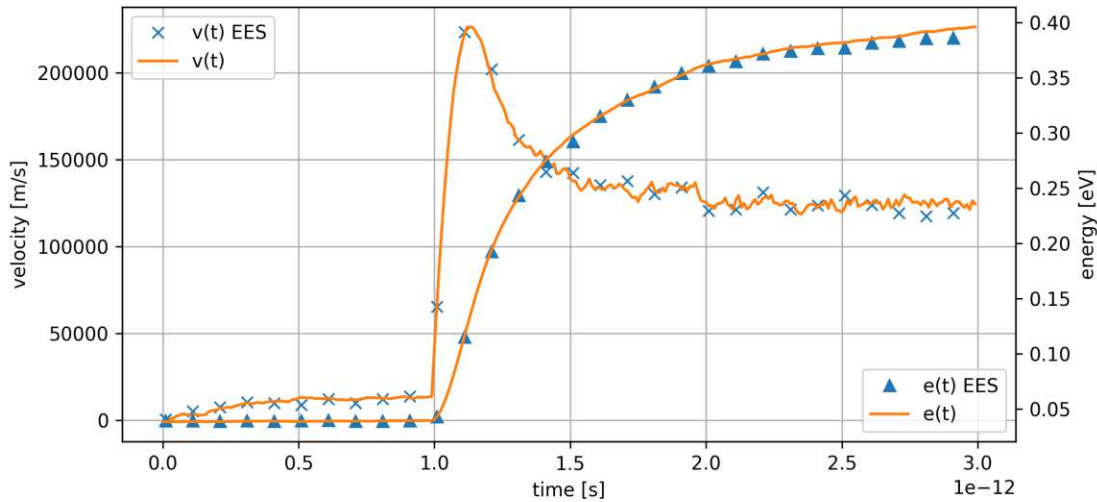


Figure 5-5: Step response of mean velocity and mean energy

## 5.2.2 Relaxation

If electrons with high energy enter a domain of electrons with low energy, there will be a relaxation process towards thermal equilibrium. This happens for example at the junction between the channel and the drain region of a MOSFET. In Figure 5-6 the relaxation process of two electron ensembles is shown. One ensemble has a high initial energy representing the hot electrons (3000 K) coming from the channel. The other ensemble has a low initial energy representing the cold drain domain (300 K). If the simulation is done without EES, one can see that the cold electron's, that already are at lattice temperature, won't change their energy throughout the simulation time. On the other hand the hot electrons relax to the lattice temperature in an exponential process. If EES is included, the behavior is different. The hot electron interact with the cold ones and heat them above the equilibrium energy. Also, the hot electrons relax much faster due to the additional interaction.

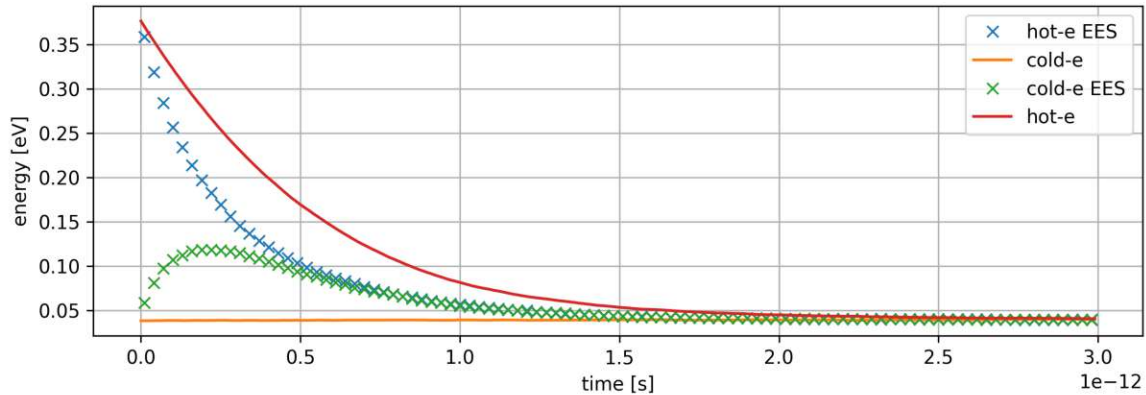


Figure 5-6: Relaxation process for  $T_L = 300 \text{ K}$  and  $n = 10^{19} \text{ cm}^{-3}$

Figure 5-7 and Figure 5-8 show the same relaxation process as 5-6. The difference is that the hot ensemble has now a temperature of 770 K and the cold one 77 K. The simulation was done with two different carrier densities  $n = 10^{19} \text{ cm}^{-3}$  and  $n = 10^{16} \text{ cm}^{-3}$ . In the simulation with the higher carrier densities hot and cold electrons relax faster, due to the higher EES rate. In the simulation with the higher carrier densities  $n = 10^{19} \text{ cm}^{-3}$ , it can also be seen, that curves approaches each other much faster in the beginning. This is because from 0 ps to 0.5 ps relaxation happens mostly

due to EES. Afterwards phonon scattering is dominant.

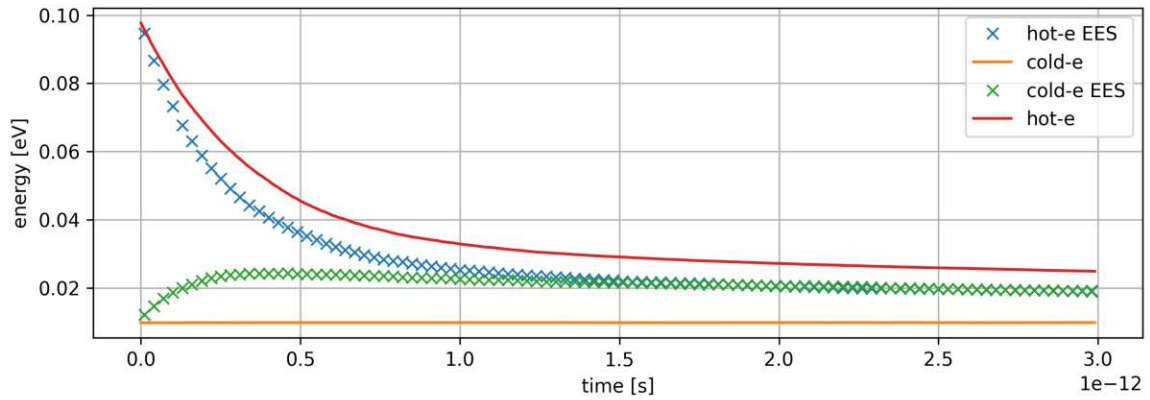


Figure 5-7: Relaxation process for  $T_L = 77$  K and  $n = 10^{19} \text{ cm}^{-3}$

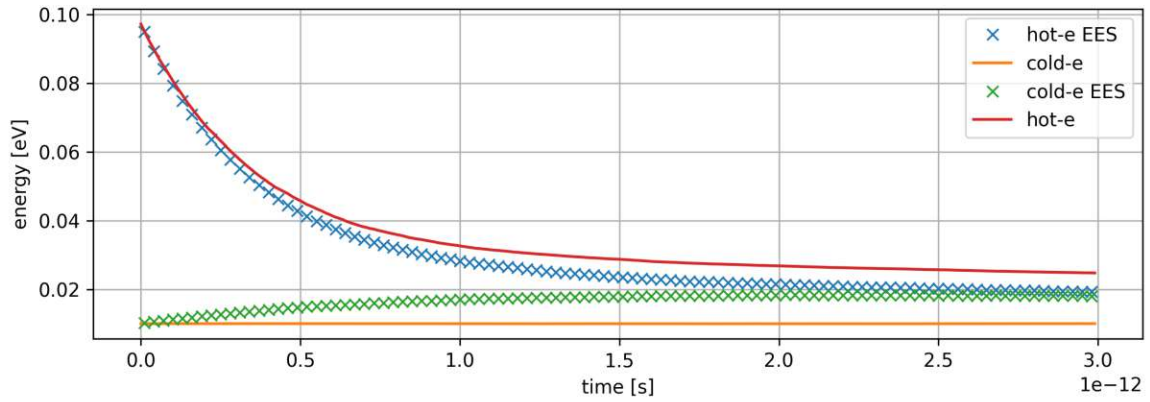


Figure 5-8: Relaxation process for  $T_L = 77$  K and  $n = 10^{16} \text{ cm}^{-3}$

# Appendix A

## Code

The Code was structured in three files: `topfile.py`, `MonteCarlo.py`, `parameter.py`. The file `topfile.py` holds the core MC loop. It is the entry point of the program. From here, the desired simulation can be selected by setting the according if condition true.

The file `MonteCarlo.py` holds all deeper intelligence and functionality of the code. There are classes to calculate rates, flight and scattering behavior as well as classes which manage the recording of data.

The file `parameter.py` holds all parameters in a data structure similar to JSON (Python dict). Parameters will be scaled as described in [A.1](#) and preconstants will be evaluated at the beginning of the program in this file.

In the following the most important Code snippets are shown.

## A.1 System of units

In Order to improve numerical accuracy, all variables need to be scaled close to 1. Therefore a distinction between units from the user input (external) and units used for the actual calculations (internal) has to be made. The unit system for the user input is chosen in a way to match common used units in literature. Every value is divided by its unit, which leads to unitless calculations. Since the calculations inside the code are done unitless, the results at the end of the simulation need to be multiplied by the according unit in order to obtain meaningful output.

physical quantity	unit
<i>length</i>	1 cm
<i>mass</i>	1 g
<i>time</i>	1 s
<i>voltage</i>	1 V
<i>current</i>	1 A
<i>energy</i>	1 eV
<i>temperature</i>	1 K

Table A.1: External units

physical quantity	unit
<i>length</i>	1 nm
<i>mass</i>	1 g
<i>time</i>	1 ns
<i>voltage</i>	1 $\mu$ V
<i>current</i>	1 $\mu$ A
<i>energy</i>	1 $\times 10^{-21}$ J
<i>temperature</i>	1 K

Table A.2: Internal units

constant	value
$\hbar$	$6.582\,119\,569 \times 10^{-16}$ eV s
$K_B$	$8.617\,333\,262 \times 10^{-5}$ eV K <sup>-1</sup>
$e$	$1.602\,176\,63 \times 10^{-19}$ A s

Table A.3: Constants [8]

## A.2 Particle state

The state of the electron is saved in a data class object. At the beginning of the code this object is shared with all other classes that need to read or overwrite the current state. In this way the object does not have to be passed or returned at every function call.

```
1 @dataclass
2 class State:
3     energy: np.double=0
4     k: np.double=0;    k_x: np.double=0;k_y: np.double=0;k_z: np.
      double=0
5     r_x: np.double=0
6     mech: int=0
7     Gamma: np.double=0
8     flighttime: np.double=0
9     failure: np.bool_=False
10
```

Listing A.1: State dataclass

## A.3 Scattering rates

In order to evaluate the scattering rate a class was implemented in `MonteCarlo.py`. It calculates the new rates based on the energy of the particle and constants saved in `parameter.py`.

```
1  class Rates:
2      def __init__(self, state: State=None):
3          self.state=state;
4          self.rates_array=np.zeros(13)#rates array init
5          cs=state
6          cs.energy=p["energy_max"]
7          self.rates_array_update()
8          cs.vars.Gamma=self.rates_array[12]
9          cs.energy=p["energy_init"]
10     def rate_ac(self, energy):# electron-acustical phonon scattering
11         return para.preconst_rates[12]*np.sqrt(energy)
12     def rate_intervally(self, energy, i):#Intervalley scattering
13         E_f=energy+para.dE[i]
14         if E_f<0: return 0
15         return para.preconst_rates[i]*np.sqrt(E_f)
16     def rates_array_update(self):
17         energy=self.state.energy
18         self.rates_array[0]=self.rate_intervally(energy, 0)
19         for i in range(1, 12):
20             self.rates_array[i]=self.rates_array[i-1]+self.
rate_intervally(energy, i)
21         self.rates_array[12]=self.rates_array[11]+self.rate_ac(
energy)
22
```

Listing A.2: Evaluation of phonon scatter rates



```
1 def ee_flight_time(self, cs1: State, cs2: State):
2     B=self.B
3     Kv=[cs2.k_x-cs1.k_x, cs2.k_y-cs1.k_y, cs2.k_z-cs1.k_z]
4     K=np.linalg.norm(Kv)
5     Gamma_ee=(B/2)*K/(self.beta2+K**2)
6     t_ee=-1/(Gamma_ee)*np.log(random.random())
7     return t_ee
8
9 def ee_scattering(self, cs1: State, cs2: State):
10    cs1.vars.mech=14; cs2.vars.mech=14
11    #build an local polar coordinate system with Kv as polar axis
12    K_v = [cs2.k_x-cs1.k_x, cs2.k_y-cs1.k_y, cs2.k_z-cs1.k_z]
13    e1_v = [-K_v[1], K_v[0], 0] # this vector is orthogonal to K_v
14    K=np.linalg.norm(K_v)
15    ek_v=K_v/K
16    e1_v = e1_v/np.linalg.norm(e1_v)
17    e2_v=np.cross(ek_v, e1_v) # both ek_v and e1_v are normalized
18
19    #generate momentumtransfer vector
20    r=random.random()
21    q=np.sqrt(r*(K**2)*self.beta2/(K**2*(1-r)+self.beta2))
22    cos_theta=q/K
23    sin_theta=np.sqrt(1-cos_theta**2)
24    phi=random.uniform(0, 2*np.pi)
25    e_v=cos_theta*ek_v + sin_theta*np.sin(phi)*e1_v + sin_theta*np.
cos(phi)*e2_v
26    q_v=q*e_v
27
28    #change momentum wavevektor and energy
29    cs1.k_x+=q_v[0]; cs1.k_y+=q_v[1]; cs1.k_z+=q_v[2]
30    cs2.k_x-=q_v[0]; cs2.k_y-=q_v[1]; cs2.k_z-=q_v[2]
31
32    energy_old = cs1.energy+cs2.energy
33    k2=cs1.k_x**2+cs1.k_y**2+cs1.k_z**2
34    cs1.k=np.sqrt(k2)
35    cs1.energy=k2*self.k2toE
```

```
36
37     k2=cs2.k_x**2+cs2.k_y**2+cs2.k_z**2
38     cs2.k=np.sqrt(k2)
39     cs2.energy=k2*self.k2toE
40     energy_new = cs1.energy+cs2.energy
41
```

Listing A.3: Evaluation of EES flighttime and rates

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# Eidesstattliche Erklärung

Hiermit erkläre ich, dass ich die vorliegende Arbeit gemäß dem Code of Conduct – Regeln zur Sicherung guter wissenschaftlicher Praxis, insbesondere ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel, angefertigt wurde. Die aus anderen Quellen direkt oder indirekt übernommenen Daten und Konzepte sind unter Angabe der Quelle gekennzeichnet. Die Arbeit wurde bisher weder im In- noch im Ausland in gleicher oder in ähnlicher Form in anderen Prüfungsverfahren vorgelegt.

Wien, 14.9.2022

Unterschrift