An optimised algorithm for ionized impurity scattering in Monte Carlo simulations

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We present a new optimised model of Brookes-Herring ionized impurity scattering for use in Monte Carlo simulations of semiconductors. When implemented, it greatly decreases the execution time needed for simulations (typically by a factor of the order of 100), and also properly incorporates the great proportion of small angle scatterings that are neglected in the standard algorithm. It achieves this performance by using an anisotropic choice of scattering angle which accurately mimics the true angular distribution of ionized impurity scattering.

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I. INTRODUCTION

Ionized impurity scattering dominates the transport properties of highly doped semiconductors, but accurate modeling of this scattering process is difficult because of the long range of the Coulomb force. The method in general use is that by Brookes-Herring, which is regarded as sufficiently accurate when simulating carrier mobilities in semiconductors. However, Brookes-Herring scattering is very anisotropic, so the standard overestimation-rejection algorithm for implementing this in Monte Carlo simulations is hugely inefficient.

The overestimation-rejection algorithm works as follows. The overestimated scattering rate is used to determine the free flight time of the particle, and at the end of every period of free flight a check is made to see if a scattering event has occurred. This, of course, leads to more checks being made than needed, but this problem is unavoidable since we cannot know in advance what the exact rate, for whatever final state that eventuates, will be. Each check involves three stages: selection of a possible final state, a calculation of the scattering rate into that final state would be, and a decision as to whether the scattering occurs or not.

This means that despite the fact that a scattering event does not occur at the end of every free flight, we still have to calculate the exact differential scattering rate for some particular choice of scattering event. If the overestimation is too great, this means the program will calculate far more differential scatterings that are neglected in the standard algorithm, and those scatterings will run the same simulation faster than one with the standard isotropic algorithm; or, alternatively, could run a much more accurate simulation in a comparable time. An early version of this algorithm was used recently to obtain manageable execution times in simulations of hot-hole lasers in III-V semiconductors.

The paper is organised as follows: section II describes the different algorithms; section III describes their comparative performance, and finally, in section IV we present our conclusions.

II. IONIZED IMPURITY SCATTERING

Here we are interested in optimising the algorithm for the Brookes-Herring model of ionized impurity scattering. This looks at the likelihood of the particle of interest (electron or hole) being deflected by the screened Coulomb field from a charged impurity. The Brookes-Herring rate for ionized impurity scattering is

\[ W_{diff} = \frac{2\pi n_{ii} e^4}{\hbar^2 \varepsilon_0 \varepsilon_r^2} \frac{1}{(q^2 + q_0^2)^2} N_d(P_{fi}^m, \theta_f, \phi_f) \left| \langle nk_i | mk_f \rangle \right|^2 \]

(1)

Here \( n_{ii} \) are the ionized impurity and hole (or electron) concentrations, \( q_0^2 \) is the square of the minimum change of the \( k \)-vector, \( k_B \) is Boltzman’s constant, \( T \) the temperature, \( \varepsilon_0 \varepsilon_r \) the permittivity, \( e \) the electron charge, \( i \) is the number of the initial band, \( f \) is the number of the final band. The so-called overlap factor is the square of the scalar product of the eigenvectors corresponding to the initial and final state respectively, and is \( \left| \langle nk_i | mk_f \rangle \right|^2 \).

Note in particular that the rate \( W_{diff} \) is proportional to

\[ \frac{1}{(q^2 + q_0^2)^2} = \frac{1}{\left| k_f - k_i \right|^2 + q_0^2} \]

(2)

We would usually assume that \( q_0 \) is just the inverse of the Debye screening length, which is given by

\[ q_d^2 = \frac{e^2 N_{ii}}{\varepsilon_0 \varepsilon_r k_B T} \]

(3)
although in subsection II C we introduce an additional contribution $q_{\min}^2$, where $q_0^2 = q_d^2 + q_{\min}^2$.

The difficulty with ionized impurity scattering is that the scattering rate becomes very large for small values of $q = |k_f - k_i|$. We can distinguish two situations leading scattering rates that are very large compared to the average scattering rate:

1. small angle scattering, i.e. $q$ is small compared to the absolute value of the incoming wave vector $k_i = |k_i|$. Note that $k_i$ is of the same order of magnitude as the absolute value of the outgoing wave vector $k_f = |k_f|$.

2. low hole or electron energy, i.e. where $k_i$ is small by itself.

A. Standard Isotropic Algorithm

The great variation in the scattering rate by angle and wave vector means that it is not straightforward to efficiently model the scattering process. If we take the simple approach of an isotropic choice of scattering angle, the usual algorithm overestimates the differential scattering rate $W_{p}^{\text{diff}} (E_k (t), \theta, \phi)$ by its maximum value $W_{\text{max}}^{\text{diff}}$. Therefore our Monte Carlo program will select an ionized impurity scattering for any particle at the overestimated rate $W_{\text{diff}}^{\text{max}}$, then reject those for which the combination of exact scattering rate $W_{p}^{\text{diff}} (E_k (t), \theta, \phi)$ and choice of random number do not lead to a scattering.

To choose a possible final state for an ionized impurity scattering process, we start by choosing a random direction for $k_f$ with all possible final directions have the same statistical weight $f (\theta, \phi) = 1/(4 \pi)$. Once we have chosen this direction, we can then work out the final $k$ vector, and hence the true scattering rate. We compare this true rate to the overestimated differential scattering rate, and use the normal rejection procedure to determine statistically whether the scattering has occurred or not.

For ionized impurity scattering $W_{\text{max}}^{\text{diff}}$ is much and much larger than $W_{p}^{\text{diff}} (E_k (t), \theta, \phi)$ for about any angle; and also this maximum value $W_{\text{max}}^{\text{diff}}$ depends sensitively on the screening length. This means that $W_{\text{max}}^{\text{diff}}$ is an inefficient overestimation, and as a result we do many calculations which do not lead to a scattering process. This significantly lengthens the execution times for our simulations.

B. New Anisotropic Algorithm

We have improved significantly on the execution times of simulations by introducing an anisotropic choice of the scattering angle, whilst compensating for this by adjusting the final scattering rate. The angular dependence of the scattering rate is centered on the direction of the initial $k$ vector, so it is useful to transform to angular coordinates $(\theta, \phi)$ centered on this direction. For this purpose we first define

$$Q_1 = \frac{|k_f - k_i|}{k_f - k_i}$$

so

$$Q_1 = 2 \sin(\theta/2) = \sqrt{2(1 - \cos \theta)}$$

where $\theta$ is the scattering angle. We now introduce an anisotropic weighting function $f (\theta, \phi)$ for the probability of finding the direction of the final $k$-vector. This same factor will then be used to compensate for this weighting by subsequently dividing the differential scattering by $f (\theta, \phi)$. At first sight one would be inclined to choose

$$f (\theta, \phi) \propto \frac{1}{Q_1} = \frac{1}{16 \sin^4 (\theta/2)} = \frac{1}{4(1 - \cos \theta)^2}$$

but this function cannot be normalised properly because the integral of $f (\theta, \phi)$ over $\theta$ and $\phi$ diverges. We could try to solve this problem by assuming a minimum scattering angle $\theta_0$, so we get a minimum value for $Q_1$ equal to $Q_0 = 2 \sin(\theta_0/2)$ and to choose for $Q_0$ e.g. the approximate Debye-value of Ridley [1], we have

$$(Q_0 k_i)^2 = q_0^2$$

We would then assume $\theta_0$ to be so small that we may assume the absolute value of the incoming and outgoing wave vectors to be the same. However, excluding scatterings with $q < q_0$ leads to erroneous results because it is exactly these small angle scatterings which dominate ionized impurity scattering. Test simulations confirm that the normalisation procedure has an equally important influence on the final result as the way screening is implemented.

To avoid erroneous results we choose $f (\theta, \phi)$ to have the Brookes-Herring shape (see eqn. [2]) –

$$f (\theta, \phi) \propto \frac{1}{(Q_1^2 + Q_0^2)^2} = \frac{1}{(4 \sin^2 (\theta/2) + Q_0^2)^2} = \frac{1}{2(1 - \cos \theta) + Q_0^2}$$

The function can be normalised because

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \frac{1}{(Q_1^2 + Q_0^2)^2} = \frac{4\pi}{Q_0^2 (4 + Q_0^2)}$$

is finite. As a result the normalised statistical weight of finding a given direction is given by

$$f (\theta, \phi) = \frac{Q_0^2 (4 + Q_0^2)}{4\pi} \frac{1}{(Q_1^2 + Q_0^2)^2} = \frac{Q_0^2 (4 + Q_0^2)}{4\pi [2(1 - \cos \theta) + Q_0^2]^2}$$

The next problem is to enter this statistical weight in the algorithm. To determine $\theta, \phi$ we choose two random numbers,
r1 and r2, between 0 and 1. In the case of an isotropic choice of direction we would have \( f(\theta, \phi) = 1/4\pi \), and we would choose

\[
\begin{align*}
  r_1 &= \frac{\phi}{2\pi} \\
  r_2 &= 2\pi (1 - \cos \theta) f(\theta, \phi).
\end{align*}
\]

For our new algorithm, we choose \( r_1 \) as in eqn. (11), and

\[
  r_2 = \pi \left[ 2(1 - \cos \theta) + Q_0^2 \right] f(\theta, \phi) - \frac{Q_0^2}{4}.
\]

The extra terms with \( Q_0^2 \) are needed to ensure that \( r_2 \) lies between 0 and 1, so that \(-1 < \cos \theta < 1\). The weighed random choice of \( \phi \) and \( \theta \) is now obtained by solving \( \phi = 2\pi r_1 \) and

\[
\cos \theta = 1 + \frac{Q_0^2}{2} \left( 1 - \frac{4 + Q_0^2}{4r_2 + Q_0^2} \right)
\]

Note that \( \cos \theta \to 1 \) for \( r_2 \to 1 \), so small angle scattering is not excluded.

In the new algorithm we need to compensate for the higher occurrence of small scattering angles caused by the introduction of a weighing function \( f(\theta, \phi) \neq 1/4\pi \) by multiplying the differential scattering rate by

\[
\frac{4\pi}{f(\theta, \phi)} = \frac{(Q_1^2 + Q_0^2)^2}{Q_0^2(4 + Q_0^2)}
\]

We construct an overestimated differential scattering rate by starting to look for the largest differential ionized impurity scattering rate including the factor \( f(\theta, \phi) \). The overlap factor is always less than one. The term

\[
\frac{1}{(q^2 + q_0^2)^2}
\]

can be overestimated by

\[
\frac{C}{(Q_1^2 + Q_0^2)^2k_i^4}
\]

where \( C \) is equal to 1 if the band is isotropic, but may need to be larger for anisotropic bands. In practice, \( C \) needs to be determined by computer experiment, which in our simulations was set equal to 1.2. There is also our new weighting factor \( f(\theta, \phi) \), which with the previous factor (eqn. 13) may both be overestimated by

\[
\frac{(Q_1^2 + Q_0^2)^2}{Q_0^2(4 + Q_0^2)} \approx \frac{C}{Q_0^2(4 + Q_0^2)} \frac{1}{k_i^4} \sim \frac{C}{q_0^2(4k_i^2 + q_0^2)}
\]

Note that this is the point where choosing a good way to normalise the weighing function \( f(\theta, \phi) \) pays off. The resulting function becomes extremely simple! Finally, the differential density of states is replaced by the total density of states divided by 4\( \pi \). Thus the overestimated scattering rate is given by

\[
W_{\text{tot}} = \frac{2\pi n_i e^4}{\hbar E_0^2 q_0^2 (4k_i^2 + q_0^2)} N_{\text{tot}}(E_0^2) \frac{C}{4\pi}
\]

Almost always \( k_i^4 \gg q_0^4 \), so this overestimation is orders of magnitude smaller than that from the standard isotropic algorithm, leading to far fewer calculations of the differential scattering rate that are followed by rejection.

C. Modified Anisotropic Algorithm

Ionized impurity scattering is an elastic process, which means that small changes of the \( k \)-vector imply a small change of the state of the hole or electron. A minimum change \( q_0 \) of the \( k \)-vector follows immediately from the implementation of the Debye screening through eqns. (11) and (16). The resulting minimum value of \( q_0 \) is proportional to \( \sqrt{\eta} \), so it becomes very small for low ionized impurity concentrations. As a result, despite the anisotropic scattering angle selection, the fraction of overestimations and hence the execution times of the simulation will still become very large for low concentrations. We can therefore improve the overestimation by introducing a second criterion determining whether the change of the \( k \)-vector is small or not. Now the average energy of an electron or hole is given by

\[
\frac{3}{2} k_B T = \frac{\hbar^2}{m_e m^*} k^2 >
\]

so the average value of \( k^2 \) is given by

\[
<k^2> = \frac{3m_e m^* k_B T}{\hbar^2}
\]

This induces us to propose that we consider \( k \) small if its square is much smaller than this value. So we set

\[
k_{\text{min}}^2 = D \frac{3m_e m^* k_B T}{\hbar^2}
\]

where we choose \( D \) to be a small number. In practice we find that \( D = 0.01 \) is acceptable. We can now set the minimum change in wave vector to be

\[
q_0^2 = q_d^2 + k_{\text{min}}^2
\]
influence on the mobility since the motion of the carrier is largely unaffected. E.g. if $\Delta k < c_0$, where $k_0^2/2m^* = k_0T$ and $c = 0.1$, then on the average such a scattering changes the component of $k$ in the direction of the electric field by less than 1%. To verify this argument we repeated a number of the simulations as varying $c$ from 0.1 to 1.6. For $c \leq 0.3$ we saw no significant effect on the calculated mobilities.

### III. RESULTS

To check the relative efficiency of these algorithms, we took an existing Monte Carlo code (used in Dijkstra and Wenckebach[5]) and rewrote one of the subroutines in two ways: first, in accordance with the isotropic algorithm, and second, according to the modified anisotropic algorithm. We could then compare the performance of the two algorithms by comparing the performance of the two codes compiled with either of the two coded algorithms. In all other aspects the two codes were the same. However, with the isotropic choice of the scattering angle, small angle scatterings such that $\sin \theta < q_0$ had to be excluded in order to let the program run within finite time.

Both the material parameters we used, and the general method followed by the code were the same as those of Hinckley and Singh [6, 7]. The codes were compiled with GNU g77 and run on a 500 MHz Pentium III running RedHat Linux 6.2. The calculation was of the drift velocities of holes in unstrained silicon, where the magnetic field was equal to zero, the electric field equal to 5 kV/cm and the temperature 300 K. Only the $k$-vector was integrated during free flight. Each simulation consisted of either 25 blocks of 1000 real scatterings each or of 2 blocks of 100 real scatterings. Only in the former set of simulations could mobilities be determined.

A comparison of execution times and mobilities for the isotropic and anisotropic algorithms. The material system was unstrained silicon with an electric field equal to 5 kV/cm and a temperature 300 K. Note that in almost all cases, the simulations averaged over 25 × 1000 scatterings take hours using the isotropic algorithm, but only minutes using the anisotropic one.

| Conc. cm$^{-3}$ | Exec. time hh:mm:ss | Mobility (simul.) cm$^2$/Vs | Mobility (Sze) cm$^2$/Vs |
|----------------|----------------------|-----------------------------|--------------------------|
| $10^{19}$      | 00.27.50             | 132 ± 13                    |                          |
| $10^{18}$      | 00.22.18             | 196 ± 21                    | 150                      |
| $10^{17}$      | 00.22.34             | 334 ± 24                    | 300                      |
| $10^{16}$      | 00.36.29             | 400 ± 19                    | 430                      |
| $10^{15}$      | 01.06.43             | 418 ± 14                    | 460                      |
| $10^{14}$      | 01.17.14             | 422 ± 14                    | 470                      |
| $10^{13}$      | 01.19.12             | 430 ± 12                    |                          |
| 0              | 01.02.28             | 428 ± 14                    |                          |

As a final check, table II shows simulation results compared with experimental values for the mobility in silicon as given in Sze[8]. For more precision each simulation consisted of 50 blocks of 5000 real scatterings, and the electric field was kept at 5 kV/cm. Note that again the stated errors correspond to a 95% certainty level, and that we have good agreement between our code with the optimised ionized impurity scattering algorithm and the values given by Sze.

### IV. CONCLUSIONS

We have demonstrated a new way of significantly reducing execution times in simulations of systems involving Brooks-Herring ionized impurity scattering. This was done by introducing a carefully calculated anisotropic scattering angle for these ionized impurity processes, thus avoiding the usual problem of a large fraction of inefficient overestimations. Execution times of hole mobility calculations in silicon showed that the speedup was strongly dependent on impurity concentration, and generally well in excess of a factor of 5, typically being of the order of 100. The method is applicable to any simulation in which Brookes-Herring ionized impurity scattering is implemented, and it could be usefully generalised to other strongly anisotropic scattering processes, such as polar optical phonon and piezoelectric scatterings.
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