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# The hot-electron distribution of two-dimensional electrons in a polar semiconductor at zero temperature

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**Abstract.** An analytic solution is found for the most simple but realistic model of hot-electron transport in two dimensions. Only emission of longitudinal optical phonons is taken into account. Results are presented for the electron momentum and energy distribution functions, the average velocity and the electron temperature parallel and perpendicular to the electric field.

## 1. Introduction

The study of non-linear transport [1] is of paramount importance in modern electronics. With the decreasing size of electronic components, voltages are applied over smaller distances which results in larger electric fields. Transport will occur under conditions of high electric field and will be non-linear.

The equation governing transport under high (but not extreme) electric field is the Boltzmann equation. This is a non-linear integro-differential equation. The most popular way to solve this equation is by the Monte Carlo method [2], which is a purely numerical technique.

In a polar semiconductor with no impurities and lattice imperfections the only important process limiting the electric conductivity at zero temperature is the emission of longitudinal optical phonons (LO phonons). Under the action of an electric field the electron gains energy and will emit an LO phonon when its energy is larger than the LO-phonon energy $\hbar\omega_{\rm LO}$. The latter process is inelastic. The electron velocity falls back to around zero and the process of acceleration can start again. The average velocity of the electron is about half the critical speed, which is given by $v_{\rm LO} = (2\hbar\omega_{\rm LO}/m^*)^{1/2}$, and depends very little on the electric field ($m^*$ is the electron effective mass). Thus a saturation [3] in the average electron velocity versus the field is found. This type of electron transport leads to a pure streaming motion which has an anisotropic electron-momentum distribution. This was first suggested by Bray and Pinson [4] and later elaborated by Vosilius and Levinson [5] who introduced a 'needle-like' distribution for the electron momentum.

The Boltzmann equation for the situation of zero temperature was solved quasi-analytically for the case of electrons moving in three dimensions (3D) by Devreese and Evrard [6]. They invoked the so-called 'two-circle' model approximation. The basic idea is to separate the momentum space into two circles (called polaron circles) with radius $p_1 = (2m^*\hbar\omega_{\rm LO})^{1/2}$ and $p_2 = (4m^*\hbar\omega_{\rm LO})^{1/2} = \sqrt{2}p_1$, respectively. Then the

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Boltzmann equation can be solved under the assumption that there is a negligible probability of the electron reaching the second polaron circle. In [7] an asymptotic expression of the results of [6] was presented.

The aim of the present paper is to present a solution of the Boltzmann equation for transport in two dimensions (2D) in the extreme situation of low electron concentration at zero temperature and in the absence of impurities and lattice imperfections. In this case non-linear effects will be most pronounced and the electron velocity will only be limited by the process of LO-phonon emission. There is no thermal averaging and no re-distribution of the electron energy due to electron–electron collisions. We show that under these limits a quasi-analytic solution of the Boltzmann equation is possible. The present solution is useful: (i) in testing various approximations for non-linear electron transport, and (ii) as an extreme model for non-linear transport in two dimensions. In this paper the electron distribution function is studied within the 'two-circle' model adopted to the ideal two-dimensional situation. The analytic results are presented in section 3. The present results for the electron average velocity and average electron temperature are compared in section 4 with a solution of the Boltzmann equation by the Monte Carlo technique.

## 2. The transition and scattering rate for interaction with LO phonons

Applying Fermi's golden rule to the Fröhlich Hamiltonian, for a perfect 2D electron system [8] with only LO-phonon interaction in a parabolic band, we find for the transition probability $P(\boldsymbol{p}',\boldsymbol{p})$ from state $|p_x, p_y\rangle$ to state $|p'_x, p'_y\rangle$

$$P(\boldsymbol{p}',\boldsymbol{p}) = \frac{\alpha}{\sqrt{2}}\begin{bmatrix} N_0 \\ N_0+1 \end{bmatrix} \frac{\delta(p'^2/2 - p^2/2 \mp 1)}{|\boldsymbol{p}'-\boldsymbol{p}|} \tag{1}$$

where the minus (plus) sign refers to absorption (emission) of a phonon, which is proportional to the LO-phonon occupation number: $N_0 = 1/\exp(\hbar\omega_{\rm LO}/k_{\rm B}T - 1)$. $\alpha$ is the electron–phonon coupling constant. Above and in the following we use units such that $\hbar = m^* = \omega_{\rm LO} = 1$.

The scattering rate for a state $|p_x, p_y\rangle$ is denoted by $\lambda(p)$ and becomes

$$\lambda_\pm(p) = \frac{4\pi\alpha}{\sqrt{2}}\begin{bmatrix} N_0 \\ N_0+1 \end{bmatrix} \sum_{q_\parallel} \frac{1}{\sqrt{q_\parallel{}^4 + 4(p^2 \pm 1)q_\parallel{}^2 + 4}} \tag{2a}$$

which after performing the summation results in

$$\lambda_\pm(p) = 2\alpha\begin{bmatrix} N_0 \\ N_0+1 \end{bmatrix} \frac{\Theta(p\pm\sqrt{2})}{\sqrt{p^2/2} + \sqrt{p^2/2 \pm 1}} K\left(\frac{2[p^2/2(p^2/2\pm 1)]^{1/4}}{\sqrt{p^2/2}+\sqrt{p^2/2\pm 1}}\right) \tag{2b}$$

where $K(k)$ is the complete elliptic integral and $\Theta(x)$ the theta function. $\alpha$ is the Fröhlich coupling constant which is 0.068 for GaAs. $\lambda_-(p)$ $(\lambda_+(p))$ refers to the process of emission (absorption) of an LO phonon. In this paper we neglect size effects (the finite width of the 2D electron layer) in the scattering rate which were studied e.g. by Leburton [9] and Ridley [10].

## 3. The electron momentum distribution function

The Boltzmann equation in the presence of an electric field $\boldsymbol{E}$ along the $x$ direction is, for non-degenerate electrons, given by

$$\frac{\partial f(p_x,p_y)}{\partial p_x}eE = \int f(p'_x,p'_y)P(\boldsymbol{p}',\boldsymbol{p})\,\mathrm{d}\boldsymbol{p}' - \int f(p_x,p_y)P(\boldsymbol{p},\boldsymbol{p}')\,\mathrm{d}\boldsymbol{p}' \quad (3)$$

where $P(\boldsymbol{p}',\boldsymbol{p})$ is the probability that the electron makes a transition from the state $|p'_x,p'_y\rangle$ to the state $|p_x,p_y\rangle$ and is given by (1). Further we introduce

$$\lambda(p) = \int P(\boldsymbol{p},\boldsymbol{p}')\,\mathrm{d}\boldsymbol{p}'$$

which is the scattering rate for a state $|p_x,p_y\rangle$ and is given by (2).

In the following we limit ourselves to the situation of $T = 0$ where an analytic solution of the Boltzmann equation can be obtained. Because of the specific nature of the electron–LO-phonon interaction, the electron momentum distribution between two polaron circles is only coupled to the distribution function in adjacent circles. Under the assumption that $f(p_x,p_y) \approx 0$ when $p^2 \geq 4$, which is satisfied for electric fields that are not extremely high, the Boltzmann equation in the region $p^2 = {p_x}^2 + {p_y}^2 \geq 2$ takes the simple form

$$\frac{\partial f_>(p_x,p_y)}{\partial p_x}eE = -\lambda_-(p)f_>(p_x,p_y) \quad (4)$$

where $\lambda_-(p)$ is the scattering rate for emission of LO phonons at $T = 0$ K and $f_>(p_x,p_y)$ is the electron distribution between the two circles $2 < p^2 < 4$. Thus only 'scattering-out' into the inner circle with emission of a LO phonon is considered.

The electron momentum distribution located inside the first polaron circle, i.e. $p^2 \leq 2$, is determined by the Boltzmann equation

$$\frac{\partial f_<(p_x,p_y)}{\partial p_x}eE = \int f_>(p'_x,p'_y)P(\boldsymbol{p}',\boldsymbol{p})\,\mathrm{d}\boldsymbol{p}' \quad (5)$$

where $f_>(p'_x,p'_y)$ is the solution of (4). Electrons in the inner circle can only reach the outer circle through the acceleration effect of the electric field.

Solving equation (4) we obtain for the momentum distribution function in the strip $2 < p^2 < 4$

$$f_>(p_x,p_y) = C\exp\left[-A\int_0^1 \frac{\mathrm{d}x}{x\sqrt{1-x^2}}\ln\left(\frac{|p_x|}{\sqrt{2}}x + \sqrt{1+\frac{p^2-2}{2}x^2}\right)\right] \quad (6)$$

where $C$ is a constant which is determined by the continuity of the distribution at the polar circle, and $A = 2\sqrt{2}\alpha/eE$.

The function given by (6) falls off very rapidly with increasing $p$. Therefore the logarithmic term in (6) can be expanded in powers around $p = \sqrt{2}$. To first order this leads to

$$f_>(p,\theta) = C\exp(\theta^2 A/2)\exp[-Ag(\theta)(p/\sqrt{2}-1)] \quad (7)$$

with $g(\theta) = (\pi - 2\theta\sin\theta)/2\cos\theta$, and where now we have introduced polar coordinates with $\theta$ the angle between $p$ and the $x$ direction.

In order to obtain the momentum distribution function inside the circle $p^2 = 2$, we rewrite (5) as follows:

$$\frac{\partial f_<(p_x,p_y)}{\partial p_x} = \frac{A}{4\sqrt{2}}\int_0^{\pi/2} \mathrm{d}\theta'\, f_>(\sqrt{p^2+2},\theta')\left[\frac{1}{\sqrt{1+p^2-p\sqrt{p^2+2}\cos(\theta'+\theta)}} + \frac{1}{\sqrt{1+p^2-p\sqrt{p^2+2}\cos(\theta'-\theta)}}\right]. \tag{8}$$

We know that $f_>(p,\theta)$ falls off very rapidly with increasing $p$, which implies that the main contribution to the integration of (8) comes from the region $p \ll 1$. With this approximation the momentum distribution function inside the circle $p^2 = 2$ is obtained as

$$f_<(p_x,p_y) = \frac{C}{2}\int_0^{\pi/2} \mathrm{d}\theta\, \exp[-(\pi^2/8 - \theta^2/2)A]\exp[-Ap_y^2 g(\theta)/4] \times \sqrt{\frac{A\pi}{2f(\theta)}}\left[1 \pm \mathrm{erf}\left(\sqrt{Ag(\theta)}\frac{|p_x|}{2}\right)\right]. \tag{9}$$

where erf $(x)$ is the error function and the upper and lower symbols ($\pm$) refer to $p_x \geq 0$ and $p_x \leq 0$, respectively. One of the integration constants was determined by the condition that the distribution function has to be zero when $p_x \to -\infty$.

The constant C can be obtained from the continuity condition $f_>(\sqrt{2},\theta) = f_<(\sqrt{2},\theta)$ on the first polaron circle $p^2 = 2$. Finally we find for the momentum distribution function

$$f(p_x,p_y) = \begin{cases} CF(\theta)\exp[-Ag(\theta)(p/\sqrt{2}-1)] & p^2 \geq 2 \\ C\displaystyle\int_0^{\pi/2} \mathrm{d}\phi\, \frac{\exp\{[\phi^2 - g(\phi)p_y^2/2]A/2\}}{\sqrt{g(\phi)}}[1 \pm \mathrm{erf}(\sqrt{Ag(\phi)}|p_x|/2)] & p^2 \leq 2. \end{cases} \tag{10}$$

where we defined $f_<(0,0)/C = \int_0^{\pi/2} \mathrm{d}\phi\, \exp(\phi^2 A/2)/\sqrt{g(\phi)}$, and

$$F(\theta) = \int_0^{\pi/2} \mathrm{d}\phi\, \frac{\exp\{A[\phi^2 - g(\phi)\sin^2\theta]/2\}}{\sqrt{g(\phi)}}\left[1 \pm \mathrm{erf}\left(\sqrt{Ag(\phi)}\frac{|\cos\theta|}{\sqrt{2}}\right)\right].$$

## 4. Numerical results and discussion

In figures 1($a$) and 1($b$) the momentum distribution function obtained within the present 'two-circle' approximation are shown for the different values of AEM $= 2\sqrt{2}\alpha/eE$ and in the direction parallel (figure 1($a$)) and perpendicular (figure 1($b$)) to the electric field. For GaAs the values AEM = 1000, 200, 50, 20 and 10 correspond

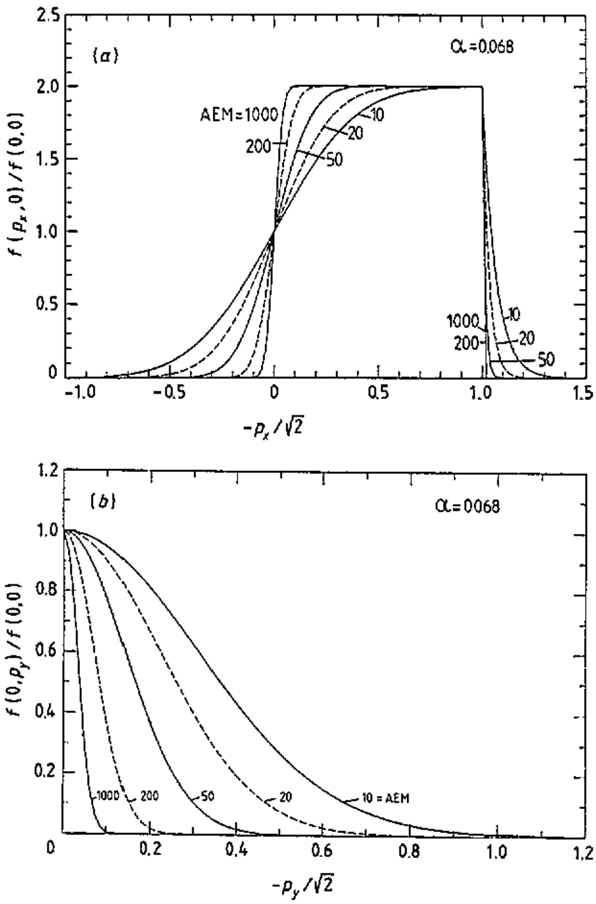


**Figure 1.** The momentum distribution function normalized to $f(0,0)$ for different values of AEM $= 2\sqrt{2}\alpha/eE$ at $T = 0$ K. The distribution function is plotted in (*a*) the $(p_x, 0)$ plane (i.e. along the electric field) and (*b*) the $(0, p_y)$ plane (i.e. perpendicular to the electric field).

to the electric fields, $E = 12.58$, 62.9, 251.6, 629 and 1258 V cm$^{-1}$, respectively. The momentum distribution function $f(p_x, p_y)$ is shown in figure 2 for: (*a*) low electric field (AEM = 200), (*b*) intermediate field (AEM = 50), and (*c*) high field (AEM = 10). From figures 1 and 2 it is apparent (i) that the distribution function goes to zero at the second polaron circle for the above values of AEM, and consequently our starting assumption of $f_>(p_x, p_y) \approx 0$ when $p^2 > 4$ holds. Since equation (10) is valid up to AEM = 10, this 'two-circle' model is more suitable for the case of 2D than for the 3D situation where the 'two-circle' approximation breaks down for AEM smaller than 20 as stated in [7]; (ii) that similar to the 3D case the smaller the electric field the more the distribution function approaches a rectangle in the $x$ direction and a delta function in the $y$ direction. In the limit of zero electric field we found the simple result

$$\lim_{E \to 0} f(p_x, p_y) = \delta(p_y)\Theta(p_x)\Theta(\sqrt{2} - p_x)/\sqrt{2} \tag{11}$$

where $\Theta(x) = 0$ $(x < 0)$, $1$ $(x > 0)$; (iii) that compared with the 3D case, as presented in [6] and [7], for the same values of AEM the distribution is sharper in 2D than in 3D.

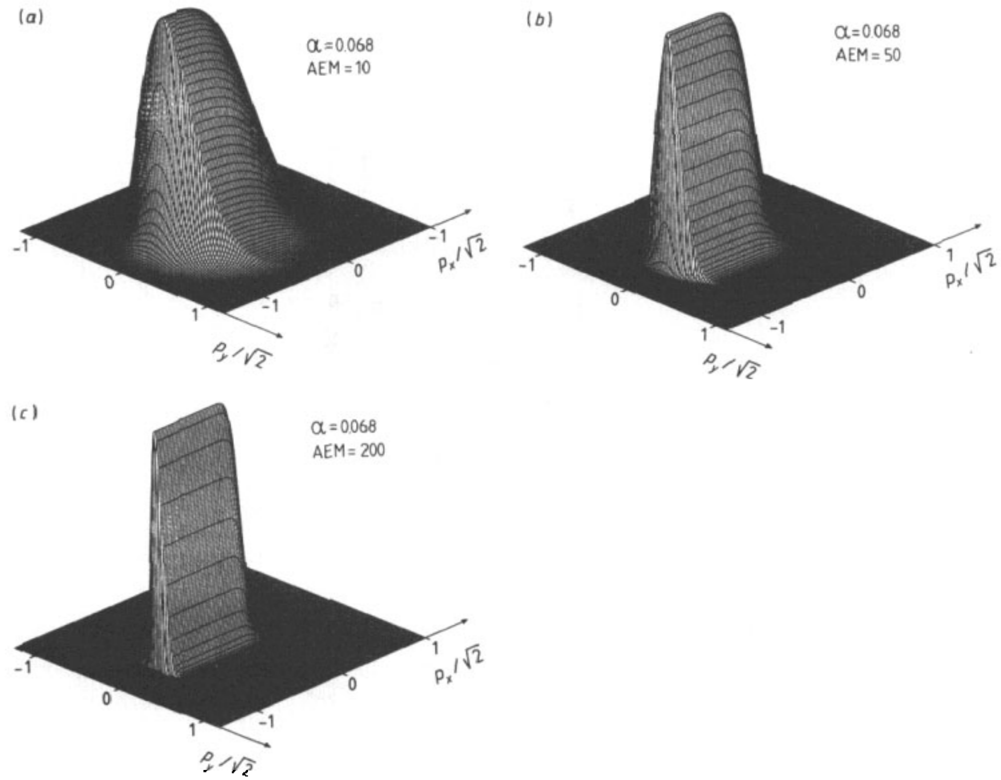


**Figure 2.** The momentum distribution function $f(p_x, p_y)$ normalized to $f(0,0)$ as obtained within the present model for: ($a$) high electric field, AEM = 10; ($b$) intermediate field, AEM = 50; ($c$) low field AEM = 200.

In figure 3 the contours of constant $f(p_x, p_y)$ are shown which correspond to the same values of electric field as in figure 2. The distribution function drops sharply past the first polaron circle $p = \sqrt{2}$. With decreasing electric field the distribution function becomes more concentrated inside a narrow range of momentum space.

The electron *energy* distribution function can be obtained from the momentum distribution function through

$$f(\epsilon) = \int \mathrm{d}p_x \int \mathrm{d}p_y \, f(p_x, p_y) \delta[\epsilon - ({p_x}^2 + {p_y}^2)] \tag{12}$$

which can be reduced to one integration

$$f(\epsilon) = 2 \int_0^{\epsilon^{1/4}} \mathrm{d}x \, \frac{f(x\sqrt{2\sqrt{\epsilon} - x^2}, \sqrt{\epsilon} - x^2) + f(-x\sqrt{2\sqrt{\epsilon} - x^2}, \sqrt{\epsilon} - x^2)}{\sqrt{2\sqrt{\epsilon} - x^2}} . \tag{13}$$

The numerical results for the energy distribution function corresponding to those of figure 2 are shown in figure 4($a$). In order to bring out the non-Maxwellian shape of the electron distribution more clearly we show in figure 4($b$) the same distribution function on a logarithmic scale. Note the rapid decrease of the energy distribution for $\epsilon > \hbar\omega_{\mathrm{LO}}$. Inserting equation (7) into (13) we find $f_{>}(\epsilon) \sim \exp(-a\sqrt{\epsilon})$ for $\epsilon > \hbar\omega_{\mathrm{LO}}$ where $a \sim$ AEM is large in low electric fields.

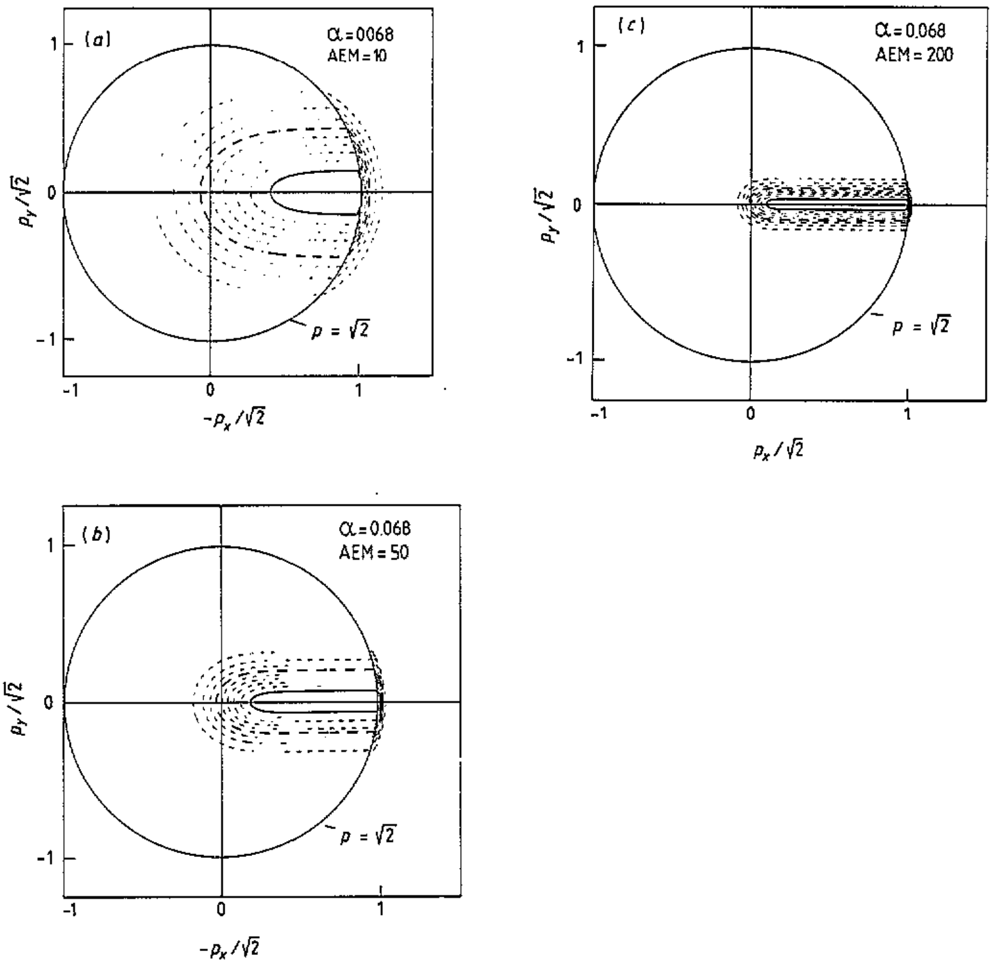


**Figure 3.** Contour plots of constant momentum distribution function $f(p_x, p_y)$ for the same parameters as in figure 2 for: (*a*) AEM = 10, (*b*) AEM = 50 and (*c*) AEM = 200.

Given the distribution function $f(p_x, p_y)$, all physical observables of interest can be obtained by numerical integration. In figure 5 we show the results for the electron average velocity. The electron temperatures parallel and perpendicular to the electric field defined by $T_{\parallel} = \langle p_x{}^2 \rangle / (2k_B m^*)$ and $T_{\perp} = \langle p_y{}^2 \rangle / (2k_B m^*)$, respectively, are shown in figure 6 in units of $T_D = \hbar\omega_{LO}/k_B$. The average $\langle \cdots \rangle$ is over the electron momentum distribution function. For comparison the Monte Carlo results are given by the symbols, this corresponding to an 'exact' numerical solution of the Boltzmann equation. In the limit of an infinitely long simulation time the Monte Carlo approach will lead to the exact result. Note that for the present model, at $T = 0$, there is no linear regime. The velocity approaches $v_{LO}/2$ in the limit $E \to 0$. The reason is that for velocities $v < v_{LO}$ the electron behaves like a free particle and under the action of an electric field the electron performs an accelerated motion until $v = v_{LO}$. This is

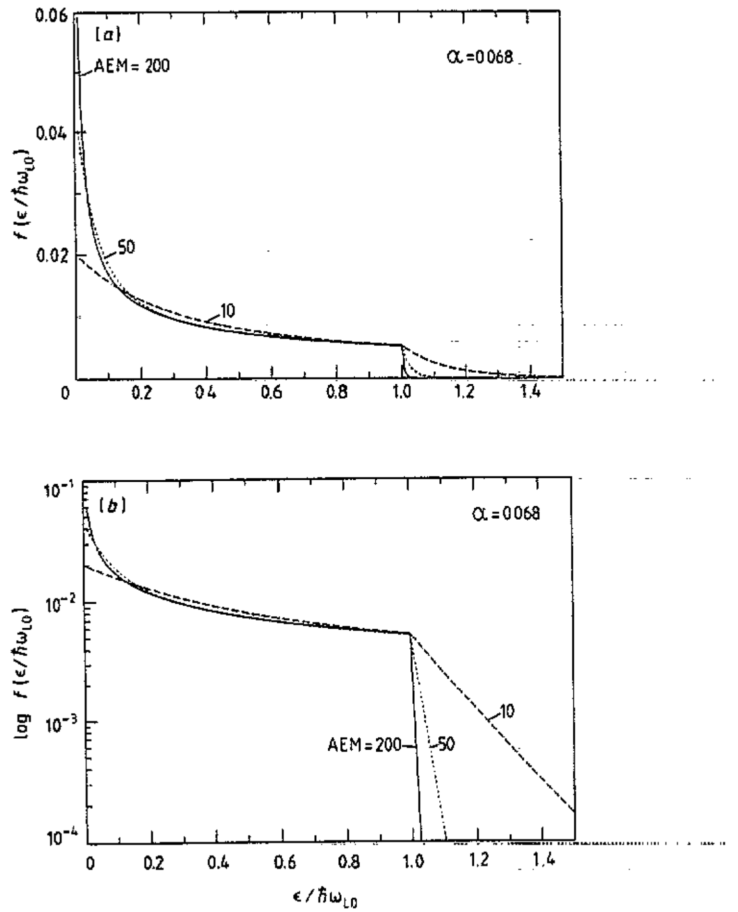


**Figure 4.** (*a*) The normalized energy distribution function $f(\epsilon)$ versus the electron energy $\epsilon$ for the same values of AEM as in figure 2. (*b*) the same energy distribution function $f(\epsilon)$ shown on a logarithmic scale.

also the reason why $T_{\parallel}$ approaches

$$\frac{1}{2}k_{\mathrm{B}}T_{\parallel} = \frac{m^*}{2}\frac{1}{t_0}\int_0^{t_0} \mathrm{d}t\, v^2(t) = \frac{1}{3}k_{\mathrm{B}}T_D$$

which is non-zero and independent of the electric field. We used the fact that $v(t) = eEt$ for $v < v_{\mathrm{LO}}$ and $t_0 = v_{\mathrm{LO}}/eE$. Of course $T_{\perp} \to 0$ for $E \to 0$.

## 5. Conclusion

An analytic solution of a model system for hot-electron transport in a non-degenerate two-dimensional electron gas was presented in the case of zero temperature. This calculation can be applied to high mobility and very low electron density heterostructures at low temperature and high electric field where transport is non-linear and dominated by LO-phonon emission.

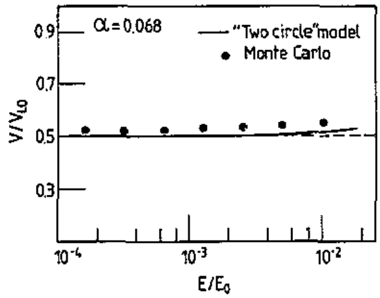


**Figure 5.** The average electron velocity as a function of the electric field. The results of the 'two-circle' model are shown by the full curve and the full circles are the results from a exact solution of the Boltzmann equation obtained with the Monte Carlo method. For GaAs $v_{LO} = 4.40 \times 10^7$ cm s$^{-1}$ and $E_0 = 9.25 \times 10^4$ V cm$^{-1}$.

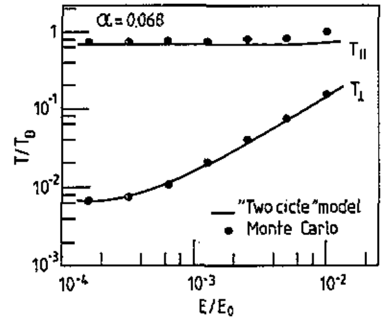


**Figure 6.** As figure 5, but for the average electron temperature parallel ($T_{\|}$) and perpendicular ($T_{\perp}$) to the electric field. For GaAs $T_D = 425$ K and $E_0 = 9.25 \times 10^4$ V cm$^{-1}$.

The results of this paper can also be used to test various approximations for non-linear electron transport, i.e., the displaced Maxwellian approach. A comparison of the results of the 'two-circle' model was made with the results of a Monte Carlo simulation. We presented an explicit analytic expression for the electron momentum distribution function which was also plotted. From this function the energy distribution function, the average electron velocity and average electron temperature parallel and perpendicular to the electric field was calculated. It was found that for the present zero-temperature model the non-linear regime extends to zero electric field.

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## References

[1] Sze M 1981 *Physics of Semiconductor Devices* (New York: Wiley)
[2] Jacoboni C and Reggiani L 1983 *Rev. Mod. Phys.* **55** 645
[3] Shockley W 1950 *Bell System Tech. J.* **30** 990
[4] Bray R and Pinson W E 1964 *Phys. Rev.* **136** A1449
[5] Vosilius I I and Levinson I B 1966 *Sov. Phys.-JETP* **23** 1104
[6] Devreese J T and Evrard R 1976 *Phys. Status Solidi* b **78** 85
[7] Peeters F M and Devreese J T 1981 *Phys. Status Solidi* b **108** K23
[8] Sak J 1972 *Phys. Rev.* B **6** 3981
[9] Leburton J P 1984 *Appl. Phys.* **56** 2850
[10] Ridley B K 1982 *J. Phys. C: Solid State Phys.* **15** 5899