Computational Electronics

Relaxation Time Approximation

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Relaxation-time approximation

Analytical solutions of the Boltzmann equation are possible only under very restrictive assumptions [1]. Direct numerical methods for device simulation have been limited by the complexity of the equation, which in the complete 3-D time-dependent form requires seven independent variables for time, space and momentum. In recent times, more powerful computational platforms have spurred a renewed interest in numerical solutions based on the spheroidal harmonics expansion of the distribution function [2]. To-date, most semiconductor applications have been based on stochastic solution methods (Monte Carlo), which involve the simulation of particle trajectories rather than the direct solution of partial differential equations.

Most conventional device simulations are based on approximate models for transport which are derived from the Boltzmann equation, coupled to Poisson's equation for self-consistency. In the simplest approach, the relaxation time approximation is invoked, where the total distribution function is split into a symmetric term in terms of the momentum (which is generally large) and an asymmetric term in the momentum (which is small). In other words,

$$f(\mathbf{r},\mathbf{k},t) = f_S(\mathbf{r},\mathbf{k},t) + f_A(\mathbf{r},\mathbf{k},t) \quad . \tag{1}$$

Then, for non-degenerate semiconductors $(1 - f) \approx 1$, the collision integral may be written

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sum_{\mathbf{k}'}\left[f(\mathbf{k}')S(\mathbf{k}',\mathbf{k}) - f(\mathbf{k})S(\mathbf{k},\mathbf{k}')\right]$$
$$= \underbrace{\sum_{\mathbf{k}'}\left[f_S(\mathbf{k}')S(\mathbf{k}',\mathbf{k}) - f_S(\mathbf{k})S(\mathbf{k},\mathbf{k}')\right]}_{(\partial f_S/\partial t)_{coll}} + \underbrace{\sum_{\mathbf{k}'}\left[f_A(\mathbf{k}')S(\mathbf{k}',\mathbf{k}) - f_A(\mathbf{k})S(\mathbf{k},\mathbf{k}')\right]}_{(\partial f_A/\partial t)_{coll}} \tag{2}$$

We now consider two cases:

(a) Equilibrium conditions: $f_S = f_0, f_A = 0 \rightarrow \left(\frac{\partial f}{\partial t}\right)_{coll} = \left(\frac{\partial f_S}{\partial t}\right)_{coll} = 0$

(b) Non-equilibrium conditions when $f_A \neq 0$. In this case, we must consider two different situations:

- Low-field conditions, where f_S retains its equilibrium form with $T_C = T_L$. In this case $(\partial f_S/\partial t)_{coll} = 0$.
- High-field conditions when $T_C \neq T_L$ and f_S does not retain its equilibrium form. In this case $(\partial f_S/\partial t)_{coll} \neq 0$.

In all of these cases, a plausible form for the term $(\partial f_A/\partial t)_{coll}$ is

$$\left(\frac{\partial f_A}{\partial t}\right)_{coll} = -\frac{f_A}{\tau_f}, \tag{3}$$

where τ_f is a characteristic time that describes how the distribution function relaxes to its equilibrium form. With the above discussion, we may conclude that

- At low fields: $\left(\frac{\partial f}{\partial t}\right)_{coll} = \left(\frac{\partial f_A}{\partial t}\right)_{coll} = -\frac{f_A}{\tau_f}$.
- At high fields: $\left(\frac{\partial f}{\partial t}\right)_{coll} = \left(\frac{\partial f_S}{\partial t}\right)_{coll} + \left(\frac{\partial f_A}{\partial t}\right)_{coll} = \left(\frac{\partial f_S}{\partial t}\right)_{coll} - \frac{f_A}{\tau_f}$.

To understand the meaning of the relaxation time, we consider a semiconductor in which there are no spatial and momentum gradients. With the gradient terms zero, the BTE becomes

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f_A}{\partial t}\right)_{scatt} = -\frac{f_A}{\tau_f} = -\frac{f - f_0}{\tau_f} \tag{4}$$

i.e.

$$\frac{\partial f}{\partial t} + \frac{f}{\tau_f} = \frac{f_0}{\tau_f} \tag{5}$$

The solution of this first-order differential equation is

$$f(t) = f_0 + [f(0) - f_0]e^{-t/\tau_f} \quad . \tag{6}$$

This result suggests that any perturbation in the system will decay exponentially with a characteristic time constant τ_f. It also suggests that the RTA is only good when $[f(0) - f_0]$ is not very large. Note that an important restriction for the relaxation-time approximation to be valid is that τ_f is independent of the distribution function and the applied electric field.

Solving the BTE in the Relaxation Time Approximation

Let us consider the simple case of a uniformly doped semiconductor with a constant electric field throughout. Since there are no spatial gradients, $\nabla_{\mathbf{r}} f = 0$. Under steady-state conditions we also have $\partial f / \partial t = 0$. With the above simplifications, the BTE reduces to

$$\mathbf{F} \cdot \nabla_{\mathbf{p}} f = \frac{1}{\hbar} \mathbf{F} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{coll} \tag{7}$$

For parabolic bands and choosing the coordinate system such that the electric field is along the *z*-axis, one can expand the distribution function into Legendre polynomials

$$f(z, p) = f_0(z, p) + \sum_{n=1}^{\infty} g_n(E) P_n(\cos\theta) \tag{8}$$

where $P_0 = 1$, $P_1 = \cos\theta$, $P_2 = \frac{3}{2}\cos^2\theta - \frac{1}{2}$, … . In the above expressions, θ is the angle between the applied field (along the symmetry axis), and the momentum of the carriers. For sufficiently low fields, we expect that only the lowest order term is important, so that

$$f(p) \cong f_0(p) + g_1(p)\cos\theta = f_0(p) + f_A(p) \quad . \tag{9}$$

Substituting the results on the LHS of the BTE and using parabolic dispersion relation gives

$$
\begin{aligned}
LHS &= -\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}\left[f_0(p)+g_1(p)\cos\theta\right] \\
&\approx -\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f_0(p) = -e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon} = -eEv\cos\theta\frac{\partial f_0}{\partial\varepsilon}
\end{aligned}
\tag{10}
$$

where, as previously noted θ is the angle between the electric field and **v**.

We now consider the collision integral on the RHS of the BTE. Substituting the first order approximation for $f(\mathbf{p})$ gives

$$
\begin{aligned}
\left.\frac{\partial f}{\partial t}\right|_{coll} &= \sum_{k'}\left[S(k',k)f_0(k') - S(k,k')f_0(k)\right] \\
&+\sum_{k'}\left[S(k',k)g_1(k')\cos\theta' - S(k,k')g_1(k)\cos\theta\right] \\
&= -g_1(k)\cos\theta\sum_{k'}S(k,k')\left[1-\frac{S(k',k)g_1(k')\cos\theta'}{S(k,k')g_1(k)\cos\theta}\right] \\
&= -g_1(k)\cos\theta\sum_{k'}S(k,k')\left[1-\frac{f_0(k)g_1(k')\cos\theta'}{f_0(k')g_1(k)\cos\theta}\right]
\end{aligned}
\tag{11}
$$

where in the last line of the derivation we have used the principle of detailed balance. We can further simplify the above result, by considering the following coordinate system:

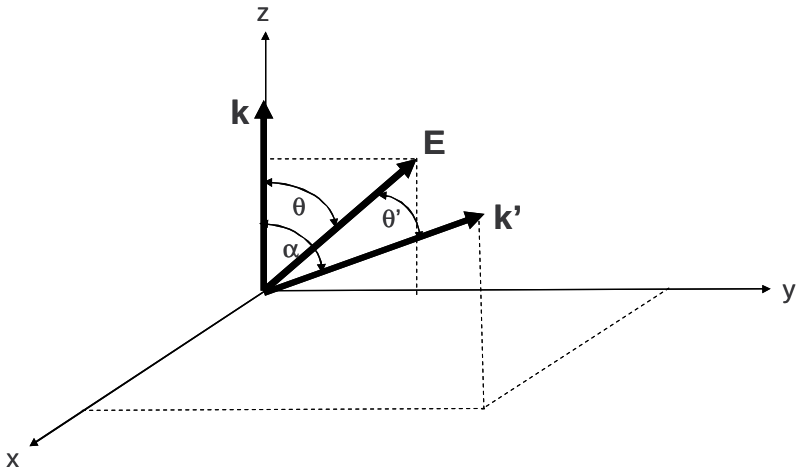

Figure 1. Coordinate system used in the rest of the derivation.

Within this coordinate system, we have:

$$k = (0, 0, k)$$
$$k' = (k' \sin\alpha \cos\varphi, k' \sin\alpha \sin\varphi, k' \cos\alpha)$$
$$E = (0, E\sin\theta, E\cos\theta) \tag{12}$$

which leads to:

$$E \cdot k' = Ek' \cos\theta' = Ek' \left(\sin\alpha \sin\varphi \sin\theta + \cos\alpha \cos\theta\right). \tag{13}$$

The integration over φ will make this term vanish, and under these circumstances we can write:

$$\frac{\cos\theta'}{\cos\theta} = tg\theta \sin\alpha \sin\varphi + \cos\alpha \rightarrow \cos\alpha \tag{14}$$

To summarize:

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -g_1(k)\cos\theta \sum_{k'} S(k,k') \left[1 - \frac{f_0(k) g_1(k')}{f_0(k') g_1(k)} \cos\alpha\right] \tag{15}$$

Note that for the relaxation approximation to be valid, the term in the brackets inside the summation sign should not depend upon the distribution function.

- Consider now the case of elastic scattering process. Then $|k| = |k'|$ and $\frac{f_0(k) g_1(k')}{f_0(k') g_1(k)} = 1$. Under these circumstances:

  $$\left.\frac{\partial f}{\partial t}\right|_{coll} = -g_1(k)\cos\theta \sum_{k'} S(k,k')(1-\cos\alpha) = -\frac{g_1(k)\cos\theta}{\tau_m(k)} = -\frac{f_A(k)}{\tau_m(k)}$$

  Hence, when the scattering process is ELASTIC, the characteristic time τ_f equals the momentum relaxation time.

- If the scattering process is ISOTROPIC, then *S*(**k**,**k'**) does not depend upon α. In this case, the second term in the square brackets averages to zero and

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -g_1(k)\cos\theta\sum_{k'} S(k,k') = -\frac{g_1(k)\cos\theta}{\tau(k)} = -\frac{f_A(k)}{\tau(k)}$$

Thus, in this case, the characteristic time is the scattering time or the average time between collision events.

To summarize, under low-field conditions, when the scattering process is either isotropic or elastic, the collision term can be represented as $-f_A/\tau_f(k)$, where in general $\tau_f(k)$ is the momentum relaxation time that depends only upon the nature of the scattering process. Following these simplifications, the BTE can thus be written as

$$-eEv\cos\theta\left(\frac{\partial f_0}{\partial E}\right) = -\frac{g_1(k)\cos\theta}{\tau_m(k)} \tag{16}$$

or

$$g_1(k) = eEv\tau_m(k)\left(\frac{\partial f_0}{\partial E}\right) \tag{17}$$

The distribution function is, thus, equal to

$$\begin{aligned} f(k) &= f_0(k) + eEv\cos\theta\tau_m(k)\left(\frac{\partial f_0}{\partial E}\right) \\ &= f_0(k) + eEv_z\tau_m(k)\left(\frac{\partial f_0}{\partial E}\right) \end{aligned} \tag{18}$$

To further investigate the form of this distribution function, we use $\frac{\partial f_0}{\partial E} = \frac{1}{\hbar v_z}\frac{\partial f_0}{\partial k_z}$. This leads to

$$f(k) = f_0(k) + \frac{e}{\hbar}E\tau_m(k)\frac{\partial f_0}{\partial k_z} \tag{19}$$

The second term of the last expression resembles the linear term in the Taylor series expansion of $f(\mathbf{k})$. Hence, we can write

$$f(k_x, k_y, k_z) = f_0\left(k_x, k_y, k_z + \frac{e}{\hbar} E\tau_m(k)\right) \tag{20}$$

To summarize, the assumption made at arriving at this last result for displaced Maxwellian form for the distribution function is that the electric field E is small. Hence, the displaced Maxwellian is a good representation of the distribution function under low-field conditions

References

1 P. A. Markowich and C. Ringhofer, *Semiconductor Equations* (Springer-Verlag, Wien New York).

2 C. Ringhofer, "Numerical Methods for the Semiconductor Boltzmann Equation based on Spherical Harmonics Expansions and Entropy Discretizations", *Transp. Theory and Stat. Phys.*, Vol. 31, pp. 431-452 (2002).