# Analytic formulae for the impact ionization rate for use in compact models of ultra-short semiconductor devices


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## ABSTRACT

This paper presents a new approximate compact formulae for the impact ionization (I.I.) generation rate ($G_{II}$) in ultra-short-channel devices.


## 1 INTRODUCTION

For ultra short length devices it is vital to accurately account for hot electron effects such as impact ionization. By means of a Fermi Golden Rule calculation with a screened Coulomb interaction, Quade, Schöll and Rudan [1] have shown that, in the limit of large screening length, the impact ionization rate per unit time can be expressed in the form

$$G_{II} = \frac{n}{(2\pi)^3} \int_{k_{th}}^{\infty} \frac{f(k)}{\tau_{II}(k)} d^3k \tag{1}$$

where $n$ is the electron density

$$n = \frac{2}{(2\pi)^3} \int f(k) d^3k \tag{2}$$

and $\tau_{II}(k)$is the isotropic ionization scattering time of the kth moment given by

$$\frac{1}{\tau_{II}(k)} = \frac{1}{2\tau_0}\left(\frac{k}{k_{th}} + \frac{k_{th}}{k} - 2\right) \tag{3}$$

where the parameter $\tau_0$ is called the characteristic inverse time constant [1].

If the density function $f(k)$ is modelled by a heated Maxwellian of the form

$$f(k) = \frac{\hbar^3}{2(2\pi m^* k_B T_e)^{3/2}} \exp\left(-\frac{\hbar^2 k^2}{2m^* k_B T_e}\right) \tag{4}$$

in which $T_e$ is the electron temperature, determined by the electric field within the device [2]. For a direct semiconductor, (1) yields the Schöll-Quade impact ionization rate formula

$$G_{II}(n, T_e) = \frac{n}{\tau_0}\left[\sqrt{\frac{u}{\pi}} \exp\left(-\frac{1}{u}\right) - \mathrm{erfc}\left(\frac{1}{\sqrt{u}}\right)\right] = \frac{n}{\tau_0} G_{SQ}(u) \tag{5}$$

involving the variable $u = {k_B T_e}/{E_{th}}$ where $E_{th}$ is the threshold energy for impact ionization. This parameter is frequently approximated by the band gap energy $E_g \approx 1.12$ ev. The parameter $\tau_0 \approx 1.26 \times 10^{-14}$ sec. In general we expect $\tau_0$ to be a function of the lattice temperature $T_L$. Selberherr et. al. [3], [4] have proposed new models for $f(k)$ that improve upon the heated Maxwellian (4) and provide a more accurate parameterization of the hot electron population. The analog of the integral (1) can be evaluated in terms of special functions and but these can be difficult to evaluate. We propose the use of the Gauss-Laguerre integration technique introduced in [5] as an effective way to generate simple analytic formulae that involve only elementary functions and provide a practical accurate formula for the impact ionization rate.

## 2 THE HEATED MAXWELLIAN

For the heated Maxwell case the impact ionization rate (1) is given by

$$G_{II}(n, T_e) = \frac{n}{\tau_0} G_{SQ}(u) \tag{6}$$

where $G_{SQ}(u)$ is defined by the integral

$$\frac{2}{\sqrt{\pi}} \frac{\hbar^3}{(2m^* k_B T_e)^{\frac{3}{2}}} \int_{k_{th}}^{\infty} k^2\left(\frac{k}{k_{th}} + \frac{k_{th}}{k} - 2\right) \exp\left(-\frac{\hbar^2 k^2}{2m^* k_B T_e}\right) dk \tag{7}$$

By introducing the change of variable $z = \sqrt{\frac{\hbar^2}{2m^* k_B T_e}} k$ this integral can be expressed as the sum

$$\sqrt{u} I_3(u) + \frac{1}{\sqrt{u}} I_1(u) - 2I_2(u) \tag{8}$$

with the moment functions $I_n(u)$ defined by

$$I_n(u) = \frac{2}{\sqrt{\pi}} \int_{\frac{1}{\sqrt{u}}}^{\infty} z^n \exp(-z^2) dz \tag{9}$$

The three moments required can be exactly evaluated

$$I_1(u) = \frac{2}{\sqrt{\pi}} \int_{\frac{1}{\sqrt{u}}}^{\infty} z \exp(-z^2) dz = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{u}} \tag{10}$$

$$I_2(u) = \frac{1}{2}\left(\mathrm{erfc}\left(\frac{1}{\sqrt{u}}\right) + \frac{2}{\sqrt{\pi}} \frac{1}{\sqrt{u}} e^{-\frac{1}{u}}\right) \tag{11}$$

$$I_3(u) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{u}} (\frac{1}{u} + 1) \quad (12)$$

and substitution of these into (8) yields the Schöll-Quade function $G_{SQ}$.

## 3 AN INTEGRATION TECHNIQUE

In order to capture the parameter dependence of the integral (1) we cannot use regular quadrature technique such as an adaptive Simpson rule. Instead we use the Gauss-Laguerre formulae [6]. The general form of this integration technique is

$$\int_0^\infty e^{-x} f(x)dx = \sum_{k=1}^{n} \omega_k \cdot f(x_k) + \frac{(n!)^2}{(2n)!} f^{(2n)}(\zeta) \quad (13)$$

where $0 < \zeta < \infty$ and $x_k$'s are the zeros (the nodes) of the Laguerre polynomials.

Using this integral approximation technique we can construct practical, closed-form, solutions that preserve the analytical dependence on parameters in the integral.

For the Schöll-Quade formula we need to evaluate three members of the family of integrals (9). Introducing the new variable $\zeta + \frac{1}{u} = z^2$ the integral $I_n(u)$ can be written in the form

$$I_n(u) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{u}} \int_0^\infty (\zeta + \frac{1}{u})^{\frac{n-1}{2}} e^{-\zeta} d\zeta \quad (14)$$

A two node approximation is given by

$$\widehat{I}_n^{(2)} = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{u}} (\omega_1 (x_1 + \frac{1}{u})^{\frac{n-1}{2}} + \omega_2 (x_2 + \frac{1}{u})^{\frac{n-1}{2}}) \quad (15)$$

The parameters $\omega_1, \omega_2, x_1$ and $x_2$ are fixed numerical constants given by

$$x_1 = 0.585786437626905$$
$$x_2 = 3.414213562373095$$
$$\omega_1 = 8.535533905932735e-01$$
$$\omega_2 = 1.464466094067262e-01$$

The factor $e^{-\frac{1}{u}}$ enhances the convergence greatly so even the two node approximation (15) produces the fit shown in figure 1.

## 4 THE TAIL DISTRIBUTION

For short channel devices, the Maxwellian form (4) has to be modified. A possible generalization is given by

$$f = \frac{b\sqrt{\pi}}{4\Gamma(\frac{3}{2b})} \frac{h^3}{(2\pi m^* k_B T)^{\frac{3}{2}}} \exp(-(\frac{\hbar^2 k^2}{2m^* k_B T})^b) \quad (16)$$

This form can accurately reproduce the Monte Carlo simulations of turned-on MOSFET's [3]. When the parameter $b = 1$ the expression (16) reduces to the heated Maxwellian form. However, when $b \neq 1$, $T$ can no longer

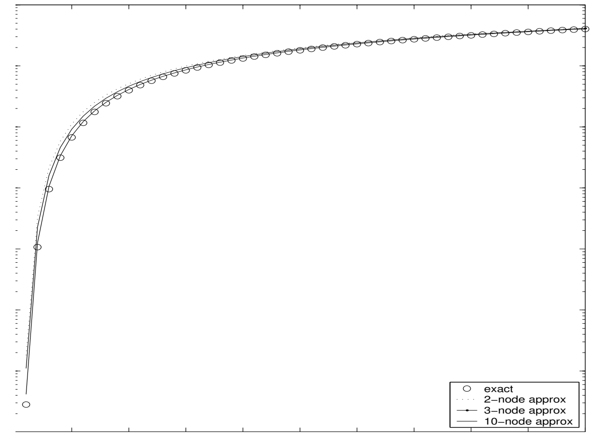


Figure 1: A fit of the exact Schöll-Quade function $G_{SQ}$ with $u \in [0, 5]$ by Gauss-Laguerre approximation with node numbers $N = 2, 3$ and 10.

be interpreted as the electron temperature. In this paper we will regard $b$ and $T$ as fitting parameters. The generalization $G_{GSQ}$ of the Schöll-Quade function $G_{SQ}$ to arbitrary $b$ is given by

$$\begin{aligned} G_{GSQ}(u,b) &= \frac{1}{2\Gamma(\frac{3}{2b})}[u^{\frac{1}{2}}\Gamma(\frac{2}{b})(1-\Gamma_{\text{inc}}(u^{-b},\frac{2}{b})) \\ &\quad + u^{-\frac{1}{2}}\Gamma(\frac{1}{b})(1-\Gamma_{\text{inc}}(u^{-b},\frac{1}{b})) \quad (17) \\ &\quad - 2\Gamma(\frac{3}{2b})(1-\Gamma_{\text{inc}}(u^{-b},\frac{3}{2b}))] \end{aligned}$$

involving the incomplete gamma function $\Gamma_{\text{inc}}(x, a)$ defined by

$$\Gamma_{\text{inc}}(x,a) = \frac{1}{\Gamma(a)} \int_0^x \exp(-z) z^{a-1} dz \quad (18)$$

The parameter $u = \frac{k_B T}{E_{th}}$ is determined by the tail distribution parameter $T$. The impact ionization rate is now given by

$$G_{II}^{\text{gen}}(n, T_e, b) = \frac{n}{\tau_0} G_{GSQ}(u,b) \quad (19)$$

Figure 2. shows the a semilogarithmic plot of the function $G_{II}^{\text{gen}}/n$ with $u \in [0, 5]$ for three values of $b$ close to the regular value $b = 1$. The plots are produced using the exact form of the incomplete gamma function. The incomplete gamma function is not trivial to evaluate and so we utilize the integration technique introduced in section three to obtain a simple analytic approximation to $G_{GSQ}$. Using our integration method we can approximate the incomplete gamma function (18) by the formula

$$1 - \exp(-\xi) - \frac{\exp(-\xi)}{\Gamma(a)} \sum_{k=1}^{N} w_k [(\xi + x_k)^{a-1} - x_k^{\ a-1}] \quad (20)$$

Formula (20) provides a source of simple formulae $G_{GSQ}^N(u, b)$ that approximate $G_{GSQ}(u, b)$. Figure 3 shows the the

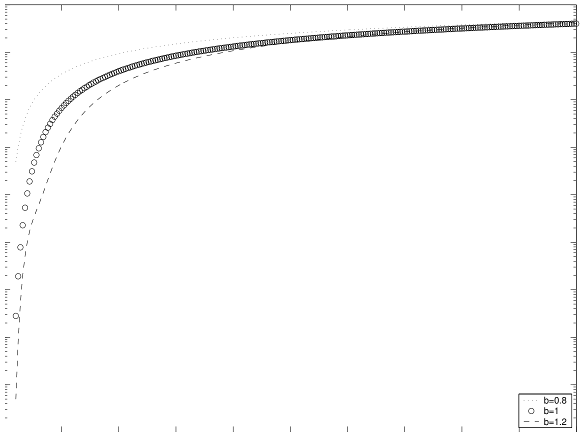


Figure 2: A semilogarithmic plot of the function $G_{II}^{\text{gen}}/n$ with $u \in [0,5]$ for $b = 0.8, 1$ and $1.2$.

Gauss-Laguerre approximations to $G_{GSQ}^N(u,b)$ with $u \in [0,5]$ for $N = 2,3$ and 10 nodes when $b = 1.2$. From this

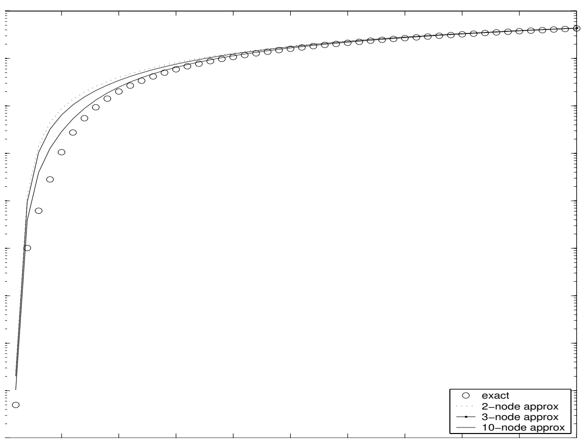


Figure 3: A fit of the function $G_{GSQ}^N$ with $u \in [0,5]$ with $b = 1.2$ for Gauss-Laguerre approximation with node numbers $N = 2,3$ and 10.

figure it is clear that we require a large numberof nodes if we require accuracy for small $u$ but the qualitative shape is well captured by even the 2-node approximation.

## 5 A GENERALIZED MODEL

In [4] the following analytical expression for the distribution function

$$\begin{aligned} f(k) &= \frac{h^3}{2(2\pi m^* k_B T_e)^{\frac{3}{2}}}[(1-c)\exp(-\frac{\hbar^2 k^2}{2m^* k_B T_e}) \\ &\quad + c\frac{b\sqrt{\pi}}{2\Gamma(\frac{3}{2b})}(\frac{T_e}{T})^{\frac{3}{2}}\exp(-(\frac{\hbar^2 k^2}{2m^* k_B T})^b) \qquad (21) \end{aligned}$$

has been proposed. When $c = 0$, $f(k)$ reduces to the heated Maxwellian (4) and when $c = 1$ it becomes the tail distribution function (16). For $0 \le c \le 1$ it allows an interpolation between the two forms. The impact ionization rate is a linear function of $f$ and so we obtain the new combined formula $G_{II}^{\text{new}}$ given by

$$G_{II}^{\text{new}}(u_1,u_2) = \frac{n}{\tau_0}G_{GSQ}^{\text{new}}(u_1,u_2) \qquad (22)$$

where

$$G_{GSQ}^{\text{new}}(u_1,u_2) = (1-c)G_{SQ}(u_1) + cG_{GSQ}(u_2) \qquad (23)$$

and the variables $u_1$and $u_2$ are defined by

$$u_1 = \frac{k_B}{E_{th}}T_e,\ u_2 = \frac{k_B}{E_{th}}T \qquad (24)$$

This new model has four parameters $c, b, T_e$ and $T$. In the next section we propose a special case of this general model that has fewer parameters and is easier to implement.

## 6 AN IMPROVED MODEL

To reduce the number of parameters we will make some reasonable assumptions about the values of the model parameters $c, b, T_e$ and $T$. From the reasoning behind the ansatz (21), it is reasonable to suppose that $T_e$ is the lattice temperature $T_L$ and that the 'tail temperature' $T = \alpha T_L$ with $1 \le \alpha \le 2$. We set $c = \frac{1}{2}$ so that the distributions are combined in a balanced way. This means that we only have a two parameters $b$ and $\alpha$ in our new model. The resulting expression for the impact ionization rate is given by

$$G_{II}^N(u,\alpha) = \frac{n}{\tau_0}G_{GSQ}^N(u,\alpha) \qquad (25)$$

with

$$G_{GSQ}^N(u,\alpha) = \frac{1}{2}(G_{GSQ}^N(u,b) + G_{GSQ}^N(\alpha u,b)) \qquad (26)$$

The variable $u$ is the standard Schöll-Quade variable

$$u = \frac{k_B}{E_{th}}T_L \qquad (27)$$

The approximation (26) with $b = 1$ was first introduced by Pop in [7]. Pop implemented the model in the context of the FIELDAY device simulation program and determined $\alpha = 1.8$ by data fitting. Figure 4 shows the improved model curves with $u \in [0,5]$ for the regular case $b = 1$ for $\alpha = 1$, the standard Quade formula, and $\alpha = 1.5$ and $\alpha = 2$.

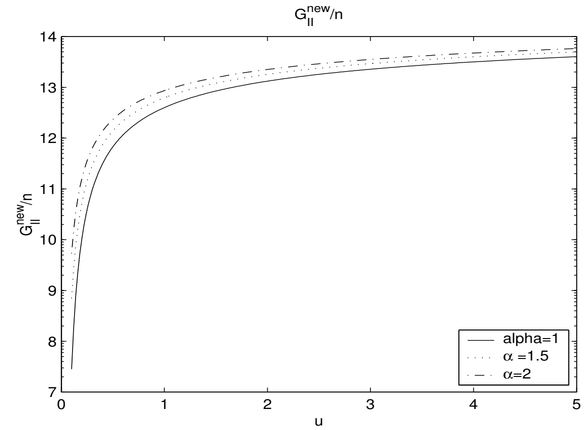


Figure 4: The generalized Schöll-Quade function $G_{II}^{\text{new}}(u, \alpha)$ with $u \in [0, 5]$ for $\alpha = 1$ (Quade) and $\alpha = 1.5$ and $\alpha = 2$.

## 7 CONCLUSION

We have presented a method for obtaining new accurate formulae for the impact ionization rate for use in compact modelling. We have combined an approach based on fundamental physics with the classical technique of Gauss-Laguerre integration. We have proposed both a general four parameter model and a simpler version we called the improved model. In our improved model, there are only two parameters. This latter model is a generalization of the model introduced by Pop [7]. In each case we have provided a family simple approximate formule for the impact ionization rate obtained by retaining a reduced number of Gauss-Laguerre nodes. This yields a series of models ranging from the lowest level 2-node approximation to the exact answer. We conjecture that the 2-node approximation may be adequate for most purposea as it captures the qualitative shape of the exact solution.

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