MASTER

Monte Carlo simulation of electron transport in GaAs

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MONTE CARLO SIMULATION OF ELECTRON TRANSPORT IN GAAS

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SUMMARY

This thesis deals with the modeling of electron transport in N-type bulk GaAs. Especially it deals with the influence of ionized impurities on electron mobility. The used model is derived from first order perturbation theory. It accounts for the possibility of space correlated impurities such as clusters of impurities and dipoles. For this purpose the Ensemble Monte Carlo (EMC) method is used. In this method the Boltzmann transport equation is solved with help of statistical techniques. This technique is outlined in chapter 3.

The original high-field EMC program was modified to make it more suitable for low-field simulations. A new concept of 'overestimation' not found yet in the literature was introduced in order to speed up the program. With this technique it is possible to avoid the time-consuming numerical calculation of difficult integrals and iterative procedures needed to calculate the scatter rate and scatter angle. The error made by the overestimation is accounted for by a simple rejection technique, which adds an extra self scattering. It is proved in chapter 3 that this technique does not affect the solution of the Boltzmann transport equation.

The program based on this principle of overestimation proved to have two advantages over the old program. First the ionized impurity scattering model can be implemented easily in full detail and if the overestimated expressions are chosen such that the extra self scatter rate is 'small' it runs much faster.

The program produces mobility data which are in accordance with the literature. Furthermore it shows that the influence of clustered impurities can be neglected at room temperature. However at 77K it becomes detectable.

In addition the effect of dipole scattering has been investigated. The formulas predict that there will be hardly any influence for the slow electrons, but that instead fast electrons will be
scattered more.

Investigation of the formulas, corresponding to this effect, shows that the product of dipole length and inverse screening length should be less than a critical value. The combination of this critical value and a cutoff value for the reciprocal vector leads to three important restrictions.

First the dipole length should be about the lattice constant. Secondly the free carrier concentration should be high, about $10^{19} \text{ cm}^{-3}$. The last restriction concerns the actual influence on the distribution function. The momentum relaxation due to dipole scattering has to be relevant. This leads to a dipole concentration of about $10^{20} \text{ cm}^{-3}$.

It is almost impossible to meet all these constraints in GaAs-technology. However in other semiconductor materials it may be easier to meet these constraints.

In chapter 6 a model is derived for self-consistent screening in the first-order perturbation approximation. In chapter 7 a more sophisticated model concerning ionized impurity scattering, called partial phase shift analysis, is discussed. Especially the implementation of the semi-classical approximation in a Monte Carlo program is investigated.

Investigations show that implementation is possible. However more investigations are needed to determine the validity of the semi-classical approximation and the bound on the input variables for which the program produces reliable data.
CONTENTS

1. INTRODUCTION 1

2. THE BOLTZMANN TRANSPORT EQUATION 3

3. THE MONTE CARLO METHOD 5
   3.1 Selection of the free flight time 6
   3.2 Choosing the scatter process 8
   3.3 Choosing the state after scattering 8
   3.4 Technique based on overestimation 10
   3.5 Overestimation 11
   3.6 Discussion of the overestimation method 12

4. SCATTER PROCESSES 13
   4.1 Piezo-electric scattering 13
      4.1.1 Overestimation 16
      4.1.2 Discussion 17
   4.2 Acoustic phonon scattering 17
      4.2.1 Overestimation 18
      4.2.2 Discussion 20
   4.3 Polar optical phonon scattering 20

5. IONIZED IMPURITY SCATTERING 22
   5.1 Ionized impurity scattering due to clusters of correlated impurities. 22
      5.1.1 Limits 23
      5.1.2 The scatter rate and state after scattering 24
      5.1.3 Ridley model 25
         5.1.3.1 Overestimation 27
         5.1.3.2 Calculation of the angle after scattering 29
         5.1.3.3 Rejection technique 30
      5.1.4 Conclusion 32
   5.2 Dipole scattering 32
      5.2.1 Overestimation 34
      5.2.2 Discussion 36
5.2.3 Estimation of the effects

6. SELF CONSISTENT SCREENING
   6.1 Theory
   6.2 Approximations
   6.3 Discussion

7. PARTIAL PHASE SHIFT ANALYSIS
   7.1 Theory
   7.2 Implementation of the partial phase shift
      method into a Monte Carlo program
   7.3 Friedel Sum Rule

8. RESULTS
   8.1 The influence of screening on electron-acoustic phonon scattering
      8.1.1 The model
      8.1.2 Simulation
      8.1.3 The Results
      8.1.4 Conclusions
   8.2 Ionized impurity scattering
      8.2.1 Temperature dependence
      8.2.2 Clusters of ionized impurities
      8.2.3 Dipole scattering
         8.2.3.1 Simulation
         8.2.3.2 Discussion
      8.2.4 Self consistent screening
         8.2.4.1 Conclusion
   8.3 Partial phase Shift analysis
      8.3.1 Conclusion

9. CONCLUSIONS

LITERATURE
APPENDIX A: DIPOLE SIMULATIONS
APPENDIX B: SELF-CONSISTENT SCREENING
APPENDIX C: PARTIAL PHASE SHIFT ANALYSIS
1. INTRODUCTION

The subject for my master thesis was the investigation of the influence of ionized impurity scattering due to clusters of correlated impurities on the mobility in bulk GaAs. An old Monte Carlo program, developed for high-field GaAs bulk simulations, was given. Unfortunately documentation was not available. Therefore it took me an enormous amount of time to discover how it worked and more important which formulas and approximations were used.

The fact that this program was written for high-field simulations was disastrous for my kind of simulations. The approximations which are valid for high fields are not necessary good for low field simulations. The calculations of mobilities take place with very low fields. The program produced dubious data in the low field region.

The solution for this problem was to make the program suitable for low field simulations. All scatter processes of importance in GaAs were reconsidered and implemented correctly. Also the nucleus of the program, the subroutine which calculates the duration of the free flight, was adapted. Furthermore a new concept, suggested by F.P.Widdershoven, called "Overestimation Method" was introduced successfully.

This thesis has three main parts. The first part gives a short introduction concerning the Boltzmann transport equation, the Monte Carlo method and the overestimation method. In the second part the scatter processes are discussed. In this part the concept of overestimation will be used many times. The last part is reserved for results. These results are mainly concerned with the subject of ionized impurity scattering.

It was planned that during three months, I should perform measurements at Philips Research Laboratories, Eindhoven, on MBE grown Sb-doped Si samples. During that period only one sample could be grown. Unfortunately no usable measurements were possible,
due to many dislocations and deep traps in that sample. So the time was mainly spend on improving the Monte Carlo program.
2. THE BOLTZMANN TRANSPORT EQUATION

The most important physical phenomenon in semiconductor materials is the charge carrier transport under influence of external fields. These fields may be electrical or magnetic. In this paper we only deal with charge carrier transport under influence of electrical fields.

If an external field is applied the conduction electrons will be accelerated and gain energy. This extra energy will be passed to the lattice by inelastic scatter processes. After some time a new steady state will be reached.

The distribution function $f(k,r,t)$ is defined as the occupation probability of a state characterized by a wave vector $k$, at a position $r$, at a time $t$. In the following bold face indicates vector quantities. This function gives a complete description of the electron system. The above distribution function is the solution of the well known Boltzmann Transport Equation (BTE).

$$\frac{\partial f(k,r,t)}{\partial t} = \frac{\partial}{\partial k} \left[ \frac{\partial f(k,r,t)}{\partial k} \right] + \frac{\partial}{\partial r} \left[ \frac{\partial f(k,r,t)}{\partial r} \right] - \frac{\partial f(k,r,t)}{\partial t} _{sc} \quad (2.1)$$

The first term on the right hand accounts for the external forces and the second term describes the influence due to diffusion. The third term, called the collision or scatter term, accounts for all possible scatter processes. The number of electrons $dN$ in in a volume $(r,dr)$ of the r-space and $(k,dk)$ of the k-space at a certain time $t$ is:

$$dN(r,dr,k,dk,t)=f(k,r,t) \ dr \ dk \quad (2.2)$$

The electron is described as a wave packet. This wave packet is formed out of Bloch-functions $\psi_k(r)=u_k(r)\exp(ik.r)$, being the unperturbed solutions of the Schrödinger equation. The electron is described as a quasi particle called 'crystal electron'. The crystal electron faces only external forces and the potential perturbations of the imperfect crystal. These potential perturbations originate from impurities,
Usually the velocity $\frac{\partial \mathbf{r}}{\partial t}$ in the diffusion term is replaced by the group velocity of the wave packet:

$$\frac{\partial \mathbf{r}}{\partial t} = \mathbf{v}(k) = \frac{1}{\hbar} \nabla_{\mathbf{k}} W(k)$$

(2.3)

where $W(k)$ is the kinetic energy of an electron with wave vector $k$. The external forces (only electrical fields are considered) are accounted for by:

$$\frac{\partial \mathbf{k}}{\partial t} = -\frac{e}{\hbar} \mathbf{E}$$

(2.4)

This description of the dynamics is referred as quasi classical. The role of momentum is represented by $\hbar \mathbf{k}$, which is called the crystal momentum.

Analogous to the electron system a BTE can be set up for the phonon system. This phonon BTE is coupled with the BTE for electrons by means of annihilation and creation of phonons through electrons. The Bloch approximation states that BTE's can be uncoupled. The underlying reason is that the phonon system sets up an equilibrium so quickly that the disturbances in the phonon system can be neglected. Under this assumption and the assumption of non-degenerate statistics, the scatter term of (2.1) may be written as:

$$\frac{\partial f}{\partial t}_{\text{ac}} = \frac{V}{(2\pi)^3} \iiint \mathrm{d}k' \frac{1}{k'} \left[ S(k,k')f(k') - S(k,k)f(k) \right]$$

(2.5)

were $S(k,k')$ is the transition rate from state $k$ to $k'$. Generally the BTE can be only solved for very special cases.
3. THE MONTE CARLO METHOD

In order to investigate the charge transport in semiconductor materials we have to solve the Boltzmann Transport equation. Analytically it is only possible for a few simple cases. The obvious for the other cases is to do it numerically. There are several numerical methods, e.g. the iterative technique and a statistical technique called the Ensemble Monte Carlo (EMC) method. "Solving" the BTE with an EMC method means that a distribution in phase space is obtained that hopefully approximates the distribution function.

The last method has the advantage that no a priori simplifying assumptions have to be made. Complicated band structures may be implemented and it is possible to follow the evolution of the distribution function in time.

The model for electron transport in the EMC-method is a sequence of free flights interrupted by scatter processes. The motion of the electron during the free flight is governed by the external forces. The duration of the free flight, the choice of the scatter process and the state after scattering is determined with help of random numbers. The scatter processes themselves are assumed to be instantaneous. An ensemble of electrons is simulated simultaneously, therefore the method is called Ensemble Monte Carlo (EMC) method.

The art of Monte Carlo simulation is the generation of random numbers with a certain probability distribution \( f(x) \). In general the random variable \( \tilde{x} \) can be obtained with help of an uniformly distributed variable \( \tilde{r} \):

\[
\int_{0}^{\tilde{r}} dr = \int_{0}^{\tilde{x}} f(x) dx \quad (3.1)
\]

or

\[
\tilde{r} = F(\tilde{x}) \quad (3.2)
\]
were $F(x)$ is the cumulative distribution function.

The required $\tilde{x}$ is obtained by inversion,

$$\tilde{x} = F^{-1}(\tilde{r}).$$

(3.3)

With help of this technique we only need a random generator which produces uniformly distributed numbers between zero and one.

3.1 Selection of the free flight time

The free flight time is related to the scatter probability $\nu_i(k)$. For each scatter process $i$ this probability is described by $S_i(k,k')$.

$$\nu_i(k) = \frac{V}{(2\pi)^3} \iiint dk' S(k,k'),$$

(3.4)

where $dk'$ stands for $dk' \, dk' \, dk'$.

In spherical coordinates expression (3.4) is given according:

$$\nu_i(k) = \frac{V}{(2\pi)^3} \iiint dk' d\phi \, d\theta \, k'^2 \sin(\theta) \, S_i(k,k').$$

(3.5)

The total scatter rate $\gamma(k)$ is given according to

$$\gamma(k) = \sum_i \nu_i(k).$$

(3.6)

The value $\gamma(k(t)) \, dt$ is the probability that an electron experiences a scatter process in a time $dt$. The probability that the electron has not undergone a scattering during the time interval $(t_0, t)$ is [1]
\[
P_0(t_0, t) = \exp\left[-\int_{t_0}^{t} \gamma(k(t')) \, dt'\right]. \quad (3.7)
\]

So the free flight time, \( \bar{t} - t_0 \), can be obtained from

\[
P_0(t_0, \bar{t}) = \bar{r} \quad (3.8)
\]

This leads to the implicit expression

\[
\int_{t_0}^{\bar{t}} dt' \gamma(k(t')) = -\ln(\bar{r}) \quad (3.9)
\]

The problem of (3.9) is that \( k \) changes in the time due to the external forces and \( \gamma(k(t)) \) is not an analytical function of \( k \). Therefore the expression can only be evaluated at high computational cost.

Rees [2,3] proposed a solution for this problem. He introduced a dummy scatter process called self scattering. This process does not affect the state of the electron. The rate of this process is chosen in such way that during the period of interest the new total scatter rate \( \gamma'(k(t)) \) is constant. This constant is denoted with \( \Gamma \). The rate of the dummy process is \( \Gamma - \gamma(k(t)) \), which should be always larger or equal to zero. The calculation of the free flight time reduces now to

\[
\bar{t} = -\frac{\ln(1 - \bar{r})}{\Gamma} \quad (3.10)
\]
3.2 Choosing the scatter process

After the free flight has ended a scattering occurs. The decision of which process will take place is done with help of the conditional probabilities

\[ P_i = P( \text{process } i | k(t) ) = \frac{\nu_i(k)}{\Gamma} \]  \hspace{1cm} (3.11)

The process \( j \) is selected by choosing the process \( j \) for which

\[ \sum_{i=1}^{i-1} P_i < \tilde{r} \leq \sum_{i=1}^{j} P_i \]  \hspace{1cm} (3.12)

is true and \( \tilde{r} \) an uniformly distributed number between zero and one.

3.3 Choosing the state after scattering

After the scattering process has been selected the state \( k' \) after scattering has to be determined. If the process was self scattering no scattering occurs (\( k' = k \)). For all other cases the new state \( k' \) can be determined with the following procedure:

- The modulus \( k' \) of \( k' \) is calculated from the new kinetic energy \( W' \).
- The direction of \( k' \) is derived with help of the normalized distribution functions \( P_\theta(\theta) \) and \( P_\phi(\phi) \), (3.13) and (3.14). The angles (3.15) and (3.16) are selected with two uniformly distributed numbers \( \tilde{u}_1 \) and \( \tilde{u}_2 \).
If we choose a local coordinate system with the z-axis along the k-direction the distribution of \( \phi \) becomes uniformly distributed

\[
\tilde{\phi} = \frac{1}{\pi} \left( \tilde{\phi} \right)
\]

\( \tilde{\phi} = 2\pi\tilde{u}_1 \),

where \( \tilde{u}_1 \) is a random number between 0 and 1.

The angles \( \tilde{\phi} \) and \( \tilde{\theta} \) are determined in the local system. They are subsequently transformed back to the original system.
3.4 Technique based on overestimation

F.P. Widdershoven suggested a technique which enables to calculate the scatter rate and the state after scattering in full detail without numerical calculations of integrals and without numerical inversion techniques. He called this technique 'Overestimation'.

The idea behind this technique is to add self-scattering on each transition from \( k \to k' \). The self-scattering is chosen in such a way that the resulting expressions are analytically solvable. If a transition \( k \to k' \) happens a simple rejection scheme is enough to get rid of the overestimation. The big advantage is that although no simplifying assumptions have been made the program runs fast.

Before we discuss this technique we calculate the scatter rate and angle distribution for two different combined processes. We assume that process one and two are described by \( S_1(k,k') \) and \( S_2(k,k') \). We define a third process by combining one and two:

\[
S_3(k,k') = S_1(k,k') + S_2(k,k') \tag{3.18}
\]

The total scatter rate is easily found as:

\[
\nu_3(k) = \frac{V}{(2\pi)^3} \iiint dk'.S_3(k,k') \tag{3.19}
\]

It is clear from formula (3.19) that the scatter probability from \( k \) to \( k' \) is proportional to \( S_3(k,k') \). The modulus of \( k' \) is easily derived from the new kinetic energy after scattering. The angles \( \theta \) and \( \phi \) are derived with help of their distribution functions and pseudo-random uniformly distributed numbers \( \tilde{u}_1 \) and \( \tilde{u}_2 \) (3.17) and (3.16).

After calculating the new state \( k' \) for the combined process, we do not know which process was responsible for the change in \( k \). However we do know that the probability of this change is proportional to \( S_3(k,k') \). With this and (3.18) we can define conditional probabilities which describe the probability the
process was actually one or two:

\[
\begin{align*}
P(\text{process}=1|k,k') &= \frac{S_1(k,k')}{S_3(k,k')} \quad (3.20) \\
P(\text{process}=2|k,k') &= \frac{S_2(k,k')}{S_3(k,k')} \\
&= 1 - P(\text{process}=1|k,k') \quad (3.21)
\end{align*}
\]

We can use an algorithm (3.12) similar to the one which chooses the scatter process after a free flight. This algorithm in pseudo FORTRAN is, with \texttt{RAW} a uniformly distributed variable:

\[
\text{IF } \texttt{RAW} \text{.LT. } \frac{S_1(k,k')}{S_3(k,k')} \\
\text{THEN } \quad \text{process=1} \\
\text{ELSE } \quad \text{process=2} \quad (3.22)
\]

### 3.5 Overestimation

If we want to implement a scatter process in the program we need to calculate the total scatter rate and the new state after scattering. If we include the model in full detail the resulting expressions are often not analytically solvable. Equations and integrals have to be solved numerically. The price we pay for a more detailed model is an enormous consumption of cpu-time.

If we use the algorithm described in the previous section it is possible to avoid the difficult expressions. This technique is called overestimation.

The procedure is as follows:

1) Model of the process in full detail \(\rightarrow S(k,k')\)

2) If needed define a dummy process (which will lead to self-scattering) such that:

\[
S(k,k') = S(k,k') + S_d(k,k')
\]
- the calculation of $\hat{\nu}(k)$ and the state after scattering is possible analytically and if possible
- $S_d(k,k') \ll S(k,k')$.

3) Implementation of the scatter process is as follow:
- The overestimated version $\hat{S}(k,k')$ of $S(k,k')$ is implemented. After determining the new state with the simple formulas valid for the overestimated version we can decide which process was actually active using (3.8). If we find that the real process was active the calculated scattering occurs. If the dummy process was active we take self-scattering.

3.6 Discussion of the overestimation method

It is clear that with help of the concept of overestimation it is possible to arrive at a simple model for a highly complex process. Having simple expressions leads to a decreased use of cpu-time. However, it should be noted that the simple model leads to an extra amount of self scattering. Higher scatter rates lead to shorter free flight times, and thus higher computational costs. This is the reason why the constraint $S_d(k,k') \ll S(k,k')$ has to be met if possible. In general there will be a trade-off (figure 3.1) between model and cpu-time.

![Figure 3.1: Trade-off between cpu-time and model](image-url)
4. SCATTER PROCESSES DUE TO PHONONS

In this chapter we discuss the different scatter processes which are important in GaAs. We are only interested in low-field simulations. Therefore we will not discuss intervalley scattering and scatter processes in satellite valleys. We derive the different formulas. Our starting point is the scatter probability $S(k,k')$ which is found from first-order perturbation theory. These calculations can be found in many textbooks which discuss quantum phenomena in semiconductors, e.g. \[4,5,6\]. We will use the concept of 'overestimation' many times.

The scatter processes of interest are:

- Piëzo-electric scattering
- Acoustic deformation potential scattering
- Polar optical mode scattering
- Ionized impurity scattering.

In this chapter only the inelastic scatter processes are discussed. The elastic processes will be discussed in chapter 5.

4.1 Piëzo-electric scattering

Piëzo-electric scattering is caused by acoustic phonons of long wavelength. The perturbing potential is proportional to the gradient of the strain caused by the vibrating lattice. The energy associated with the phonon is low. The energy of a phonon with wave vector $q$ is:

$$W = \hbar \omega_q = \hbar v_q q$$  \hspace{1cm} (4.1)

with $q = |q|$ and $v_q$ the sound velocity which is assumed isotropic here. The state after scattering is defined through $k' = k \pm q$. The upper sign is for absorption and the lower sign is for
emission. The number of phonons with wave vector \( q \), \( \eta_q \), is given according to the Bose-Einstein distribution:

\[
\eta_q = \left[ \exp \left( \frac{\hbar \omega_q}{k_B T} \right) - 1 \right]^{-1}
\]

(4.2)

The piezo-electric constant, the relative dielectric constant, the reciprocal screening length and the non parabolicity factor are denoted respectively by \( K_p \), \( \epsilon_r \), \( \gamma \) and \( \alpha \).

The transition probability is given by

\[
S_n(k,k') = \frac{2\pi \hbar \nu \epsilon_r}{\epsilon_0 \epsilon_0 V q} \left[ \eta_q + \frac{1}{2} \mp \frac{1}{2} \right] \cdot \frac{q^4}{(q^2 + \gamma^2)^2} \cdot S(k,k') \cdot \delta \left[ W(k) \pm \hbar \nu q^2 - W(k') \right].
\]

(4.3)

with \( S(k,k') \) the overlap function

\[
S(k,k') = \left[ \frac{(1+\alpha W)(1+\alpha W')}{(1+2\alpha W)(1+2\alpha W')} + \alpha \cos(\theta) \cdot \frac{W W'}{(1+2\alpha W)(1+2\alpha W')} \right]^{2}
\]

(4.4)

and \( W = W(k) \) and \( W' = W(k') \), with \( W(k)(1+\alpha W(k)) = \frac{\hbar^2 k^2}{2m^*} \). The reciprocal screening length \( \gamma \) is defined as \( \gamma^2 = \frac{n e^2}{\epsilon_0 \epsilon_r k_B T} \), with \( n \) the electron concentration, \( k_B \) the Boltzmann constant and \( T \) the lattice temperature.

The energy-conserving \( \delta \)-function in (4.3) makes that only certain phonons \( (q) \) can be absorbed or emitted. If we use the definitions of figure 4.1, and combine these with the condition of energy conservation we can derive (4.5) and (4.6).

![Figure 4.1: Relation between k and k'](image)
\[
\begin{align*}
\hbar q &= \pm \frac{(1+2\alpha W)v_s m^* v_s \pm \hbar \cos(\beta)}{(1 - 2am^* v_s^2)^2}, \text{ with } \hbar q \geq 0 \quad (4.5)
\end{align*}
\]

and
\[
\mathbf{k} \cdot \mathbf{k}' - \mathbf{k} \cdot \mathbf{k}' \cos(\theta) = k^2 + kq \cos(\beta) \quad (4.6)
\]

In order to derive the scatter rate we use
\[
\nu^s(k) = \frac{V}{(2\pi)^3} \iiint \mathbf{d}k' \cdot S^s(k, k') = \frac{V}{(2\pi)^3} \iiint \mathbf{d}q' \cdot S^s(k, k')
\]
or in spherical coordinates
\[
- \frac{V}{(2\pi)^3} \int d\phi \int \sin(\beta) d\beta \int q^2 dq \cdot S^s(k, k+q) \quad (4.7)
\]

After some lengthy calculations it is possible to convert (4.7) into:
\[
\nu^s(k) = \frac{e^2 K^2 m^* v_s}{4\pi \varepsilon_0 \varepsilon_r \hbar^2 k} \int_{x_{\min}}^{x_{\max}} \left\{ \left[ \frac{1}{\exp(x)-1} + \frac{1}{2} \right] \right\} \cdot \mathcal{F}(k', k') \cdot \frac{k T}{\hbar v_s} x \left( \frac{k T}{\hbar v_s} \right)^2 \left( \frac{k T}{\hbar v_s} \right)^2 + \gamma^2 \right} \cdot dx \quad (4.8)
\]

with
\[
x = \frac{hv_s}{k T} q
\]

\[
x_{\min} = \begin{cases} 
0, & \text{emission} \\
\frac{2v_s}{k T} \frac{(1+2\alpha W)v_s - \hbar k}{(1 - 2am^* v_s^2)^2}, & \text{absorption}
\end{cases}
\]

\[
x_{\max} = \begin{cases} 
\frac{2v_s}{k T} \frac{\hbar k - (1+2\alpha W)v_s}{(1 - 2am^* v_s^2)^2}, & \text{emission} \\
\frac{2v_s}{k T} \frac{(1+2\alpha W)v_s + \hbar k}{(1 - 2am^* v_s^2)^2}, & \text{absorption}
\end{cases}
\]
4.1.1 Overestimation

In order to obtain a more simple expressions we use the concept of overestimation. Note that if we construct a probability density for the variable \( x \) the new state after scattering can be obtained. With a certain \( \bar{x} \) the new kinetic energy can be calculated (4.9) and with help of (4.6), the angles \( \bar{\beta} \) and \( \bar{\theta} \) are easily derived.

\[
W(k') = W(k) \pm k_B T x
\]  

(4.9)

The cumulative density function is given as:

\[
P_x(x) = \frac{P(x)}{P(0)}
\]  

(4.10)

with

\[
\tilde{x}
\]

\[
I(x) = \int_{x_{\text{min}}}^{\tilde{x}} \left[ \frac{1}{\exp(x) - 1} + \frac{1}{2} \right] \cdot \mathcal{G}(k,k').
\]

(4.11)

The following overestimations are used:

\[\frac{1}{\exp(x) - 1} \rightarrow \frac{1}{x}\] absorption

\[\frac{1}{\exp(x) - 1} + 1 \rightarrow \frac{1 + x_{\max}}{x}\] emission

\[\mathcal{G}(k,k') \rightarrow 1\] absorption

\[-(1 + 2\alpha(W \pm k_B T x)) \rightarrow \begin{cases} (1 + 2\alpha(W + k_B T x_{\max}) & \text{absorption} \\ (1 + 2\alpha W) & \text{emission} \end{cases}\]

\[\left( \frac{k_B T}{\hbar v_s} x \right)^4 \rightarrow \left( \frac{k_B T}{\hbar v_s} x \right)^2 \cdot \left( \left( \frac{k_B T}{\hbar v_s} x \right)^2 + \gamma^2 \right)\]

This leads to \( \hat{I}(x) \):
\[ I(\bar{x}) = \frac{1}{2} c \left\{ \frac{1}{\left( \frac{k_B T}{\hbar \nu_s} x_{\text{min}} + \gamma^2 \right)^2} + \frac{1}{\left( \frac{k_B T}{\hbar \nu_s} \bar{x} + \gamma^2 \right)^2} \right\} \] (4.12)

with
\[ c = \begin{cases} (1 + 2\alpha W) & \text{absorption} \\ (1 + 2\alpha(W + k_B T x_{\text{max}}))(1 + x_{\text{max}}) & \text{emission} \end{cases} \]

The cumulative distribution function is given as:
\[ P_x(x) = \frac{x}{I(0)} \] (4.13)

(4.13) can be easily inverted. The rejection step is straightforward.

### 4.1.2 Discussion

The implementation of piezoelectric scattering is easy if we use the concept of overestimation. The big advantage of the overestimation technique is that not one simplifying assumption has been used. Therefore the model accounts for non-parabolic bands, screening, the overlap function, inelastic scattering and the correct Bose-Einstein distribution.

### 4.2 Acoustic phonon scattering

Acoustic phonon scattering is scattering due to the deformation potential \( (E_{ac}) \). The process is taken to be inelastic. The energy relation for acoustic phonons is exactly the same as the one for piezoelectric scattering. The formulas derived for the modulus of \( q \), the minimal value of \( x \) and the max value of \( x \) are the same.

The transition probability is given by
Sem. \( S_{ac}^{(k,k')} = \frac{\pi \frac{\hbar^2}{\rho \hbar^2_s k} q}{V_{ac}} \left[ \eta_q + \frac{1}{2} \mp \frac{1}{2} \right] \left( \frac{q^2}{q^2 + \gamma^2} \right)^2 \)

\[ \mathcal{S}(k,k') \delta \left( W(k) - W(k') \pm \hbar \omega_{ac} \right) \] \hspace{1cm} (4.14)

with \( \rho \) the specific density.

The influence of screening is also taken into account. We use for the screening again the Debye-Hückel model. Although this model is not correct for time-varying potentials it may be used because the frequency of the disturbing potential is relatively low.

If we use the relations (4.1), (4.5), (4.6) and (4.14) we find for the scatter rate:

\[
\nu^{ab}(k) = \frac{\Xi^2 m}{4\pi v_s k} \left( \frac{k_B T}{\hbar} \right) \int_{x_{\min}}^{x_{\max}} dx \left\{ \left[ \frac{1}{\exp(x)-1} + \frac{1}{2} \mp \frac{1}{2} \right] \right\} \cdot \mathcal{S}(k,k') \cdot \left( 1 + 2\alpha(W \pm k_B T x) \right) \] \hspace{1cm} (4.15)

4.2.1 Overestimation

In order to get simple expressions we use the concept of overestimation. The following overestimations are used:

\[
* \left( \frac{q^2}{q^2 + \gamma^2} \right)^2 \longrightarrow 1
\]

\[
* \frac{1}{\exp(x)-1} \longrightarrow \frac{1}{x} \hspace{1cm} \text{absorption}
\]

\[
* \frac{1}{\exp(x)-1} + 1 \longrightarrow \frac{1 + x_{\max}}{x} \hspace{1cm} \text{emission}
\]

\[
* \mathcal{S}(k,k') \longrightarrow 1
\]
Following the same procedure we also used in the case of piezoelectric scattering we define an overestimated integral as:

\[
I(x) = \frac{\Xi^2}{4\pi v_s h^2 k} \left( \frac{k_B T}{h v} \right)^3 C \int_{x_{min}}^x x'.dx' \\
= \frac{\Xi^2}{8\pi v_s h^2 k} \left( \frac{k_B T}{h v} \right)^3 C \left[ x^2 - x_{min}^2 \right] \tag{4.16}
\]

with

\[
C = \begin{cases} 
(l+2\alpha(W + k_{T_{max}})) & \text{for absorption} \\
(l+2\alpha W)(1+x_{max}) & \text{for emission} 
\end{cases}
\]

and \( x \in (x_{min}, x_{max}). \)

The overestimated scatter rate is found as

\[
\nu_{\text{ab}}(k) = \frac{\Xi^2}{4\pi v_s h^2 k} \left( \frac{k_B T}{h v} \right)^3 C \left[ x_{max}^2 - x_{min}^2 \right] \tag{4.17}
\]

The cumulative distribution function for the variable \( x \) is constructed as follows

\[
P_x(\tilde{x}) = \frac{\hat{I}(\tilde{x})}{I(0)} = \frac{\tilde{x}^2 - x_{min}^2}{x_{max}^2 - x_{min}^2} \tag{4.18}
\]

With help of the cumulative distribution function it is easy to find a random variable \( \tilde{x} \). With this \( \tilde{x} \) it is easy to calculate the new energy (4.9), and with the formulas (4.5), (4.6) also the state after scattering. The overestimation is corrected with the help of a straightforward rejection technique.
4.2.2 Discussion

Scattering due to acoustic phonons can be implemented very easily if we use the concept of overestimation. In the overestimated version the disturbing potential is assumed to be unscreened. This approach leads not only to simple formulas, but has also one big advantage, it opens the possibility to introduce dynamic screening, and to use tabulated scatter rates at the same time.

If during the Monte Carlo simulation the screening length is calculated dynamically it varies. When acoustic scatter events take place it is possible to use the actual screening length in the rejection. The advantage of tabulated scatter frequencies is that they lead to a fast running program.

4.3.1 Polar optical scattering

In polar materials such as III-V compounds polar optical phonon scattering is a dominant scatter mechanism. The process is inelastic. According to first order perturbation theory the transition rate is given by:

\[
\begin{align*}
S_{ab}^{\text{p}}(k, k') &= \frac{2\pi}{\hbar} \frac{2\pi e^2 \hbar \omega_0}{4\pi \epsilon_0 V} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_v} \right) \frac{\mathcal{G}(k, k')}{q^2} \\
&\quad \times \left( \eta_q + \frac{1}{2} \pm \frac{1}{2} \right) \delta(\mathcal{W}(k') - \mathcal{W}(k) \pm \hbar \omega_0) 
\end{align*}
\]

(4.19)

With the phonon energy equal to \( \hbar \omega_0 \) and \( \epsilon_\infty \) the high frequency dielectric constant.

The expression for the transition probability is rather complex. Although application of the overestimation method is possible it was not implemented. The reason for this is that this scatter process was already implemented correctly. The scatter rate for
this process is given by:

\[
\nu(k) = \frac{(2m^*)^{1/2} e^2 \omega_0^2}{8\pi e_0^2 \hbar} \left( \begin{array}{cc} 1 & 1 \\ \epsilon_\infty & \epsilon_i \end{array} \right) \left( 1 + 2aW' \right)^{-1/2} \frac{F(W,W')}{y^{1/2}} \left( \eta + \frac{1}{2} \right)_{2/2} \text{ (4.20)}
\]

with

\[ W' = W \pm \hbar \omega_0, \ y = W(1+aW), \text{ and} \]

\[
F(W,W') = \frac{1}{C} \left[ A \ln \left( \frac{y^{1/2} + y'^{1/2}}{y^{1/2} + y'^{1/2}} \right) + B \right] \text{ (4.21)}
\]

\[ A = \left[ 2(1+aW)(1+aW') + \alpha(y+y') \right]^2 \text{ (4.22)}
\]

\[ B = -2\alpha(yy')^{1/2} \left[ 4(1+aW)(1+aW') + \alpha(y+y') \right] \text{ (4.23)}
\]

and \[ C = 4(1+aW)(1+aW')(1+2aW)(1+2aW') \text{. (4.24)} \]

The scatter angle \( \theta \) is not easily derived. However it is possible to make use of the combined technique [1]. This method, which looks like the overestimation method also uses random numbers to evaluate the expressions. This problem has been worked out by Widdershoven [7].
5. IONIZED-IMPURITY SCATTERING

Ionized-impurity scattering is an important scattering mechanism. It has been studied theoretically by many authors. Without doubt the two most important models are the Conwell-Weisskopf [8], and the Brooks-Herring model [9]. Many extensions and improvements have been made by other authors. Most of them have been reviewed in a paper of Chattopadhyay and Queisser [10].

Some of the extensions deal with coherent multiple center scattering [11-13]. These effects are important for compensated semiconductors where the positions of the donor and accepter atoms can be correlated, due to the formation of clusters during crystal growth. Widdershoven [14] modeled correlated impurity clusters for the case of an uncompensated material. This model is with a simple adaptation also applicable for dipole scattering.

In order to investigate the effects on mobility of clusters with correlated impurities on the mobility we used the model derived by Widdershoven. We expect that the adapted model, valid for dipole scattering, has serious effects on the electron distribution function. Therefore the influence on the distribution function is investigated.

5.1 Ionized-impurity scattering due to clusters of correlated impurities

If we use first order perturbation theory and assume that the impurities in a cluster have an isotropic Gaussian distribution, with standard deviation $\sigma$ we can derive [14]:

$$\left\{ S(k,k') \right\} = \frac{2 \pi}{h} \frac{e^4 M N_c}{V(\epsilon_0 \epsilon_r)^2} \frac{1+(M-1)\exp(-q^2\sigma^2)}{(q^2 + \gamma^2)^2} \cdot$$

$$\left( \delta(k,k') \right) \delta(W(k') - W(k)) \quad (5.1)$$
In this formula the (*) means that all cluster configurations are averaged. \( M \) is the number of impurities in one cluster, \( N_c \) the cluster concentration and \( \sigma \) is the standard deviation of the isotropic Gaussian distribution of the donor atoms in one cluster. We shall use this formula as a starting point for further investigation.

### 5.1.1 Limits

To get some understanding what the effects of correlated clusters are it is useful to investigate some limits of (5.1). The first limit is that we take simply \( M = 1 \). This means that we have no clusters. As we expect the transition probability (5.2) is equal to the one of the Brooks-Herring model, with \( N_d = N_c \):

\[
\begin{align*}
\{ S(k,k') \} &= -\frac{2\pi}{h} \frac{e^4 N_d}{V(\epsilon_0 \varepsilon_r)^2} \frac{\delta(k,k')}{(q^2 + \gamma^2)^2} \delta(W(k') - W(k)) \quad (5.2)
\end{align*}
\]

Another limit is the case that there is no correlation \( (\sigma \to \infty) \), which leads also to (5.2). A third case is that the correlation is so strong \( (\sigma \to 0) \) that the cluster acts like one \( M \) times ionized impurity. This leads to the Brooks-Herring transition probability with \( \epsilon = M \) the valence of the impurity:

\[
\begin{align*}
\{ S(k,k') \} &= \frac{2\pi}{h} \frac{Z^2 e^4 N_c}{V(\epsilon_0 \varepsilon_r)^2} \frac{\delta(k,k')}{(q^2 + \gamma^2)^2} \delta(W(k') - W(k)) \quad (5.3)
\end{align*}
\]

If we look at the two extreme cases, very compact clusters (5.3) and no clusters (5.2), we see that the transition probability differs a factor \( M \). All that happens between these cases is described by (5.1).
5.1.2 The scatter rate and state after scattering.

The scatter rate for ionized-impurity scattering is given according to:

\[ \nu(k) = \frac{V}{(2\pi)^3} \iiint dk' \left\{ \mathcal{S}(k, k') \right\} \] (5.4)

If we use the the dispersion relation

\[ \mathcal{W}(k) = \frac{\hbar^2 k^2}{2m^*} \] (5.5)

we find:

\[ \nu(k) = \frac{M N c m^* (1+2\alpha \mathcal{W})}{2\pi (\varepsilon_0 \varepsilon_r)^2 \hbar^3 k} \int_0^\pi d\theta \sin(\theta) \frac{1 + (M-1)\exp(-2k^2(1-\cos(\theta)\sigma^2))}{(2k^2(1-\cos(\theta) + \gamma^2)^2).\mathcal{G}(k, k')} \] (5.6)

with

\[ \mathcal{G}(k, k') = \frac{(1+\alpha \mathcal{W}(1+\cos(\theta)))^2}{(1+2\alpha \mathcal{W})^2} \] (5.7)

Calculation of (5.6) leads to exponential integrals. The expressions which determine the state after scattering are not analytically solvable, even if the overlap function is not taken into account. In order to simplify the problem we use the overestimation method to solve the problem statistically. We can use the following overestimations:

- \[ \mathcal{G}(k, k') \leq 1 \rightarrow 1 \]
- \[ 1 + (M-1)\exp(-q^2\sigma^2) \rightarrow M \]
  or \[ \rightarrow 1 + (M-1)\exp(-4k^2\sigma^2) \]
The last overestimation is somewhat more complex but it may be interesting especially if \( 1 < 1 + (M-1)\exp(-4k^2\sigma^2) < M \). If we use the simple expression we find:

\[
\nu(k) = M^2 \frac{N m^*e^4(1+2aW)}{\pi(\varepsilon_0\varepsilon_r)^2\hbar^3\gamma^2} \frac{k}{4k^2 + \gamma^2} \tag{5.8}
\]

If we use the general expressions we can easily derive a random angle \( \theta \) with help of an uniformly distributed number \( \bar{u} \):

\[
\cos(\bar{\theta}) = 1 - \frac{2\gamma^2\bar{u}}{4k^2(1-\bar{u}) + \gamma^2} \tag{5.9}
\]

In the rejection technique we can get rid of the overestimation. This is done with the following algorithm:

IF ( \( M \cdot \text{RAN.GT.} (1-\exp[-2k^2(1-\cos(\bar{\theta})]) \cdot \nu(k,k') \) )

THEN SELF SCATTERING

ELSE SCATTER WITH \( \bar{\theta} \) \tag{5.10}

5.1.3 Ridley model

The big disadvantage of the Brooks-Herring model is that the scatter rate can become very high. Ridley [15] suggested that ionized impurity scattering is actually not a two-body problem. He introduced a concept which he called statistical screening. If a scatter process occurs it is possible that a second scatterer is nearer. He proposed that if that was the case the scatter process does not take place. He derived for this model a modified cross section. This modified cross section leads to a much lower scatter rate, especially when the impact parameter is large, that is for those scatterings where the deflection of the electron is small.

Instead under the name of statistical screening model this model is also known as the Ridley model. Although the physical base of statistical screening is not physical and therefore questionable, it is nice for Monte Carlo purposes and it works very well [16]. In
the next section we will derive a Ridley model for scattering due to clusters of ionized impurities.

As a starting point we use the transition probability according to (5.1). In order to derive the Ridley model for clusters of ionized impurities it is important that we take a whole cluster as one scatterer. If we do not do this we are not able to define an average distance between the scatterers. We shall use the subscripts \( b \) and \( r \) respectively for Brooks-Herring and Ridley quantities.

Classically [4] the scatter rate is given by

\[
\nu_B(k) = n_c \nu(k) \Sigma_B. \tag{5.11}
\]

The total cross section \( \Sigma_B \) is given by

\[
\Sigma_B = \int_0^\pi 2\pi \sin(\theta) \sigma_B(\theta) \, d\theta. \tag{5.12}
\]

If we combine (5.4), (5.11) and (5.12) we find for the differential cross section \( \sigma_B(\theta) \)

\[
\sigma_B(\theta) = \frac{1}{N_c \nu(k)} \frac{V}{(2\pi)^3} \int_0^\infty k'^2 \, dk' S_B(k, k'). \tag{5.13}
\]

Integrating over the energy conserving \( \delta \)-function leads to

\[
\sigma_B(\theta) = M \frac{m^* e^4 (1+2\alpha \omega)^2}{4\pi^2 h^4 (\epsilon_0 \epsilon_r)^2} \frac{1 + (M-1)\exp(-q^2\sigma^2)}{(q^2 + \lambda_D^{-2})^2} \cdot \mathcal{G}(k, k'). \tag{5.14}
\]

with \( q^2 = 2k^2(1-\cos(\theta)) \) and \( \mathcal{G}(k, k') \) given by (5.7). According to Ridley we introduce a modified cross section

26
\[ \sigma_R(\theta) = \sigma_B(\theta) \cdot \exp\left(-a N_c \int_0^\pi 2\pi \sin(\theta') \cdot \sigma_B(\theta') \cdot d\theta' \right) \] (5.15)

with \( a = N_c^{-1/3} \) the average distance between the scatterers. If we integrate \( \sigma_R(\theta) \) over the space angle we find for the total cross section \( \Sigma_R \):

\[ \Sigma_R = \frac{1}{a N_c} \left[ 1 - \exp\left( -\frac{a}{v(k)} \nu_B(k) \right) \right]. \] (5.16)

The Ridley scatter rate is found if we substitute (5.16) into (5.12), the classical definition

\[ \nu_R(k) = \frac{v(k)}{a_c} \left[ 1 - \exp\left( -\frac{a}{v(k)} \nu_B(k) \right) \right]. \] (5.17)

For the calculation of the angle after scattering we can use the cumulative angle distribution function

\[ P_{R,\theta}(\theta) = 1 - \frac{\nu_{R,\theta}(\theta)}{\nu_{R,\theta}(0)} \] (5.18)

with

\[ \nu_{R,\theta}(\theta) = \int_0^\pi 2\pi \sin(\theta') \cdot \sigma_R(\theta') \cdot d\theta' \] (5.19)

The problem with (5.17) and (5.18) is that the expressions are complex and can be calculated only at high computational costs.

5.1.3.1 Overestimation

In this section we will derive an efficient algorithm based on overestimation which is implemented in the Monte Carlo program. If we look at the Ridley cross section there are two obvious overestimations:
1) \( \hat{\sigma}_R(\theta) = \hat{\sigma}_B(\theta) \), and

2) \( \hat{\sigma}_R(\theta) = \hat{\sigma}_B(\theta) \). exp \left\{ -a N \int_0^\pi 2\pi \sin(\theta) \hat{\sigma}_B(\theta) d\theta \right\}

with \( \hat{\sigma}_B(\theta) \) an overestimated version and \( \hat{\sigma}_B(\theta) \) an underestimated version of the Brooks-Herring differential cross section. The first overestimation is not interesting because it leads to the Brooks-Herring scatter rate. We have to use the second one.

Note that it is only possible to calculate the total cross section (5.16) easily if \( \hat{\sigma}_B(\theta) = C \hat{\sigma}_B(\theta) \). C should be independent of \( \theta \). Therefore the following estimations were used:

\[
\hat{\sigma}_B(\theta) = \frac{m^2 e}{4\pi^2 \hbar^2 (\epsilon_0 \epsilon_r)^2} \cdot \frac{M^2}{(q^2 + \lambda_D^{-2})^2} \tag{5.20}
\]

and

\[
\hat{\sigma}_B(\theta) = \frac{m^2 e}{4\pi^2 \hbar^2 (\epsilon_0 \epsilon_r)^2} \cdot \frac{M}{(q^2 + \lambda_D^{-2})^2}. \tag{5.21}
\]

With the above estimation it is easy to calculate the scatter rate \( \hat{\nu}_R(k) \) and the cumulative angle distribution function \( P_{R, \theta}(\theta) \) with help of

\[
\hat{\nu}_{R, \theta}(\theta) = \int_0^\pi 2\pi \sin(\theta'). \hat{\sigma}_R(\theta'). d\theta'
\]

\[
= M(1+2\alpha W)^2 \frac{\nu(k)}{a_c} \left[ 1 - \exp \left\{ -\frac{a_c}{\nu(k)} \hat{\nu}_{B, \theta}(\theta) \right\} \right] \tag{5.22}
\]

with

\[
\hat{\nu}_{B, \theta}(\theta) = \frac{M m^* e^4}{\pi \hbar^3 (\epsilon_0 \epsilon_r)^2} \frac{1}{4k} \left\{ \frac{1}{2k^2(1-\cos(\theta)) + \lambda_D^{-2}} - \frac{1}{4k^2 + \lambda_D^{-2}} \right\} \tag{5.23}
\]

The overestimated scatter rate is found using \( \hat{\nu}_R(k) = \hat{\nu}_{R, \theta}(0) \). The angle after scattering can be determined with help of the cumulative distribution function.
\[ P_{R,\theta}(\theta) = 1 - \frac{\nu_{R,\theta}(0)}{\nu_{R,\theta}(\theta)}. \] (5.24)

5.1.3.2 Calculation of the angle after scattering

We can determine the angle \( \bar{\theta} \) after scattering with help of an uniformly distributed number \( \bar{u} \):

\[ \bar{\theta} = R_{R,\theta}^{-1}(\bar{u}). \] (5.25)

If we define \( \bar{y} = y(\bar{\theta}) = \frac{a}{v(k)} \nu_{B,\theta}(\theta) \), then \( \bar{y} \) is related to \( \bar{u} \) according to:

\[ \bar{y} = -\ln\left[ 1 - (\bar{u}-1)\left( 1 - \exp\left[ -\frac{a}{v(k)} \nu_{B,\theta}(0) \right] \right) \right]. \] (5.26)

If we use this new variable and combine this with the definition we find

\[ \cos(\bar{\theta}) = 1 + \frac{\gamma^2}{2k^2} - \frac{1}{\frac{2k^2}{4k^2 + \gamma^2} + \bar{y} \frac{8 \pi \hbar^4 (\epsilon_0^2 \epsilon_r^2)^2 4k^4}{a \mathcal{N} m^2 \mathcal{E}^4}}. \] (5.27)

With help of overestimation it is possible to calculate the scatter rate and angle after scattering analytically. With help of the rejection technique we should get rid of the overestimation.

5.1.3.3 Rejection technique

The straightforward method for the rejection technique is the algorithm:

\[ \text{IF} (\hat{R}_{R,\theta}(\bar{\theta}), \sigma_{R,\theta}(\bar{\theta})) \text{ THEN SELF SCATTERING ELSE SCATTER WITH } \theta \] (5.28)

The evaluation of this expression lead to serious difficulties. Where we could avoid numerical calculation of difficult integrals
this is not possible in the rejection technique. However it is possible to cut this problem in several parts and use the concept of overestimation itself again in the rejection technique.

We define a short hand for the rejection procedure:

\[ a > b \] \text{ means if the upper inequality is true then a self-scattering occurs. If the lower inequality is true the calculated scatter process occurs.}

We can write (5.28) as

\[
\tilde{v} > \frac{\sigma_B(\tilde{\theta})}{\sigma_B(\tilde{\theta})} \cdot \exp \left\{ - a N \pi \int_{\theta}^{\pi} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta \right\}
\] (5.29)

We know that if \( \tilde{u} > A > A.B \) that a self-scattering occurs. If this is not the case we can define a new random variable \( \tilde{v} \)

\[
\tilde{v} = \tilde{u} \cdot \frac{\sigma_B(\tilde{\theta})}{\sigma_B(\tilde{\theta})}
\] (5.30)

This variable is uniformly distributed between zero and one. The check we now have to do is

\[
\tilde{v} > \frac{\sigma_B(\tilde{\theta})}{\sigma_B(\tilde{\theta})} \cdot \exp \left\{ - a N \pi \int_{\theta}^{\pi} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta \right\}
\] (5.31)

or

\[
\tilde{w} = -\ln(\tilde{v}) < a N \pi \int_{\theta}^{\pi} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta
\] (5.32)

Again we can limit our problem if we define a boundary \( w_b \).

\[
w_b = a N \pi \int_{\theta}^{\pi} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta \geq -\ln(B)
\] (5.33)
Note that this boundary can be calculated analytically. Now we know that if \( \tilde{w} \geq w_b \geq -\ln(B) \) then the calculated scatter process happens. If this is not the case then \( w \in (0, w_b) \). We describe the remaining problem as:

\[
\tilde{w} = a N_c \int_{\theta_1}^{\theta_2} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta = a N_c \int_{\theta_1}^{\theta_2} 2\pi \sin(\theta) \left[ \sigma_B(\theta) - \hat{\sigma}_B(\theta) \right] d\theta
\]

We can write (5.34) as \( \cos(\theta) \leq \cos(\theta) \). The remaining problem can be solved if we interpreted the expression with \( \theta_1 \) and \( \theta_2 \) as cumulative distribution function, see figure 5.1.

![Figure 5.1: The distribution functions](image)

In this context we can evaluate (5.34) statistically. If we calculate with the overestimated formula the angle \( \theta_1 \), which is always bigger than \( \theta \), we put \( \theta_2 \) equal to \( \theta_1 \). With help of the rejection technique (5.35) we can derive the right distribution of \( \theta_1 \) for \( \theta_1 > \theta \).
If\( u_{1} \cdot \hat{L} \cdot T \left( \frac{\sigma_{B}(\theta_{1}) - \sigma_{B}(\theta_{1})}{\sigma_{B}(\theta_{1})} \right) \) THEN \( \theta_{1} \) is accepted  
ELSE \( \theta_{1} \) is not accepted \( (5.35) \)

It is clear that when \( \theta_{1} \) is accepted than a self scattering occurs. If \( \theta_{1} \) is not accepted then the calculated scatter process with angle \( \theta \) occurs.

5.1.4 Conclusion

If we use the Brooks-Herring model in the Monte Carlo program we get very high scatter rates. These high scatter rates lead to short free flight times and thus high computational costs. An alternative scatter mechanism, proposed by Ridley, does not have this disadvantage.

This model is more complex, but with help of overestimation it is possible to derive analytical solutions for the scatter rate and state after scattering. The rejection technique is not straightforward. If we cut this problem into parts and use the concept of overestimation itself again it is possible to arrive at a simple algorithm.

5.2 Dipole scattering

A special case of ionized impurity scattering is scattering due to dipoles. A dipole is a scatterer which consists of two oppositely charged impurities. We assume that both impurities have valence \( |Z|=1 \). The field of the dipole can be characterized with the distance \( \Lambda \) between the impurities.

We can use the transition probability derived for clusters of ionized impurities, with a simple adaptation, also for dipole scattering. The adaptations are that we take \( M=2 \), and that the influence of the neighbors, i.e. the term with \((M-1)\exp(-q^{2}a^{2})\), is
in the opposite direction. Further we change the cluster density $N_c$ into the dipole density $N_{di}$. We now find for the transition probability:

$$
\left\{ S(k, k') \right\} = \frac{2 \pi}{h} \frac{e^4}{V(\epsilon_0 \epsilon_r)^2} \frac{2 N_{di}}{\frac{N_{D} + N_{A}}{(q^2 + \gamma^2)^2}} 1 - \exp(-q^2 \sigma^2) .
$$

$$
\Psi(k, k') \delta(\mathcal{W}(k') - \mathcal{W}(k)) \quad (5.36)
$$

It is clear that the role of $\Lambda$ is accounted for by $\sigma$. The averaging procedure over all dipole configurations leads to an isotropic transition probability.

One understandable limit of (5.36), $\sigma \rightarrow \infty$, is the case that we do not have dipoles but separate acceptors and donors instead, as is the case in compensated semiconductors. In this case the total transition probability, is simply the sum of the rate due to the acceptors $N_A$ and donors $N_D$.

$$
\left\{ S(k, k') \right\} = \frac{2 \pi}{h} \frac{e^4}{V(\epsilon_0 \epsilon_r)^2} \frac{N_{D} + N_{A}}{(q^2 + \gamma^2)^2} 1 - \exp(-q^2 \sigma^2) .
$$

$$
\Psi(k, k') \delta(\mathcal{W}(k') - \mathcal{W}(k)) \quad (5.37)
$$

Another limit is not physical but interesting. If we take $\sigma \rightarrow 0$ we have an dipole with length $\Lambda = 0$. Such a dipole is not active. The transition probability is given by $(S(k, k')) = 0$.

If we use the general formula (3.5) we can find for the scatter rate the following expression

$$
\nu(k) = C(k) \int_0^{\pi} \frac{1 - \exp[-2k^2(1-\cos(\theta))\sigma^2]}{(2k^2(1-\cos(\theta)+\gamma^2)^2)} \Psi(k, k') \sin(\theta) \, d\theta, \quad (5.38)
$$

with

$$
C(k) = \frac{N_{di} e^4 m*(1+2\alpha W) k}{\pi h^3 (\epsilon_0 \epsilon_r)^2} \quad (5.39)
$$
In order to derive the scatter rate and the state after scattering analytically we use the concept of overestimation. We introduce \( v = (1 - \cos(\theta)) \) and try to find a suitable overestimation for the integral in (5.38). We make use of \( I(v) \) defined according

\[
I(v) = \int_{0}^{v} \frac{1 - \exp[-2k^2v'\sigma^2]}{(2k^2v' + \gamma^2)^2} \varphi(k,k') \, dv'. \tag{5.40}
\]

Note that the maximal value of \( v \) is two.

### 5.2.1 Overestimation

We want to use the concept of overestimation in order to get simple expressions. The following overestimations are possible:

- For \( \varphi(k,k') \leq 1 \)
  \[ 1 \]
- For \( \varphi(k,k') \geq 1 \)
  \[ \frac{1 - \exp[-2k^2v'\sigma^2]}{(2k^2v' + \gamma^2)^2} \xrightarrow{\text{A}} \frac{1}{(2k^2v' + \gamma^2)^2} \]
  \[ \text{or} \quad \frac{2k^2\sigma^2}{\gamma^4} v' \xrightarrow{\text{B}} \]

Of the second set is the first overestimation (A) is good for large \( v \) and the second (B) is good for small \( v \), see figure 5.2.

![Figure 5.2: Influence of the overestimation](image-url)
As can be seen easily from figure 5.2 it may be profitable to use a combination of the two overestimations (A) and (B). We should switch between the two overestimations at the boundary $v_b$. This boundary is found if expression (A) equals (B). This can be written as:

$$u. (u + \gamma \sigma^2)^2 - (\gamma \sigma^2)^2 = 0,$$

(5.41)

with $u = u(v) = 2k^2 \sigma^2 v$. If the screening parameter does not change during the program, the value $u_b = u(v_b)$ has to be calculated only once. We can do it in the preprocessing step and use a Newton-Raphson algorithm. After this is done the boundary $v_b$ can be calculated as

$$v_b = \frac{u_b}{2k^2 \sigma^2}$$

(5.42)

If $v_b$ is greater than two it is clear that overestimation (B) is not relevant. If $v > 2$ we take $v_b$ equal to two. We can construct an overestimated integral $I(v)$.

$$\hat{I}(v) = \int_0^{v_1} \frac{2k^2 \sigma^2}{\gamma^4} v \, dv' + \int_{v_1}^{v_2} \frac{1}{(2k^2v' + \gamma^2)^2} \, dv'.

(5.43)

with $v_1 = \min(v_b, v)$ and $v_2 = \max(v_b, v)$. With help of (5.43) we find for the overestimated scatter rate $\hat{\nu}(k)$

$$\hat{\nu}(k) = C(k) \left\{ \frac{k^2 \sigma^2}{\gamma^4} v_b^2 + \frac{2 - v_b}{(2k^2v_1 + \gamma^2)(4k^2 + \gamma^2)} \right\}

(5.44)

The cumulative distribution function can be constructed according to:

$$P_{\nu}(v) = \frac{\hat{I}(v)}{\hat{I}(0)}

(5.45)

The state after a scattering has occurred can be determined with the help of a uniformly distributed number $\tilde{r}$:

$$\tilde{r} = P_{\nu}^{-1} (\nu)

(5.46)

There are three possible situations if we want to calculate (5.46):

I) $v_b = 2$

II) $\tilde{v} \leq v_b$, and $v_b < 2$

III) $\tilde{v} > v_b$, and $v_b < 2$
In situation I the state after scattering is calculated according to
\[ \cos(\theta) = 1 - 2\sqrt{\frac{r}{\bar{r}}} \tag{5.47} \]
If we are in situation II or III we can define a boundary \( r_b \)
\[ r_b = \frac{\hat{I}(\nu_v)}{I(2)} \tag{5.48} \]
It is clear that if our random number \( \bar{r} \) is less than \( r_b \) then situation II is valid. If \( \bar{r} \) is greater than \( r_b \) then situation III is valid.

If situation II is valid then the angle after scattering is given by
\[ \cos(\theta) = 1 - \sqrt{\frac{\bar{r}}{I(0)} \frac{\gamma^4}{k^2\sigma^2}} \tag{5.49} \]
and if situation III is valid by
\[ \cos(\theta) = 1 + \frac{\gamma^2}{2k^2} - \frac{1}{2k^2} \frac{2k\nu + \gamma^2}{1 - 2k^2(\bar{r} - r_b)(2k\nu + \gamma^2)} \tag{5.50} \]

5.2.2 Discussion

If we compare scattering due to a dipole with a cluster of two identical charged monopoles there are some important differences. First of all there is of course the difference in the transition probabilities. The term \( 1 - \exp(q^2\sigma^2) \) reduces the transition probability, especially if \( q^2\sigma^2 = 2k^2\sigma^2(1 - \cos(\theta)) \ll 1 \). This means that slow electrons will be scattered less than would be the case with 'normal' ionized-impurity scattering. The fast electrons are scattered as they would be with 'normal' ionized-impurity scattering.

Another difference is that the dipoles do not contribute to the free electron concentration. This means that the screening does not change if the dipole concentration is changed. A semiconductor with only dipoles has almost no free electrons and hardly any screening.
This leads to extremely high scatter rates. In order to get some screening we have to implement in addition to the dipoles 'normal' impurities.

5.2.3 Estimation of the effects

Before we investigate the influence of dipoles on the electron distribution function we want to know what we can expect. Therefore we calculate the momentum relaxation time \( \tau_m(W) \) for dipole scattering. If we average this over the Maxwell-Boltzmann distribution we can find the average momentum relaxation time and the mobility. If we rewrite this expression we can find a criterion for when the influence should become detectable.

Another point of interest is the screening. The dipoles do not contribute to the free carrier concentration. This would mean that the screening parameter \( \gamma \to 0 \), and that the scatter rate becomes infinitely high. We introduce screening with help of loose donor atoms \( N_D \). The screening parameter \( \gamma^2 \) now becomes:

\[
\gamma^2 = \frac{eN_D}{\epsilon_0 \epsilon_r k T} \quad (5.51)
\]

If we want to follow the procedure described above it is easy to make some simplifying assumptions. We use a linear approximation instead of the exponential term in the transition probability:

\[ q^2 \sigma^2 = 1 - \exp(-q^2 \sigma) \text{ if } q^2 \sigma < 1. \]

Further we use parabolic bands ( \( \mathcal{E}(k,k')=1 \) and \( \alpha = 0 \)). Now the transition probability is given by

\[
\left\{ S(k,k') \right\} = \frac{2 \pi e^4 2 N_d}{h} \frac{q^2 \sigma^2}{(q^2 + \gamma^2)^2} \delta(W(k')-W(k)) \quad (5.52)
\]

Although this expression is not correct it gives a good understanding of what happens to the mobility in the case of dipoles. If we use the definition of the momentum relaxation time we find
\[
\frac{1}{\tau_m(W)} = \frac{1}{(2\pi)^3} \iiint \frac{k \cdot q}{k^2 \cdot S(k, k')} \, dk' \, dk \qquad (5.53)
\]

or

\[
\frac{1}{\tau_m(W)} = \frac{\sqrt{2m}}{4\pi \hbar^2 (\varepsilon_o \varepsilon_r)^2 \sqrt{W(k)}} \left[ 1 - \frac{\gamma^2}{2k^2} \ln \left( 1 + \frac{2k^2}{\gamma^2} \right) + \frac{1}{1 + \frac{4k^2}{\gamma^2}} \right] \quad (5.54)
\]

with \( u = \frac{W(k)}{k_B T} \) and \( \beta = \frac{1}{h \gamma} \sqrt{\frac{24m}{k_B T}} \).

Averaging (5.54) over \( f_0(k) \), the Maxwell-Boltzmann distribution function with energy as weighting factor, leads to:

\[
< \tau_m > = \frac{2}{3} \int \int \int \frac{d^3k}{k_B T} \cdot \tau_m(W(k)) \cdot W(k) \cdot f_0(k) \quad (5.55)
\]

with

\[
f_0(k) = \frac{\hbar^3}{(2\pi m k_B T)^{2/3}} \exp(-u) \quad (5.56)
\]

of which the result is approximated by:

\[
< \tau_m > = \frac{128\sqrt{2\pi m k_B T} (\varepsilon_o \varepsilon_r)^2 k_B T}{e^4(2N_{DA})(\gamma^2 \sigma^2) \left[ \beta^2 - 3.1 \ln \left( 1 + 2\frac{\beta^2}{3} \right) + \frac{\beta^2}{1 + 2\frac{\beta^2}{3}} \right]} \quad (5.57)
\]
The corresponding dipole mobility can be found according to

$$
\mu_{\text{dip}} = \frac{e^{<r>}}{m^*} \frac{\mathcal{L}(\beta^2) \cdot \mu_{\text{BH}}(N_D, T, 2N_D \cdot N_A)}{(\gamma^2 \alpha^2) \left[ \beta^2 - 3.1 \ln \left( 1 + \frac{2}{3} \beta^2 \right) + \frac{\beta^2}{1 + \frac{2}{3} \beta^2} \right]} 
$$

(5.58)

with

$$
\mathcal{L}(x) = \ln(1+x) - \frac{1}{1+x} 
$$

(5.59)

and

$$
\mu_{\text{BH}}(N_D, T, N_A) = \frac{256 \pi (\epsilon_0 \epsilon_r)^2 (k_B T)^{2/3}}{e^3 N^3 \sqrt{2 \pi m^*} \mathcal{L}(\beta^2)} 
$$

(5.60)

If we look at (5.58) we can see that the dipole and normal impurity mobility will be discrepant if the correction term differs seriously from 1. This leads to a critical $(\gamma \alpha)$ value according:

$$
(\gamma \alpha)^2_{\text{crit}} = \frac{\mathcal{L}(\beta^2)}{\beta^2 - 3.1 \ln \left( 1 + \frac{2}{3} \beta^2 \right) + \frac{\beta^2}{1 + \frac{2}{3} \beta^2}} 
$$

(5.61)

It can easily be seen that if we take $(\gamma \alpha) < (\gamma \alpha)_{\text{crit}}$, we can expect for $(4k_b^2 \sigma^2) < 1$ a different relaxation behaviour compared with ordinary ionized impurity scattering. The second constraint indicates where the dipole scattering is beginning to act like ordinary ionized impurity scattering.

Both constraints lead to an interesting property. If it is possible to make a semiconductor with constraint $(\gamma \alpha) < (\gamma \alpha)_{\text{crit}}$ and $4k_b^2 \sigma^2 = 1$ with $k_b$ bigger than the average reciprocal vector then we have an selective scatter mechanism. All electrons with state vectors below $k_b$ are hardly scattered but electrons with $k$ bigger than $k_b$ are scattered like ordinary ionized impurity scattering.
An interesting possibility is the case that $k_b$ is such that the drift mobility is hardly affected. The interesting effects are detectable at the high energy region of the electron distribution function. There will be less electrons with high energy, leading to a decreased hot electron effect.

This property could be very interesting. The reason for this is that the lifetime of many devices is decreased by hot electrons effects. An added hot electron scatter mechanism could increase the lifetime of those devices.

The approximation gives a good understanding of the possible effects on the electron distribution. It is also possible to calculate the momentum relaxation time if we do not use the linear approximation for $1 - \exp(-q^2\sigma^2)$. The momentum relaxation time we now find is:

\[
\frac{1}{\tau_r(k)} = \frac{m^*e^4(2N_{d_1})}{8\pi(e_0\epsilon_0)^2h^3k^3} \left[ \mathcal{E} \left( \frac{4k^2}{\gamma^2} \right) \right] - (M - 1) \mathcal{K} \left( \frac{4k^2}{\gamma^2}, \gamma^2\right) \right] \quad (5.62)
\]

with \[
\mathcal{K}(x,y) = (1+y) \exp(y) \left[ E_1(y) - E_1(y+xy) \right] \quad -1 + \frac{\exp(-xy)}{1 + x} \quad (5.63)
\]

and

\[
E_1(x) = \int_x^\infty \frac{\exp(-z)}{z} \, dz \quad (5.64)
\]
6. SELF CONSISTENT SCREENING

A perturbing potential will collect a gas of charged carriers around itself. This results in a disturbance of the carrier distribution in its neighborhood. Charged impurities for example will attract oppositely charged carriers and repel identically charged carriers. The result is that the actual potential is screened. Usually a screened potential has a smaller range than an unscreened potential. Therefore screening reduces the scatter rate of a scatter process.

For a number of processes it is important for Monte Carlo purposes to have screening. If no screening is present the scatter rate is infinity high as is the case for ionized-impurity scattering and piezo-electric scattering.

6.1 Theory

F.P. Widdershoven derived a model which delivers self-consistent screening. This model results in a averaging procedure over the distribution function. For Monte Carlo purposes the averaging over the distribution function can be replaced by an averaging over the electron ensemble of the program.

For the derivation of the screening length we shall use first order perturbation theory. We shall derive a general model for the screening length valid for a semiconductor with different bands. We use $\nu$, as the band index.

The unperturbed wave function for an electron in band $\nu$ is given according to [22] as:

$$\Psi_{\nu,k}(r) = N^{-1/2} \cdot u_{\nu,k}(r) \cdot \exp(ik \cdot r)$$  \hspace{1cm} (6.1)

with $N$ the number of units cells in the crystal volume $\Omega_e$. The cell-periodic part of the wave function $u_{\nu,k}(r)$ is normalized in a unit cell volume $\Omega_u$: 

41
The real disturbing potential $v(r)$ is assumed to vary slowly with respect to the unit cell dimensions. The matrix element is

$$<v', k' | v(r) | v, k> = \int_{\Omega_u} \psi_{\nu', k'}(r) \psi_{\nu, k}(r) dr^3$$

$$= \sum_{j=1}^{N} \int_{\Omega_{u,j}} u_{\nu, k}(r) u_{\nu, k}(r) v(r) \exp(i(k-k').r) dr^3 \quad (6.3)$$

If we use the fact that $v(r)$ varies slowly the following approximation holds:

$$<v', k' | v(r) | v, k> = \sum_{j=1}^{N} \int_{\Omega_{u,j}} u_{\nu, k}(r) u_{\nu, k}(r) v(r) \exp(i(k-k').r) dr^3$$

$$= \int_{\Omega_u} u_{\nu, k}(r) u_{\nu, k}(r) v(r) \exp(i(k-k').r) dr^3 \quad (6.4)$$

with $r_j$ the center of unit cell $j$. With the definition of the overlap integral (6.5) (6.4) can be written as (6.6).

$$I_{\nu', \nu, k', k} = \int_{\Omega_u} u_{\nu, k}(r) u_{\nu, k}(r) dr^3 \quad (6.5)$$

$$<v', k' | v(r) | v, k> = \frac{1}{\Omega_u} \sum_{j=1}^{N} \Omega_u . v(r) . \exp(i(k-k').r) . I_{\nu', \nu, k', k}$$

$$= I_{\nu', \nu, k', k} \cdot \frac{1}{\Omega_u} \int_{\Omega_u} v(r) . \exp(i(k-k').r) . dr^3$$

$$= I_{\nu', \nu, k', k} V_{k'-k} \quad (6.6)$$

In (6.6) the sum over the units cells has been approximated by an integral over the crystal volume. Also the definition
\[
V_q = \frac{1}{\Omega_c} \int \nu(r) \exp(-i q \cdot r) \, dr^3 
\]  \hspace{1cm} (6.7)

of the Fourier components \( V_q \) of the potential \( v(r) \) has been used.

The potential \( v(r) \) causes a perturbation of the wave function \( \Psi_{\nu,k} \). The perturbed function \( \Phi_{\nu,k} \) is given by first order stationary perturbation theory:

\[
\Phi_{\nu,k}(r) = \Psi_{\nu,k}(r) + \sum_{\nu',k'} \frac{\langle \psi'_{\nu',k'} | v(r) | \psi_{\nu,k} \rangle}{\tilde{\omega}_{\nu,k} - \tilde{\omega}_{\nu',k'}} \psi'_{\nu',k'}(r) \hspace{1cm} (6.8)
\]

The prime at the summation stands for the omission of the state \( |\psi_{\nu,k} \rangle \) in the evaluation of the sum over the states \( |\psi_{\nu',k'} \rangle \). The change in probability density, induced by the action of the perturbing potential \( v(r) \) on the state \( |\psi_{\nu,k} \rangle \), is given by

\[
P_{\nu,k}(r) = |\Phi_{\nu,k}(r)|^2 - |\Psi_{\nu,k}(r)|^2 \hspace{1cm} (6.9)
\]

Up to the first order in the perturbation this can be written as

\[
P_{\nu,k}(r) = \sum_{\nu,k} \left\{ \frac{V_{k'-k} I_{\nu',\nu,k',k} \psi_{\nu',k'}(r) \psi_{\nu,k}(r)}{\tilde{\omega}_{\nu,k} - \tilde{\omega}_{\nu',k'}} \psi_{\nu',k'}(r) \psi_{\nu,k}(r) \right. \\
+ \frac{V_{k-k'} I_{\nu',\nu,k',k} \psi_{\nu')(r) \psi_{\nu,k}(r)}}{\tilde{\omega}_{\nu,k} - \tilde{\omega}_{\nu',k'}} \psi_{\nu',k'}(r) \psi_{\nu,k}(r) \right\} \hspace{1cm} (6.10)
\]

The Fourier transform

\[
P_{\nu,k,q} = \frac{1}{\Omega_c} \int P_{\nu,k}(r) \exp(-i q \cdot r) \, dr^3 \hspace{1cm} (6.11)
\]

can be evaluated by making use of (6.4), (6.5) and (6.6), where \( v(r) \) is replaced by \( \exp(-i q \cdot r) \), and of the relations

\[
V^*_{-q} = V_q \hspace{1cm} (6.12)
\]

\[
I^*_{\nu',\nu,k',k} = I_{\nu,\nu',k,k'} \hspace{1cm} (6.13)
\]

The result is
\[ P_{\nu,k,q} = \frac{1}{q^2} \sum_{\nu'} \left\{ \frac{\mathcal{G}_{\nu',\nu,k+q,k}}{\mathcal{W}_{\nu,k} - \mathcal{W}_{\nu',k+q}} + \frac{\mathcal{G}_{\nu',\nu,k-q,k}}{\mathcal{W}_{\nu,k} - \mathcal{W}_{\nu',k-q}} \right\} \]  

(6.14)

where the overlap function \( \mathcal{G}_{\nu',\nu,k',k} \) is defined as

\[ \mathcal{G}_{\nu',\nu,k',k} = |I_{\nu',\nu,k',k}|^2 \]  

(6.15)

By summing over all states, weighed by their occupation number \( f_{\nu',k'} \) we can find the induced screening density

\[ n_{sc}(r) = 2 \sum_{\nu,k} f_{\nu,k} P_{\nu,k}(r), \]  

(6.16)

The factor 2 accounts for the two possible spin directions, which have not been distinguished by a separate quantum number. The Fourier transform \( N_{sc} \) of \( n_{sc} \) is given by

\[ N_{sc,q} = V \cdot q \cdot q, \]  

(6.17)

where

\[ X_q = 2 \sum_{\nu,k} f_{\nu,k} \sum_{\nu'} \left\{ \frac{\mathcal{G}_{\nu',\nu,k+q,k}}{\mathcal{W}_{\nu,k} - \mathcal{W}_{\nu',k+q}} + \frac{\mathcal{G}_{\nu',\nu,k-q,k}}{\mathcal{W}_{\nu,k} - \mathcal{W}_{\nu',k-q}} \right\} \]  

(6.18)

This result holds for every \( q \neq 0 \) that is small compared to a reciprocal lattice vector. For \( q = 0 \) the state \( \nu' = \nu \) has to be omitted in the summation over \( \nu' \).

The potential \( v \) is the sum of the unscreened 'bare' potential \( v_b \) and the screening potential \( \pm e \phi_{sc} \) (\( + \) for holes, \( - \) for electrons):

\[ v(r) = v_b(r) \pm e \phi_{sc}, \]  

(6.19)

where \( \phi_{sc} \) is related to \( n_{sc} \) by the Poisson equation:

\[ \Delta \phi_{sc} = \frac{\epsilon_0}{\epsilon_r} n_{sc} \]  

(6.20)

Fourier transform of (6.20) yields:

\[-q^2(V_{q,b} - V_{q,b}) = \frac{\epsilon_0}{\epsilon_r} X_q \]  

(6.21)

where \( V_{q,b} \) is the Fourier transform of \( v_b \), and (6.17) and (6.18) have been used. From (6.21) \( V_q \) can be solved:

\[ V_q = \frac{q^2}{q^2 + \frac{\epsilon_0}{\epsilon_r}} V_{q,b} \]  

(6.22)
where the inverse screening length $\gamma_q$ is defined by

$$\gamma_q^2 = \frac{e^2}{\varepsilon_0 \varepsilon_r} X_q.$$  \hspace{1cm} (6.23)

### 6.2 Approximations

In order to derive the screening parameter we have to evaluate $X_q$. In general the screening length is dependent on $q$. In order to get rid of the $q$-dependence we can use the random-phase approximation in combination with the long wave length limit. A Maxwell-Boltmann distribution for one parabolic band yields:

$$X_q = \frac{2}{\Omega_c} \sum_{k} f_{0,k} \left\{ \frac{1}{W_k - W_{k+q}} + \frac{1}{W_k - W_{k-q}} \right\}$$ \hspace{1cm} (6.24)

with

$$f_{0,k} = \frac{n e^3}{(2\pi m^* k_B T)^{3/2}} \exp\left( -\frac{\hbar^2 k^2}{2m^* k_B T} \right)$$ \hspace{1cm} (6.25)

and

$$W_k = \frac{\hbar^2 k^2}{2m^*}$$ \hspace{1cm} (6.26)

and

$$\left\{ \frac{1}{W_k - W_{k+q}} + \frac{1}{W_k - W_{k-q}} \right\} = \frac{4m^*}{\hbar^2} \frac{q^2}{k^4 + 4(k.q)^2}$$ \hspace{1cm} (6.27)

If we replace the sum by an integral we find

$$X_q = 2 \int d^3 k f_{0,k} \frac{q^2}{q^4 + 4(k.q)^2} \frac{4m^*}{\hbar^2}$$ \hspace{1cm} (6.28)

Assuming an isotropic distribution function $f_{0,k}$ we can use the random phase approximation and average over the solid angle $4\pi$:

45
\[
\left< \frac{q^4}{q^4 + 4(k.q)^2} \right> = \frac{1}{\beta} \int_0^\pi \frac{2\pi \sin(\beta)}{2\pi \sin(\beta)} d\beta
\]

\[
= \frac{1}{4kq} \ln \left( \frac{2k + q}{2k - q} \right) \approx \frac{\hbar^2}{4m^*} \frac{2}{W_k}
\]  
(6.29)

Using this approximation we find

\[
< X_q >_\beta = \int dk^3 f_{0,k} \frac{2}{W_k}
\]

(6.30)

As can be seen from (6.30) we have to average \((2/W_k)\) over the distribution function. If we use the Maxwell-Boltzmann (6.25) distribution function we find

\[
< X_q >_\beta = \frac{n_e}{k_B T}
\]

(6.31)

which results into the inverse Debye screening length \(\gamma_D\):

\[
\gamma_D^2 = \frac{e^2 n_e}{\epsilon_0 \epsilon_r k_B T}
\]

(6.32)

For Monte Carlo purposes it may be interesting to use the actual distribution of the electrons. If there are \(N \gg 1\) electrons with energy \(W_i\) the distribution dependent inverse screening length \(\gamma_d\) becomes approximately:

\[
\gamma_d^2 = \frac{e^2 n_e}{\epsilon_0 \epsilon_r B_0},
\]

(6.33)

with

\[
B_0 = \frac{1}{N} \sum_{i=1}^N \frac{1}{2W_i}
\]

(6.34)

A same similar expression is found when we use the non-parabolic energy dispersion relation. Neglecting the overlap function we find
\[
\mathcal{B}_\alpha = \frac{1}{N} \sum_{i=1}^{N} \left\{ \frac{2\alpha w_i}{1 + 2\alpha w_i} + \frac{1 + 2\alpha w_i}{2w_i (1 + 2\alpha w_i)} \right\}. \quad (6.35)
\]

6.3 Discussion

The use of the Debye-Hückel screening model is justified under steady state conditions, which are not far from equilibrium. This is a consequence of the assumption of the Maxwell-Boltzmann distribution.

For transient simulations and systems far from equilibrium the screening length can be calculated self-consistently according to the random phase approximation (6.33) and (6.35). If the random phase approximation breaks down the screening parameter has to be calculated from (6.23) and (6.18).
7. PARTIAL WAVE ANALYSIS

The Born approximation assumes that the disturbance due to the impurities is weak. This is not true for electrons which have low energy. In these cases a more sophisticated description of ionized impurity scattering is needed. A good alternative is a description based on the Schrödinger equation.

One technique is based on the fact that a radial perturbing potential \( v(r) \), results in phase shift of the original wave function at great distances. The phase shifts are unique for a potential \( v(r) \). With these phase shifts it is possible to calculate the differential and the momentum relaxation cross section. This method is known as partial phase shift analysis or the partial wave analysis.

7.1 Theory

The potential is assumed to have radial symmetry. Therefore only the radial part of the wave function \( \psi(r, \theta, \phi) \) needs to be solved. The Schrödinger equation is given by:

\[
\mathcal{H} \psi = \left( \frac{\hbar^2}{2m} \nabla^2 + v(r) \right) \psi
\]

(7.1)

with \( \mathcal{H} \) the Hamiltonian operator of the system. \( \psi \) is split up into a radial part \( R_1(r) \) and a tangent part \( Y_{1,m}(\theta, \phi) \). The operator \( \nabla^2 \) is written out in radial coordinates. The resulting equation for the radial part of the Schrödinger equation can be written as

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) R_1 + \frac{2m^*}{\hbar^2} \left( W - v(r) \right) R_1 - \frac{l(l+1)}{r^2} R_1 = 0
\]

(7.2)

The quantum number \( l \) appears, see Schiff [17], if the the differential equation for \( Y_{1,m} \) is solved.

This problem can be simplified through the introduction of the function

\[
g_L(r) = r R_1(r)
\]

(7.3)
Then (7.2) can be written as:

\[
\frac{d^2}{dr^2} g_1 + \left( \frac{k^2}{\hbar^2} - \frac{2m^* v(r)}{\hbar^2} - \frac{l(l+1)}{r^2} \right) g_1 = 0 \quad (7.4)
\]

In this expression the energy-wavevector relationship for a parabolic band has been used.

For ionized impurity scattering we use the screened Coulomb potential

\[
v(r) = \frac{Ze^2}{4\pi\varepsilon_0 r} \exp\left(-\frac{r}{\lambda}\right), \quad (7.5)
\]

with \( \lambda \) the screening length. The range of the potential is roughly a few times \( \lambda \). This means that the solution of (7.4) behaves for \( r \gg \lambda \) like a sine function

\[
g_1(r) \rightarrow \text{constant} \cdot \sin\left( kr - \frac{1}{2} l\pi \right) \quad (7.6)
\]

if the perturbing potential equals zero and

\[
g_1(r) \rightarrow \text{constant} \cdot \sin\left( kr - \frac{1}{2} l\pi + \delta_1(k) \right) \quad (7.7)
\]

if the potential is not zero. (6) and (7) can be written in the exponential form. This leads for \( R_1(r) \) to

\[
R_1(r) \rightarrow \text{constant} \cdot \exp\left(i\delta_1(k)\right) \frac{1}{r} \exp\left(ikr\right) \quad (7.8)
\]

The total wave function \( \Psi \) at great distance from the impurity has the form:

\[
\Psi(r,\theta,\phi) \rightarrow \text{constant} \cdot \left\{ \exp\left(ikz\right) + \frac{1}{r} f(\theta,\phi) \exp\left(ikr\right) \right\} \quad (7.9)
\]

The first term describes the incoming wave, the second term the scattered wave. The coordinate system is chosen in such a way that the incoming wave travels along the z-axis. For this reason the function \( f(\theta,\phi) \), which describes the scattering amplitude, is only dependent on \( \theta \). From (7.8) and (7.9) it is clear that there exists a relation between the phase shifts \( \delta_1 \) and the scattering amplitude \( f(\theta) \). According to Schiff [17]
\[
    f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left( 2l + 1 \right) \left[ \exp \left( 2i\delta_l \right) - 1 \right] P_l(\cos(\theta))
\]  
(7.10)

with \( P_l \) a Legendre polynomial of the order \( l \). The differential cross section is obtained from
\[
    \sigma(\theta) = |f(\theta)|^2 .
\]  
(7.11)

7.2 Implementation of the partial phase shift method into a Monte Carlo program

The implementation of the partial phase shift method into a Monte Carlo program is not straightforward. For the calculation of the cross section (7.10) the phase shifts have to be calculated. Worse is that these phase shifts depend on \( k \) and \( \lambda \), resulting in an enormous consumption of cpu time.

The solution for this problem is the use of an interpolation table. In one direction stands the dependence on \( k \) and on the other the dependence of the screening length, see figure 7.1. This two dimensional look up table was proposed by Kay [18,19].

![figure 7.1 : look up table](image)

At every cross point the total cross section should be tabulated. For the relation determining the state after scattering a general
function with several fit parameters can be used. These parameters should also be tabulated. All these values have to be calculated only once and can be calculated in a pre-processing step.

The remaining problems are the calculation of the partial phase shifts and the problem of finding a good interpolation grid and fit for the function which determines the angle after scattering.

A program, written by D. Klaasen, Philips Research laboratories Eindhoven, is able to calculate the differential cross section for ionized impurity scattering. This program makes use of the semi-classical phase shift method. This method is outlined in [20].

In order to test the possibility of implementation of the method the program was adapted. The program delivers now the total cross section and the values of the scatter angle as function of the random number $\tilde{r}$, which determines the scatter angle.

A program was written to fit the general function to the data points of the angle dependence: $\cos(\theta) = F(\tilde{r})$. Using a simplex minimalisation algorithm from the NAG FORTRAN library we found that a good fit is possible to if we use a rational function of order two. These results can be found in appendix C.

Points of concern which are not examined yet are the constraints which have to be met:

* $|F(\tilde{r})| \leq 1$, with $\tilde{r} \in [0,1]$

\[
\frac{d}{d\tilde{r}} F(\tilde{r}) \leq 0
\]

* $F(1) = -1$

Although not all constraints are met the function fits remarkably well. We can conclude that it is possible to use the algorithm described above. However it may be nessesary to use another fit function.
7.3 Friedel Sum Rule

A point of interest is the screening. The calculation of the screening length should be consistent with the partial phase shift method. There is a relation between the phase shifts and the screening. This result is known as the Friedel Sum Rule [21].

\[
\frac{1}{\pi} \sum_{l, i} (2l + 1) g_i q_i \int_0^\infty \delta_{l,i}(W) \frac{d f_i(W)}{dW} \ dW = Z, \quad (7.12)
\]

with \( i \in \{ \text{electron, hole} \} \) and \( g_i \) the degeneracy and \( f(W) \) the occupation probability. For a N-type semiconductor (\( Z = +1, i = e, g_e = 2, q_e = -1 \)) the following equation holds:

\[
\frac{2}{\pi} \sum_{l} (2l + 1) \int_0^\infty \delta_{l,e}(W) \frac{d f_e(W)}{dW} \ dW = -1 \quad (7.13)
\]

The screening is consistent with the Friedel Sum Rule if (7.13) is met. To satisfy the sum rule we must find the correct value of \( \lambda \). Kay [19] showed that this leads to a new mapping of the look up table, which is only dependent on the lattice temperature.
8. RESULTS

In this chapter some results obtained with help of the FORTRAN programs are discussed. There are five subjects investigated. The first subject shows an application of the overestimation method: the influence of screening on acoustic phonon interaction is investigated with help of the overestimation method. The second subjects deals with the ionized-impurity scattering. The third is about the dipole scattering. The fourth is about self-consistent screening in the random-phase approximation and the last is about partial wave analysis.

8.1. The influence of screening on electron acoustic phonon scattering

In this section the influence of screening on electron-acoustic phonon interaction is examined. For this purpose we used an Ensemble Monte Carlo program, written for N-type bulk GaAs low-field mobility calculations. We are only interested in the influence of screening on electron-acoustic phonon interactions. Therefore we removed the piezo-electrical interaction and also the ionized impurity-scattering. The main reason for this was to make the program run faster.

The scatter processes still active in the program are:
- Polar Optical Phonon Interaction (Emission and Absorption)
- Acoustic Phonon Interaction (Emission and Absorption)

8.1.1 The Model

The implementation scheme used for unscreened and screened acoustic phonon interaction was derived from the scatter matrices given in respectively (8.1) and (8.2).
\[
\begin{align*}
\left\{ S_{ac}^{\text{em.}}(k,k') \right\}_{\text{n.scr.}} &= \frac{\pi \frac{q^2}{\omega_{ac}}}{\rho \Omega_s \gamma} q \left[ \eta_q + \frac{1}{2} \mp \frac{1}{2} \right]. \\
G(k,k') &= \delta \left( W(k) - W(k') \pm \hbar \omega_{ac} \right) 
\end{align*}
\] (8.1)

\[
\begin{align*}
\left\{ S_{ac}^{\text{em.}}(k,k') \right\}_{\text{scr.}} &= \left\{ S_{ac}^{\text{em.}}(k,k') \right\}_{\text{n.scr.}} \left( \frac{q^2}{q^2 + \lambda^2} \right)^2 
\end{align*}
\] (8.2)

The energy relation for a Kane type band structure is given by (8.3). The non parabolically parameter for the central valley in GaAs is approximately 0.5 eV⁻¹.

\[
W(k). (1 + \alpha W(k)) = \frac{\hbar^2 k^2}{2m^*} 
\] (8.3)

The Bose-Einstein distribution for phonons is described by:

\[
\eta_q = \frac{1}{\exp \left( \frac{\hbar \omega_{ac}}{k_B T_L} \right) - 1} 
\] (8.4)

The dispersion relation of acoustic phonons is

\[
\hbar \omega_{ac} = \hbar \omega q 
\] (8.5)

The overlap function for Kane-type conduction bands is given by:

\[
G(k,k') = \left( \frac{(1+\alpha W)(1+\alpha W')}{(1+2\alpha W)(1+2\alpha W')} \right) + \alpha \cos(\theta) \frac{W.W'}{(1+2\alpha W)(1+2\alpha W')} 
\] (8.6)

For the screening parameter we used the simple model (8.7) which leads to the Debye screening length (\(\lambda\)). Although this definition is not self consistent with the Friedel Sum Rule it gives at least an impression of what happens if the acoustic phonons are screened.
\[ \lambda^{-2} = \frac{n e^2}{\varepsilon_0 \varepsilon_r k T L} \]  

(8.7)

We used a method of overestimation to deal with the screening. The effect of screening is that the transition rate from \( k \) to \( k' = k + q \) is changed with a factor \( C(q, \lambda) \leq 1 \):

\[ C(q, \lambda) = \left( \frac{q^2}{q^2 + \lambda^{-2}} \right)^2 \]  

(8.8)

The method of overestimation is straightforward:
- Calculate the scatter rate and the scatter events if they are not screened
- If we do not include the screening we are ready. If we want to include the screening we include a rejection scheme (8.9). \( \text{RAN} \) is an uniformly distributed number between 0 and 1.

\begin{verbatim}
IF(screening)
    THEN
        IF(RAN.LT.C(q,\lambda)) THEN ACOUTIC INTERACTION
            ELSE SELF SCATTERING
        ELSE
            ACOUTIC INTERACTION
\end{verbatim}

(8.9)

8.1.2 Simulation

The effect of screening has been investigated for three different temperatures (77, 150 and 300k). The screening electrons are supplied by virtual donor atoms. The concentration of these virtual donor atoms has to be defined in order to determine the screening length (8.7).

The fact that we do not include the two other screening-dependent processes, i.e. ionized-impurity scattering and piezo-electric interaction, has two advantages. One advantage is the possibility to investigate the effect of screening on acoustic phonons while other effects do not change. The other advantage is that we need
only one Monte Carlo simulation for the unscreened case for a specific temperature.

8.1.3 The results

After the initialization of the 5000 electrons the electron gas is simulated during 50 pico-seconds. During that period the electric field has a constant value of 1 kV/cm. We assume that the new equilibrium has been reached far before 25 pico-seconds. Therefore the data concerning the drift velocity and the mobility are collected and averaged during the last 25 pico-seconds. This interval has been sampled 125 times.

The data concerning the total amount of scatter events and the loss of velocity due to these processes, here called effective scatter rate, are collected during the whole simulation. These quantities can give an impression of the effectiveness of a scatter process. The results of the simulations are given in the figures 8.1 to 8.9.

Figure 8.1: The influence of screening on the acoustic absorption rate at 77K: — no screening, total scatter rate, —Δ— no creening, effective rate, —○— screening, total catter rate, —+— screening, effective scatter rate.

*) The calculated effective scatter rate is not a weighted version of the momentum relaxation rate. Therefore this rate can be bigger than the total scatter rate.
Figure 8.2: The influence of screening on the acoustic absorption rate at 150K: — no screening, total scatter rate, --Δ-- no screening, effective rate, --○-- screening, total scatter rate, —— screening, effective scatter rate.

Figure 8.3: The influence of screening on the acoustic absorption rate at 300K: — no screening, total scatter rate, --Δ-- no screening, effective rate, --○-- screening, total scatter rate, —— screening, effective scatter rate.
Figure 8.4: The influence of screening on the acoustic emission rate at 77K: — no screening, total scatter rate, -Δ- no screening, effective rate, -○- screening, total scatter rate, -++- screening, effective scatter rate.

Figure 8.5: The influence of screening on the acoustic emission rate at 150K: — no screening, total scatter rate, -Δ- no screening, effective rate, -○- screening, total scatter rate, -++- screening, effective scatter rate.
Figure 8.6: The influence of screening on the acoustic emission rate at 300K: — no screening, total scatter rate, -Δ-- no screening, effective rate, -o-- screening, total scatter rate, +-- screening, effective scatter rate.

Figure 8.7: The influence of screening on the mobility due to acoustic scattering at 77K: — no screening scatter rate, -Δ-- screening
Figure 8.8: The influence of screening on the mobility due to acoustic scattering at 150K: no screening
--Δ-- screening

Figure 8.9: The influence of screening on the mobility due to acoustic scattering at 300K: no screening
--Δ-- screening
We may conclude that screening has hardly any influence on the drift mobility. There can be two effects which are responsible. The first effect is that screening can be neglected. Secondly the simulations have so much statistical noise that the effect of screened interaction cannot be examined properly.

For the last we decided to do the simulations again. In order to decrease the Monte Carlo noise of the screened acoustic phonon interaction we raised the total scatter rate artificially with a factor 10. The simulations are not realistic any more. However we get more statistics concerning the screening. These results are depicted in the figures 8.10 till 8.12.

![Graph showing the influence of screening on mobility due to acoustic scattering at 77K](image)

**Figure 8.10:** The influence of screening on the mobility due to acoustic scattering at 77K: — no screening, --o-- screening

The rate has been raised artificially with a factor 10.
From the results we conclude that screening becomes detectable at a donor concentration of $10^{16}$ cm$^{-3}$ or higher. For room temperature the effect of screening can be neglected.
8.1.4 Conclusion

The effect of screening can be taken very simply into account if we use the method of overestimation. The effects on the total scatter rate is detectable at the temperatures 77 and 150K, especially if we increase the acoustic scatter rate with a factor 10. At 300K there is hardly any influence left.

For more realistic simulations the effects will be more or less the same. However, the effect on the drift velocity will be hardly detectable because the value for the velocity is dominated by ionized impurity and polar optical scattering. For other semiconductors where acoustic phonon scattering is a more important process, e.g. Germanium and Silicon, there could be a stronger effect.

Summarizing the conclusions we can state that although in most cases the effects of screening can be neglected it is actually present. It depends on the desired accuracy and information if it is needed to implement the rejection scheme (8.9).

8.2 Ionized Impurity scattering

The simulations are done with help of the Ridley model. For the screening length we used the simple expression (8.8) of the Debye screening. The program further accounts for polar optical scattering, acoustic scattering, and piezo-electric scattering.

8.2.1 Temperature dependence

One group of simulations shows the temperature dependence if no clusters are presents. If we compare them with values from the literature we find that the results are rather good. The difference in mobility is mainly a consequence of the Ridley model. This model decreases the scatter rate and therefore the mobility is increased.
8.2.2 Clusters of ionized impurities

Another group of simulations was done to investigate the influence of clustering. The investigated case is that where GaAs during the MBE growth is doped with $\text{Si}_3^+$-molecules. This case was also investigated by Widdershoven [14]. The results are given in the figures 8.14 and 8.15.

![Figure 8.13: Drift mobilities](image)

Figure 8.13: Drift mobilities: 
- $N_d = 0 \text{ cm}^{-3}$
- $N_d = 10^{15} \text{ cm}^{-3}$

![Figure 8.14: Mobilities at 77K](image)

Figure 8.14: Mobilities at 77K
The results show that the influence of clustering is only detectable at lower temperatures. The reason for this is that the electron has to see the cluster as one scatterer. Although at low temperatures the reach of the disturbing potentials is less, see (8.7), the effects are stronger. The reason for this is that at low temperature the average length of the wave vector, $<k>$ is small, and therefore $q = 2k(1 - \cos(\theta))$ will be also small. It is the constraint $q \sigma \ll 1$ which indicates if the cluster will acts as one scatterer or not.

### 8.2.3 Dipole scattering

In chapter 4 it was stated that it is almost impossible to see the influence of a hot electron scatter mechanism in a real device. However in a Monte Carlo programs the constraints are easily met. In figure (8.16) and (8.17) the momentum relaxation time is plotted. The dipole distances $\sigma$ are 2.8 Å respectively 5.6Å. Note that the nearest atom distance in GaAs is 2.8Å.
These figures show that the values of $\sigma$ and screening ($N_d$), has to be chosen correctly in order to get the the predicted effect of an selective scatter mechanism.
8.2.3.1 Simulation

With help of the figures we decided to do two simulations. Both simulations had in common the lattice temperature (T=300K), the free carrier concentration $n = 10^{19} \text{ cm}^{-3}$ and the dipole concentration $N_d = 10^{20} \text{ cm}^{-3}$. The only difference is the parameter $\sigma$. One simulation is done with $\sigma=2.8$ Å and the other with $\sigma=5.6$ Å.

A steady state electron gas of 10,000 particles, in a field of 1 kV/cm, is simulated during 125 pico-seconds. This time interval is sampled 125 times. The distribution function is collected in 12 directions as function of the energy. After post processing of the data the real distribution can be obtained in twelve directions.

The resulting distributions are given below for the direction of the electric field and the direction opposite to the field:

![Distribution function graph](image)

Figure 8.18: Influence on the distribution function due to dipole scattering:
- : $\sigma=2.8$ Å, direction opposite to the field
- : $\sigma=2.8$ Å, direction along the field
- - - : $\sigma=5.6$ Å, direction opposite to the field
- - - - - - : $\sigma=5.6$ Å, direction along the field

67
As expected, see appendix A, the mobility of simulation 1 ($\sigma = 2.8 \text{ Å}$) is higher than from simulation 2 ($\sigma = 5.6 \text{ Å}$). It is clear from the figures that the selective hot-carrier mechanism is stronger in simulation 1. Although the average velocity during simulation 1 is about 1.4 bigger there are less hot carriers. With this simulation the presence of a selective hot carrier mechanism has been proved.

8.2.3.2 Discussion

The predicted effect of a selective hot electron scatter mechanism has been proved. However the simulations show that this is only the case if the average dipole length is very small and the dipole concentration is high. These constraints are difficult to be met. In other semiconductor materials it may be possible to meet these constraints more easily.

8.2.4 Self-consistent screening

In another investigation a number of simulations were done with a self-consistent screening length calculated according to the random phase approximation. The price we pay for self-consistent screening is an enormous increase use of cpu time. The reason for this is that the scatter rates cannot be tabulated anymore. As a test case a velocity-field characteristic was calculated. The simulation output can be found in appendix B. The resulting velocity-field characteristics are found in the following figure.
8.4.1 Conclusion

The results of the simulations are in accordance with reality. However we can conclude that the use of self-consistent screening is not necessary for low field simulations. The use of self-consistent screening may be important if we want information about transient behavior and systems which are far from equilibrium. If the use of self-consistent screening is important it is recommendable to optimize the program for the use of cpu-time.

8.5 Partial Phase Shift analysis

The possibility of the introduction of partial phase shift (PPS) analysis, concerning ionized impurity scattering, is investigated. If we use the construction of chapter 7 we have to calculate a two-dimensional lookup table [19]. As an investigation some parameters at the cross points are calculated. The reliability of the program which calculates the partial phase shifts according to the semi-classical approximation was not investigated.
The calculations were done for an attractive and repulsive potential. Therefore these calculations can be used to model electron transport in partly compensated material. The results are given in appendix C. In the figures (8.20) and (8.21) the total cross sections and the total scatter rates are given. The scatter angle \( \theta \) dependence of the random number \( r \) is given also in appendix C.

Figure 8.20: The total cross section

- --- analytical Born approximation
- --\( \Delta \)-- Born approximation (PPS)
- --\( \circ \)-- Attractive Potential
- --\( \blacklozenge \)-- Repulsive Potential
Figure 8.21: The total scatter rate

- analytical Born approximation
- Δ- Born approximation (PPS)
- o- Attractive Potential
- ◊- Repulsive Potential

8.5.1 Conclusion

The results show that the proposed procedure in chapter 7 is possible. However, the program which calculates the partial phase shifts and the cross section should be examined for the boundaries within which the program delivers accurate data. Also, the screening should be adapted in such a way that the Friedel Sum Rule is satisfied.
9. CONCLUSIONS

A model of ionized-impurity scattering due to clusters of ionized impurities can be implemented into a Monte Carlo program. Difficult integrals and numerical inversions can be avoided if we use the method called overestimation. This overestimation leads to extra self-scattering. If this method is implemented correctly it leads to simple expressions and may even lead to a decreased use of cpu-time. The last advantage is only true if the amount of overestimation is relative low.

Simulations show that in GaAs the effect of clustering becomes detectable especially at low values of $\sigma$ (about 10 nm.) and at low temperatures (77K). The influence at 300K is not significant.

The model for ionized-impurity scattering due to clusters of ions can easily be adapted for the case of dipole scattering. The formulas predict a selective scatter mechanism. The cold electrons are scattered less than the hot electrons. This property could increase the lifetime of devices. The reason for this is that the lifetime of most devices is strongly dependent on hot carrier effects.

Simulations show that this effect is detectable at very high dipole concentrations, and very high free carrier concentrations. The two impurities of the dipole should be approximately about one nearest atom distance (2.8Å) apart from each other. This constraint makes the use of dipoles as a hot carrier scatter mechanism almost impossible.

The use of partial phase shifts to arrive at a better model for ionized impurities can be implemented in a Monte Carlo program. This results in a pre-processing step which calculates a two-dimensional lookup table. In this table the scatter rate or total cross section be tabulated. Also the parameters of a fit function for the angle dependence could be stored. A rational function of order two gives good fits for this dependency.
LITERATURE


APPENDIX A: DIPOLE SIMULATIONS

In this appendix the two printer output files of the program dipole.f are given. These simulations produced figure 8.18.

Input Parameters dipole.f: Simulation Al

Temp (K) = 300.00  E-field (kV/cm) = 1.00
Eps0 = 12.90  Eps-inf. = 10.93
Vsound (m/s) = 5240.0  Density (kg/m3) = 5360.2

Gamma Valley
Intervalley Phon. En. = 0.00000
Intervalley Coupl. Const. = 0.00E+00
Acoustic Def. Pot. = 7.00

Ion Dens (m-3) = 0.10E+26  El. Dens. (m-3) = 0.10E+26

Input program:

Ndi = .1000E+27 [m^-3]
CSIZE = 0
Spreiding = .2800E-09 [m]

Output Data

M = 10000
MC = 0
< W > = 41.93 meV

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.3560E+05</td>
<td>0.4142E+03</td>
<td>0.7573E+03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>[V]</th>
<th>[SV]</th>
<th>[SSQV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2503E+04</td>
<td>0.2695E+04</td>
<td>0.2794E+04</td>
</tr>
</tbody>
</table>

Driftmob.(v/E) = 3560.1 cm^2/(Vs)
D-Parall. = 63.15 cm^2/sec
D-transv. = 0.00 cm^2/sec

Effective scatter rate  Total scatter rate

| SEFPOAB = -0.5910E+12 | NUPOAB = 0.2302E+13 Hz |
| SEFPOEM = -0.2109E+13 | NUPOEM = 0.2364E+13 Hz |
| SEFPEAB = -0.1055E+10 | NUPEAB = 0.8000E+09 Hz |
| SEFPEEM = -0.1755E+10 | NUPEEM = 0.3200E+10 Hz |
| SEFACAB = -0.5986E+10 | NUACAB = 0.4001E+10 Hz |
| SEFACEM = -0.1395E+11 | NUACEM = 0.6400E+06 Hz |
\[ SEFIIIMP = -0.3339E+13 \quad NUIIMP = 0.4159E+13 \quad \text{Hz} \]
\[ SEFDIPO = -0.1183E+13 \quad NUDIPO = 0.8241E+12 \quad \text{Hz} \]

Input Parameters  
\text{dipole.f: Simulation A2}

\begin{center}
\begin{tabular}{lll}
Temp (K) & 300.00 & E-field (kV/cm) = 1.00 \\
Eps0 & 12.90 & Eps-inf. = 10.93 \\
Vsouund (m/s) & 5240.0 & Density (kg/m^3) = 5360.2 \\
\end{tabular}
\end{center}

Gamma Valley
\begin{itemize}
\item Pol.Opt. Phon.Energy = 0.03536
\item Interv alley Phon. En. = 0.00000
\item Interv alley Coupl. Const. = 0.00E+00
\item Acoustic Def. Pot. = 7.00
\end{itemize}

Ion Dens (m^{-3}) = 0.10E+26 
E1. Dens. (m^{-3}) = 0.10E+26

Input program:
\begin{itemize}
\item Ndi = 1.000E+27 [m^{-3}]
\item CSIZE = 0
\item Spreiding = 0.5600E-09 [m]
\end{itemize}

Output Data
\[ M = 10000 \]
\[ MC = 2 \]

\begin{center}
\begin{tabular}{llll}
\text{[V m/s]} & \text{[SV]} & \text{[SSQV]} \\
\hline
x & -0.2683E+05 & 0.2636E+04 & 0.6949E+07 \\
y & -0.1074E+03 & 0.2674E+04 & 0.7150E+07 \\
z & 0.2139E+03 & 0.2566E+04 & 0.6582E+07 \\
\end{tabular}
\end{center}

D-Parall. = 48.75 cm^2/sec
D-transv. = 0.00 cm^2/sec
Driftmob.(V/E) = 2682.7 cm^2/(Vs)

Effective scatter rate  
Total scatter rate
\begin{itemize}
\item SEFPOAB = -0.5470E+12 
NUPOAB = 0.2299E+13 Hz
\item SEFPPOEM = -0.1958E+13 
NUPOEM = 0.2379E+13 Hz
\item SEFPPEAB = -0.1884E+10 
NUPEAB = 0.2400E+10 Hz
\item SEFPPEEM = -0.5115E+10 
NUPEEM = 0.2400E+10 Hz
\item SEFACAB = -0.1108E+11 
NUACAB = 0.4800E+10 Hz
\item SEFACEM = -0.1106E+11 
NUACEM = 0.5600E+10 Hz
\item SEFIIMP = -0.3228E+13 
NUIIMP = 0.4132E+13 Hz
\item SEFDIPO = -0.3853E+13 
NUDIPO = 0.2936E+13 Hz
\end{itemize}
APPENDIX B: SELF CONSISTENT SCREENING

In this appendix the printer output of figure 8.19 is given. The simulations are called B1, B2, B3 and B4.

Input Parameters Simulation B1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp (K)</td>
<td>300.00</td>
</tr>
<tr>
<td>Eps0</td>
<td>12.90</td>
</tr>
<tr>
<td>Vsound (m/s)</td>
<td>5240.0</td>
</tr>
<tr>
<td>E-field (kV/cm)</td>
<td></td>
</tr>
<tr>
<td>Eps-inf.</td>
<td>10.93</td>
</tr>
<tr>
<td>Dens i ty (kg/m3)</td>
<td>5360.2</td>
</tr>
<tr>
<td>Gamma Valley</td>
<td></td>
</tr>
<tr>
<td>Interval Phon. En.</td>
<td>0.00000</td>
</tr>
<tr>
<td>Interval Coupl. Const.</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>Acoustic Def. Pot.</td>
<td>7.00</td>
</tr>
<tr>
<td>Ion Dens (m-3)</td>
<td>0.10E+24</td>
</tr>
<tr>
<td>E1. Dens. (m-3)</td>
<td>0.10E+24</td>
</tr>
</tbody>
</table>

Input Program:

CSIZE = 1
Spreiding = .0000E+00 [m]

Output Data

M = 10000
MC = 1
< W > = 42.71 meV

[V m/s] [SV] [SSQV]
--- --- ---
| x   | -0.5456E+05 | 0.2639E+04 | 0.6966E+07 |
| y   | -0.4754E+03 | 0.2739E+04 | 0.7504E+07 |
| z   | 0.6890E+02  | 0.2779E+04 | 0.7723E+07 |

D-Parall. = 112.12 cm^2/sec
D-transv. = 0.00 cm^2/sec
Driftmob.(v/E) = 5456.1 cm^2/(Vs)

Effective scatter rate Total scatter rate
-----------------------------------------------
SEFPOAB = -0.6356E+12 NUPOAB = 0.2248E+13 Hz
SEFPOM = -0.2491E+13 NUPOEM = 0.2403E+13 Hz
SEFPEAB = -0.2668E+11 NUPEAB = 0.6134E+11 Hz
SEFPEEM = -0.2777E+11 NUPEEM = 0.4801E+11 Hz
SEFACAB = -0.8083E+11 NUACAB = 0.8401E+11 Hz
SEFACEM = -0.9158E+11 NUACEM = 0.6534E+11 Hz
SEFIIMP = -0.1364E+13 NUIIIMP = 0.1018E+14 Hz

77
Input Parameters Simulation B2:

Temp (K) = 300.00  E-field (kV/cm) = 2.00
Eps0 = 12.90  Eps-inf. = 10.93
Vsound (m/s) = 5240.0  Density (kg/m^3) = 5360.2

Gamma Valley
Intervalley Phon. En. = 0.00000
Intervalley Coupl. Const. = 0.00E+00
Acoustic Def. Pot. = 7.00

Ion Dens (m^-3) = 0.10E+24  El. Dens. (m^-3) = 0.10E+24

Input program:
CSIZE = 1
Spreading = .0000E+00 [m]

Output Data

M = 10000
MC = 25
< W > = 52.51 meV

<table>
<thead>
<tr>
<th>[V m/s]</th>
<th>[SV]</th>
<th>[SSQV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>-0.1096E+06</td>
<td>0.2852E+04</td>
</tr>
<tr>
<td>y</td>
<td>-0.9180E+02</td>
<td>0.3275E+04</td>
</tr>
<tr>
<td>z</td>
<td>0.3251E+02</td>
<td>0.2568E+04</td>
</tr>
</tbody>
</table>

D-Parall. = 137.72 cm^2/sec
D-transv. = 0.00 cm^2/sec
Driftmob.(v/E) = 5479.1 cm^2/(Vs)

Effective scatter rate  Total scatter rate
-------------------------------  -------------------------------
SEFPOAB = -0.5995E+12  NUPOAB = 0.2308E+13 Hz
SEFPOEM = -0.2544E+13  NUPOEM = 0.2951E+13 Hz
SEFPEAB = -0.2230E+11  NUPEAB = 0.4934E+11 Hz
SEFPEEM = -0.2798E+11  NUPEEM = 0.6667E+11 Hz
SEFACAB = -0.1007E+12  NUACAB = 0.7734E+11 Hz
SEFACEM = -0.1025E+12  NUACEM = 0.8401E+11 Hz
SEFIIMP = -0.1213E+13  NUIIMP = 0.1084E+14 Hz
Input Parameters Simulation B3

Temp (K) = 300.00  E-field (kV/cm) = 3.00
Eps0 = 12.90  Eps-inf. = 10.93
Vsound (m/s) = 5240.0  Density (kg/m3) = 5360.2

Gamma Valley
Interval Phon. En. = 0.00000
Interval Coupl. Const. = 0.00E+00
Acoustic Def. Pot. = 7.00

Ion Dens (m^-3) = 0.10E+24  El. Dens. (m^-3) = 0.10E+24

Input program:
CSIZE = 1
Spreiding = .0000E+00 [m]

Output Data

\[ H = 10000 \]
\[ H_C = 423 \]
\[ < W > = 87.55 \text{ meV} \]

\[
\begin{array}{ccc}
  \text{[V m/s]} & \text{[SV]} & \text{[SSQV]} \\
  x & -0.1698E+06 & 0.3162E+04 & 0.1000E+08 \\
y & 0.6182E+03 & 0.3228E+04 & 0.1042E+08 \\
z & 0.2806E+03 & 0.3309E+04 & 0.1095E+08 \\
\end{array}
\]

D-Paral. = 260.69 cm\textsuperscript{2}/sec
D-transv. = 0.00 cm\textsuperscript{2}/sec
Driftmob. (v/E) = 5658.9 cm\textsuperscript{2}/(Vs)

Effective scatter rate  Total scatter rate

\[
\begin{array}{ccc}
  \text{SEFPOAB} & -0.5367E+12 & \text{NUPOAB} = 0.2184E+13 \text{ Hz} \\
  \text{SEFPOEM} & -0.2481E+13 & \text{NUPOEM} = 0.3467E+13 \text{ Hz} \\
  \text{SEFPEAB} & -0.2135E+11 & \text{NUPEAB} = 0.6934E+11 \text{ Hz} \\
  \text{SEFPEEM} & -0.2294E+11 & \text{NUPEEM} = 0.5734E+11 \text{ Hz} \\
  \text{SEFAGAB} & -0.1254E+12 & \text{NUACAB} = 0.8001E+11 \text{ Hz} \\
  \text{SEFACEM} & -0.1312E+12 & \text{NUACEM} = 0.1027E+12 \text{ Hz} \\
  \text{SEFIIMP} & -0.9249E+12 & \text{NUIIMP} = 0.1213E+14 \text{ Hz} \\
\end{array}
\]
Input Parameters Simulation B4

Temp (K) = 300.00  E-field (kV/cm) = 1.00
Eps0 = 12.90  Eps-inf. = 10.93
Vsound (m/s) = 5240.0  Density (kg/m^3) = 5360.2

Gamma Valley
Intervalley Phon. En. = 0.00000
Intervalley Coupl. Const. = 0.00E+00
Acoustic Def. Pot. = 7.00

Ion Dens (m^-3) = 0.10E+25  El. Dens. (m^-3) = 0.10E+25

Gegevens met betrekking tot programma:
C SIZE = 1
Spreiding = .0000E+00 [m]

Output Data

M = 10000
MC = 3
< W > = 41.98 meV

<table>
<thead>
<tr>
<th>[V m/s]</th>
<th>[SV]</th>
<th>[SSQV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>-0.3432E+05</td>
<td>0.2770E+04</td>
</tr>
<tr>
<td>y</td>
<td>0.1753E+03</td>
<td>0.2895E+04</td>
</tr>
<tr>
<td>z</td>
<td>-0.3584E+03</td>
<td>0.2506E+04</td>
</tr>
</tbody>
</table>

D-Parall. = 71.01 cm^2/sec
D-transv. = 0.00 cm^2/sec
Driftmob.(v/E) = 3431.6 cm^2/(Vs)

Effective scatter rate

<table>
<thead>
<tr>
<th>SEFPOAB</th>
<th>NUPOAB</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.5872E+12</td>
<td>0.2226E+13 Hz</td>
</tr>
<tr>
<td>SEFPOEM</td>
<td>NUPOEM</td>
</tr>
<tr>
<td>-0.2594E+13</td>
<td>0.2348E+13 Hz</td>
</tr>
<tr>
<td>SEFPEAB</td>
<td>NUPEAB</td>
</tr>
<tr>
<td>-0.1443E+11</td>
<td>0.8003E+10 Hz</td>
</tr>
<tr>
<td>SEFPEEM</td>
<td>NUPEEM</td>
</tr>
<tr>
<td>-0.1576E+11</td>
<td>0.2000E+11 Hz</td>
</tr>
<tr>
<td>SEFACAB</td>
<td>NUACAB</td>
</tr>
<tr>
<td>-0.7326E+11</td>
<td>0.6401E+11 Hz</td>
</tr>
<tr>
<td>SEFACEM</td>
<td>NUACEM</td>
</tr>
<tr>
<td>-0.9374E+11</td>
<td>0.7067E+11 Hz</td>
</tr>
<tr>
<td>SEFIIMP</td>
<td>NUIMP</td>
</tr>
<tr>
<td>-0.4142E+13</td>
<td>0.1123E+14 Hz</td>
</tr>
</tbody>
</table>

80
APPENDIX C: PARTIAL PHASE SHIFT ANALYSIS

In this appendix the program output for the simulations of section 8.5 is given. Also the some of the \( \cos(\bar{r}) = f(\bar{r}) \) dependencies is shown.

SIMULATION Cl

SCREENING RADIUS = 0.13600E-07 M
EFFECTIVE CARRIER MASS = 0.63000E-01
WAVE NUMBER = 0.40500E+09 1/M

PARTIAL WAVES FROM 0 TO 13 ARE TAKEN INTO ACCOUNT

CROSS SECTIONS (ALL IN M**2):
ANAL. BORN APPROX.: TOTAL = 0.11975E-15 ; LIN.MOM.REL. = 0.75916E-17
BORN APPROXIMATION: TOTAL = 0.11624E-15 ; LIN.MOM.REL. = 0.84683E-17
ATTRACTIVE POTENTIAL: TOTAL = 0.12172E-15 ; LIN.MOM.REL. = 0.89147E-17
REPULSIVE POTENTIAL: TOTAL = 0.11355E-15 ; LIN.MOM.REL. = 0.79940E-17

THE FRIEDEL SUM RULE YIELDS:
BORN = -0.72193E+01 ; ATTR. = 0.73393E+01 ; REPULS. = -0.71915E+01

CROSS SECTIONS FROM INTEGRATION (ALL IN M**2):
ANAL. BORN APPROX.: TOTAL = 0.11983E-15 ; LIN.MOM.REL. = 0.75916E-17
BORN APPROXIMATION: TOTAL = 0.11628E-15 ; LIN.MOM.REL. = 0.84683E-17
ATTRACTIVE POTENTIAL: TOTAL = 0.12178E-15 ; LIN.MOM.REL. = 0.89147E-17
REPULSIVE POTENTIAL: TOTAL = 0.11359E-15 ; LIN.MOM.REL. = 0.79940E-17

The fitting relation is a rational function:

\[
2 \quad f(r) = \frac{1 + X1.r + X2.r}{1 + X3.r + X4.r}
\]

The Born approximation

The fitting parameters are:

- \( X1 = -0.20015E+01 \)
- \( X2 = 0.10015E+01 \)
- \( X3 = -0.19991E+01 \)
- \( X4 = 0.99908E+00 \)
The mean square error is:

\[
\text{m.s.e.} = 0.24109 \times 10^{-3}
\]

**PFS: Attractive potential**

The fitting parameters are:

\[
\begin{align*}
X_1 &= -0.20015 	imes 10^1 \\
X_2 &= 0.10015 	imes 10^1 \\
X_3 &= -0.19989 	imes 10^1 \\
X_4 &= 0.99894 	imes 10^0
\end{align*}
\]

The mean square error is:

\[
\text{m.s.e.} = 0.25529 \times 10^{-3}
\]

**PFS: Repulsive potential**

The fitting parameters are:

\[
\begin{align*}
X_1 &= -0.20012 	imes 10^1 \\
X_2 &= 0.10012 	imes 10^1 \\
X_3 &= -0.19990 	imes 10^1 \\
X_4 &= 0.99905 	imes 10^0
\end{align*}
\]

The mean square error is:

\[
\text{m.s.e.} = 0.33307 \times 10^{-3}
\]

**Analytical Born approximation**

The fitting parameters are:

\[
\begin{align*}
X_1 &= -0.20010 	imes 10^1 \\
X_2 &= 0.10010 	imes 10^1 \\
X_3 &= -0.19992 	imes 10^1 \\
X_4 &= 0.99922 	imes 10^0
\end{align*}
\]

The mean square error is:

\[
\text{m.s.e.} = 0.22709 \times 10^{-3}
\]
SIMULATION C2

SCREENING RADIUS = 0.13600E-07 m
EFFECTIVE CARRIER MASS = 0.63000E-01
WAVE NUMBER = 0.30000E+09 1/m

PARTIAL WAVES FROM 0 TO 10 ARE TAKEN INTO ACCOUNT

CROSS SECTIONS (ALL IN m**2):
ANAL. BORN APPROX.: TOTAL = 0.21679E-15; LIN.MOM.REL. = 0.21336E-16
BORN APPROXIMATION: TOTAL = 0.20896E-15; LIN.MOM.REL. = 0.23806E-16
ATTRACTION POTENTIAL: TOTAL = 0.22301E-15; LIN.MOM.REL. = 0.25854E-16
REPULSION POTENTIAL: TOTAL = 0.19721E-15; LIN.MOM.REL. = 0.20869E-16

THE FRIEDEL SUM RULE YIELDS:
BORN = -0.55080E+01; ATTR. = 0.56502E+01; REPULS. = -0.54297E+01

CROSS SECTIONS FROM INTEGRATION (ALL IN m**2):
ANAL. BORN APPROX.: TOTAL = 0.21687E-15; LIN.MOM.REL. = 0.21336E-16
BORN APPROXIMATION: TOTAL = 0.20901E-15; LIN.MOM.REL. = 0.23806E-16
ATTRACTION POTENTIAL: TOTAL = 0.22307E-15; LIN.MOM.REL. = 0.25854E-16
REPULSION POTENTIAL: TOTAL = 0.19726E-15; LIN.MOM.REL. = 0.20869E-16

The fitting relation is a rational function:

\[ f(r) = \frac{2}{1 + x_1 r + x_2 r^2} \]

The Born approximation

The fitting parameters are:
- \( x_1 = -0.20036E+01 \)
- \( x_2 = 0.10036E+01 \)
- \( x_3 = -0.19980E+01 \)
- \( x_4 = 0.99803E+00 \)

The mean square error is:

\[ m.s.e. = 0.15824E-03 \]
PFS: Attractive potential

The fitting parameters are:

- $X_1 = -0.20036E+01$
- $X_2 = 0.10036E+01$
- $X_3 = -0.19977E+01$
- $X_4 = 0.99770E+00$

The mean square error is:

$$m.s.e. = 0.12730E-03$$

PFS: Repulsive potential

The fitting parameters are:

- $X_1 = -0.20036E+01$
- $X_2 = 0.10036E+01$
- $X_3 = -0.19984E+01$
- $X_4 = 0.99839E+00$

The mean square error is:

$$m.s.e. = 0.35954E-03$$

Analytical Born approximation

The fitting parameters are:

- $X_1 = -0.20024E+01$
- $X_2 = 0.10024E+01$
- $X_3 = -0.19981E+01$
- $X_4 = 0.99815E+00$

The mean square error is:

$$m.s.e. = 0.17509E-03$$

SIMULATION C3:

SCREENING RADIUS = 0.13600E-07 M
EFFECTIVE CARRIER MASS = 0.63000E-01
WAVE NUMBER = 0.18160E+09 1/M
PARTIAL WAVES FROM 0 TO 7 ARE TAKEN INTO ACCOUNT

CROSS SECTIONS (ALL IN M**2):
ANAL. BORN APPROX.: TOTAL = 0.57687E-15 ; LIN.MOM.REL. = 0.11194E-15
BORN APPROXIMATION: TOTAL = 0.53959E-15 ; LIN.MOM.REL. = 0.12426E-15
ATTRACTIVE POTENTIAL: TOTAL = 0.61229E-15 ; LIN.MOM.REL. = 0.14234E-15
REPULSIVE POTENTIAL: TOTAL = 0.45950E-15 ; LIN.MOM.REL. = 0.89838E-16

THE FRIEDEL SUM RULE YIELDS:
BORN = -0.35986E+01 ; ATTR. = 0.38257E+01 ; REPULS. = -0.33907E+01

CROSS SECTIONS FROM INTEGRATION (ALL IN M**2):
ANAL. BORN APPROX.: TOTAL = 0.57695E-15 ; LIN.MOM.REL. = 0.11194E-15
BORN APPROXIMATION: TOTAL = 0.53965E-15 ; LIN.MOM.REL. = 0.12426E-15
ATTRACTIVE POTENTIAL: TOTAL = 0.61235E-15 ; LIN.MOM.REL. = 0.14234E-15
REPULSIVE POTENTIAL: TOTAL = 0.45955E-15 ; LIN.MOM.REL. = 0.89839E-16

The fitting relation is a rational function:
\[ f(r) = \frac{2}{2 + X_1 r + X_2 r + X_3 r + X_4 r} \]

The Born approximation

The fitting parameters are:
- \( X_1 = -0.20116E+01 \)
- \( X_2 = 0.10114E+01 \)
- \( X_3 = -0.19919E+01 \)
- \( X_4 = 0.99208E+00 \)

The mean square error is:
\[ m.s.e. = 0.27998E-04 \]

PFS: Attractive potential

The fitting parameters are:
- \( X_1 = -0.20128E+01 \)
- \( X_2 = 0.10126E+01 \)
- \( X_3 = -0.19920E+01 \)
- \( X_4 = 0.99213E+00 \)
The mean square error is:
\[
\text{m.s.e.} = 0.41333 \times 10^{-4}
\]

PFS: Repulsive potential

The fitting parameters are:
\[
\begin{align*}
- X_1 &= -0.20098 \times 10^1 \\
- X_2 &= 0.10098 \times 10^1 \\
- X_3 &= -0.19927 \times 10^1 \\
- X_4 &= 0.99279 \times 10^0
\end{align*}
\]

The mean square error is:
\[
\text{m.s.e.} = 0.67722 \times 10^{-4}
\]

Analytical Born approximation

The fitting parameters are:
\[
\begin{align*}
- X_1 &= -0.20098 \times 10^1 \\
- X_2 &= 0.10098 \times 10^1 \\
- X_3 &= -0.19927 \times 10^1 \\
- X_4 &= 0.99275 \times 10^0
\end{align*}
\]

The mean square error is:
\[
\text{m.s.e.} = 0.73458 \times 10^{-4}
\]

SIMULATION C4

SCREENING RADIUS = 0.13600 \times 10^{-7} M
EFFECTIVE CARRIER MASS = 0.63000 \times 10^{-1}
WAVE NUMBER = 0.11480 \times 10^9 1/M

PARTIAL WAVES FROM 0 TO 5 ARE TAKEN INTO ACCOUNT

CROSS SECTIONS (ALL IN \text{M}^2):
\[
\begin{align*}
\text{ANAL. BORN APPROX.: TOTAL} &= 0.13629 \times 10^{-14} ; \text{LIN. MOM. REL.} = 0.45248 \times 10^{-15} \\
\text{BORN APPROXIMATION: TOTAL} &= 0.12098 \times 10^{-14} ; \text{LIN. MOM. REL.} = 0.49420 \times 10^{-15} \\
\text{ATTRACTION POTENTIAL: TOTAL} &= 0.14638 \times 10^{-14} ; \text{LIN. MOM. REL.} = 0.61898 \times 10^{-15} \\
\text{REPULSION POTENTIAL: TOTAL} &= 0.87890 \times 10^{-15} ; \text{LIN. MOM. REL.} = 0.27387 \times 10^{-15}
\end{align*}
\]
THE FRIEDEL SUM RULE YIELDS:
\[ \text{BORN} = -0.24138E+01 \]; \[ \text{ATTR.} = -0.26860E+01 \]; \[ \text{REPULS.} = -0.21212E+01 \]

CROSS SECTIONS FROM INTEGRATION (ALL IN \( \text{m}^2 \)):

<table>
<thead>
<tr>
<th>ANAL. BORN APPROX.</th>
<th>TOTAL</th>
<th>LIN. MOM. REL.</th>
</tr>
</thead>
<tbody>
<tr>
<td>BORN APPROXIMATION</td>
<td>TOTAL</td>
<td>LIN. MOM. REL.</td>
</tr>
<tr>
<td>ATTRACTIVE POTENTIAL</td>
<td>TOTAL</td>
<td>LIN. MOM. REL.</td>
</tr>
<tr>
<td>REPULSIVE POTENTIAL</td>
<td>TOTAL</td>
<td>LIN. MOM. REL.</td>
</tr>
</tbody>
</table>

\[ \text{ANAL. BORN APPROX.: TOTAL} = 0.13630E-14 \]; \[ \text{LIN. MOM. REL.} = 0.45248E-15 \]
\[ \text{BORN APPROXIMATION: TOTAL} = 0.12099E-14 \]; \[ \text{LIN. MOM. REL.} = 0.49420E-15 \]
\[ \text{ATTRACTIVE POTENTIAL: TOTAL} = 0.14638E-14 \]; \[ \text{LIN. MOM. REL.} = 0.61899E-15 \]
\[ \text{REPULSIVE POTENTIAL: TOTAL} = 0.87895E-15 \]; \[ \text{LIN. MOM. REL.} = 0.27388E-15 \]

The fitting relation is a rational function:
\[
f(r) = \frac{2}{1 + \lambda_1 r + \lambda_2 r^2}
\]

The Born approximation

The fitting parameters are:
\[ - \lambda_1 = -0.20271E+01 \]
\[ - \lambda_2 = 0.10231E+01 \]
\[ - \lambda_3 = -0.19811E+01 \]
\[ - \lambda_4 = 0.98509E+00 \]

The mean square error is:
\[ \text{m.s.e.} = 0.73622E-05 \]

PFS: Attractive potential

The fitting parameters are:
\[ - \lambda_1 = -0.20292E+01 \]
\[ - \lambda_2 = 0.10245E+01 \]
\[ - \lambda_3 = -0.19801E+01 \]
\[ - \lambda_4 = 0.98488E+00 \]

The mean square error is:
\[ \text{m.s.e.} = 0.74859E-05 \]
PFS: Repulsive potential

The fitting parameters are:

- $X_1 = -0.20247E+01$
- $X_2 = 0.10241E+01$
- $X_3 = -0.19807E+01$
- $X_4 = 0.98126E+00$

The mean square error is:

$m.s.e. = 0.25743E-04$

Analytical Born approximation

The fitting parameters are:

- $X_1 = -0.20221E+01$
- $X_2 = 0.10212E+01$
- $X_3 = -0.19758E+01$
- $X_4 = 0.97671E+00$

The mean square error is:

$m.s.e. = 0.80251E-04$

SIMULATION C5

SCREENING RADIUS $= 0.13600E-07$ M
EFFECTIVE CARRIER MASS $= 0.63000E-01$
WAVE NUMBER $= 0.57400E+08$ 1/M

PARTIAL WAVES FROM 0 TO 4 ARE TAKEN INTO ACCOUNT

CROSS SECTIONS (ALL IN M**2):  
ANAL. BORN APPROX.: TOTAL $= 0.42622E-14$ ; LIN.MOM.REL. $= 0.25925E-14$
BORN APPROXIMATION: TOTAL $= 0.37005E-14$ ; LIN.MOM.REL. $= 0.27592E-14$
ATTRACTIVE POTENTIAL: TOTAL $= 0.46492E-14$ ; LIN.MOM.REL. $= 0.39517E-14$
REPULSIVE POTENTIAL: TOTAL $= 0.17529E-14$ ; LIN.MOM.REL. $= 0.95437E-15$

THE FRIEDEL SUM RULE YIELDS:
BORN $= -0.13225E+01$ ; ATTR. $= 0.17302E+01$ ; REPULS. $= -0.92694E+00$

CROSS SECTIONS FROM INTEGRATION (ALL IN M**2):  
ANAL. BORN APPROX.: TOTAL $= 0.42623E-14$ ; LIN.MOM.REL. $= 0.25925E-14$
BORN APPROXIMATION: TOTAL $= 0.37006E-14$ ; LIN.MOM.REL. $= 0.27592E-14$
ATTRACTIVE POTENTIAL: TOTAL $= 0.46493E-14$ ; LIN.MOM.REL. $= 0.39518E-14$
REPULSIVE POTENTIAL: TOTAL $= 0.17530E-14$ ; LIN.MOM.REL. $= 0.95437E-15$
The fitting relation is a rational function:

\[
\frac{2}{1 + X_1 r + X_2 r^2} = f(r) = \frac{2}{1 + X_3 r + X_4 r^2}
\]

The Born approximation

The fitting parameters are:

- \( X_1 = -0.20403E+01 \)
- \( X_2 = 0.91681E+00 \)
- \( X_3 = -0.19148E+01 \)
- \( X_4 = 0.10376E+01 \)

The mean square error is:

\( m.s.e. = 0.10603E-04 \)

PFS: Attractive potential

The fitting parameters are:

- \( X_1 = -0.20023E+01 \)
- \( X_2 = 0.69444E+00 \)
- \( X_3 = -0.19542E+01 \)
- \( X_4 = 0.12626E+01 \)

The mean square error is:

\( m.s.e. = 0.11801E-04 \)

PFS: Repulsive potential

The fitting parameters are:

- \( X_1 = -0.20731E+01 \)
- \( X_2 = 0.10617E+01 \)
- \( X_3 = -0.19265E+01 \)
- \( X_4 = 0.93781E+00 \)

The mean square error is:

\( m.s.e. = 0.62319E-04 \)

89
The Born approximation

Analytical Born approximation

The fitting parameters are:

- $X_1 = -0.20682E+01$
- $X_2 = 0.10414E+01$
- $X_3 = -0.19040E+01$
- $X_4 = 0.93055E+00$

The mean square error is:

$m.s.e. = 0.81308E-04$

In the figures C1, C2, and C3 the $\cos(\theta)$-RAN dependence is shown for a few simulation results. As can be seen the fit function fits remarkably well.

![Graph](https://via.placeholder.com/150)

**Figure C1**: $\theta$-dependence, analytical Born expression data from simulation C3.

---

Calculated: calculated

Fitted: fitted
Figure C2: $\theta$-dependence, repulsive potential data from simulation C5.

--- : calculated
----- : fitted

Figure C3: $\theta$-dependence, attractive potential data from simulation C5.

--- : calculated
----- : fitted