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ABSTRACT

An approximate, electron energy distribution function, $f(\epsilon, x, t)$, is obtained for the case of a slightly ionized gas with inelastic electron-molecule collisions, and for an external electric field with both spatial and temporal variation. A previous analysis of the Boltzmann equation, for a slightly ionized gas with time-varying electric field and inelastic collisions, has been extended to include the effect of a spatial gradient in the electric field. This paper describes the spatial variation effect by continuing the discussion on the electron distribution initiated in that previous report. An interesting feature of this analytical distribution function is its explicit dependence on both the magnitude of the field and its gradients. An example is included of the combined effect of field variations in space and time upon the local average electron energy in an idealized N_2 -like gas.

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Introduction

This report continues the discussion initiated in Reference 1, and the reader is referred to that work for introductory comments, literature references, and many definitions. The material from both Reference 1 and this report is being prepared for submission to a scientific journal.

This paper will be structured as follows. First, the analytical result for the logarithmic derivative in energy of the electron distribution function is stated. Then, a brief discussion of the derivation for a spatially varying field is given; it is quite analogous to the time-varying case. Examples of the solution are given for an idealized nitrogen-like gas where a static electric field decays exponentially with distance. Finally, the combined effect of field gradients in space and time is demonstrated by mapping out the average electron energy in the model gas for a field with sinusoidal temporal variation and exponential spatial decay.

Analytical Result

The distribution function of electron energies is denoted as $f(\epsilon, x, t)$, where electron kinetic energy ϵ is expressed in units of eV, and where the distribution function is normalized as:

$$\int f(\epsilon, x, t) \sqrt{\epsilon} d\epsilon = 1, \quad (1).$$

The function $B(\epsilon, x, t)$ is defined as:

$$B(\epsilon, x, t) = -(\partial/\partial\epsilon) \ln[f(\epsilon, x, t)], \quad (2),$$

and the distribution function is then given by:

$$f(\epsilon, x, t) = \frac{- \int_0^\epsilon B(\epsilon, x, t) d\epsilon}{\int_0^\infty \frac{- \int_0^\epsilon B(\epsilon, x, t) d\epsilon}{e} \cdot \sqrt{\epsilon} d\epsilon} \quad (3).$$

The logarithmic slope $B(\epsilon, x, t)$ is given by:

$$B(\epsilon, x, t) = \frac{\sqrt{(L + \mu)^2 + \left(\frac{4 \cdot Q_l}{\epsilon \cdot Q_m} \right) \cdot \left(U + \mu \cdot \frac{kT}{e} \right)} + (L + \mu)}{2 \cdot \left(U + \mu \cdot \frac{kT}{e} \right)} \quad (4).$$

The terms used in $B(\epsilon, x, t)$ are as follows:

$$L(\epsilon, x, t) = \left[\frac{\omega}{2 v_m} + 6 \cdot \left(\frac{\lambda_m}{\lambda_e} \right) \cdot \left(\frac{E/N}{3 \epsilon Q_m} + \frac{\lambda_m}{\lambda_e} \right) - \lambda_m^2 \frac{\partial}{\partial x} \cdot \left(\frac{1}{\lambda_e} \right) \right] \cdot \Phi \quad (5),$$

$$U(\epsilon, x, t) = \left[b(\epsilon, x, t) + \frac{E/N}{3 Q_m} \cdot \left(\frac{\lambda_m}{\lambda_e} \right) \right] \cdot \Phi \quad (6),$$

$$\Phi(\epsilon, x, t) = H(\epsilon_m(\epsilon, x, t) - \epsilon),$$

H = Heaviside Unit Step Function,

$$\epsilon_m(\epsilon, x, t) = - \frac{E(x, t) \lambda_m}{[\lambda_m/\lambda_e + 3(\mu kT/e)/(E\lambda_m)]}$$

$$@ \lambda_m/\lambda_e < -3(\mu kT/e)/(E\lambda_m),$$

$$\epsilon_m(\epsilon, x, t) = \infty$$

$$@ \lambda_m/\lambda_e \geq -3(\mu kT/e)/(E\lambda_m) \quad (7),$$

$$b(\epsilon, x, t) = [E(x, t)/N]^2 / (3\epsilon Q_m^2) \quad (8),$$

$$\frac{1}{\lambda_e(x, t)} = \frac{1}{4} \cdot \frac{\partial}{\partial x} \cdot \ln \left(\frac{E(x, t)}{N} \right) \quad (9),$$

$$\lambda_m(\epsilon) = 1 / (N Q_m(\epsilon)) \quad (10);$$

and the following originally defined in Reference 1:

$$\omega(x, t) = 3/2 * 1/[E/N] * (\partial/\partial t) [E/N], \quad (11),$$

$E(x, t)$ = electric field (V/cm) over space & time, in the form:

$$E(x, t) = |E(x, t)| + kT/e * Q_m(kT/e) * N,$$

$$E(x, t) = \text{any imposed external field}, \quad (12),$$

$$v_m(\epsilon) = N * Q_m * \sqrt{2e\epsilon/m}, \quad (13),$$

$$\begin{aligned} Q_m(\epsilon) &= \text{electron-molecule momentum transfer cross section (cm}^2\text{)}, \\ Q_i(\epsilon) &= \text{electron-molecule net inelastic cross section (cm}^2\text{)} \end{aligned} \quad (14),$$

$$\begin{aligned} \mu &= 2m/M, \\ m &= \text{electron mass,} \\ M &= \text{molecule mass,} \end{aligned} \quad (15),$$

$$kT/e = \text{gas temperature in eV,} \quad (16),$$

$$N = \text{gas mixture number density (cm}^{-3}\text{), a constant,} \quad (17).$$

For a gas mixture:

δ_s = fractional concentration of species s ,

$$Q_m(\epsilon) = \sum_s \delta_s \cdot Q_{ms}(\epsilon)$$

m = momentum transfer,

$$Q_i(\epsilon) = \sum_s \sum_i \sum_j \delta_{si} \cdot Q_{isij}(\epsilon)$$

i = inelastic process (sum) with transition indices:
 i = index of initial energy level,
 j = index of final energy level,

$$\sum_s \sum_i \delta_{si} = 1$$

$$M = \sum_s \delta_s \cdot M_s$$

(18).

Analytical Procedure

This analysis begins with a two term expansion of the electron velocity distribution function in a Boltzmann equation with three collisional effects: recoil and thermal agitation during elastic electron-molecule encounters, and inelastic collisions.²

$$\begin{aligned} \frac{\partial f_0}{\partial t} + \frac{\mathbf{v}}{3} \cdot \frac{\partial f_1}{\partial \mathbf{x}} - \frac{eE_x(\mathbf{x}, t)}{m} \cdot \frac{1}{3v^2} \cdot \frac{\partial}{\partial v} \cdot (v^2 \cdot f_1) = \\ \frac{1}{2v^2} \cdot \frac{\partial}{\partial v} \cdot \left[v^2 \cdot \left(2 \cdot \frac{m}{M} \right) (N \cdot Q_{m \cdot v \cdot r}) \cdot \left(\frac{kT}{m} \cdot \frac{\partial f_0}{\partial v} + \mathbf{v} \cdot \mathbf{f}_0 \right) \right] + S_I(v) \end{aligned} \quad (19).$$

$$\frac{\partial f_1}{\partial t} + \mathbf{v} \cdot \frac{\partial f_0}{\partial \mathbf{x}} - \frac{eE_x(\mathbf{x}, t)}{m} \cdot \frac{\partial f_0}{\partial v} = -(N \cdot Q_{m \cdot v \cdot r}) \cdot f_1 \quad (20).$$

$$\frac{4 \cdot \pi \cdot \sqrt{2}}{\left(\frac{m}{e} \right)^{\frac{3}{2}}} \cdot \sqrt{\frac{m \epsilon}{2 e}} \cdot \frac{S_I(v)}{N} =$$

$$\sum_s \sum_i \sum_j \delta_i^s \cdot \left[(\epsilon + \epsilon_{i,j}^s) f_0(\epsilon + \epsilon_{i,j}^s) \cdot Q_{i,j}^s(\epsilon + \epsilon_{i,j}^s) - \epsilon \cdot f_0(\epsilon) \cdot Q_{i,j}^s(\epsilon) \right] \quad (21).$$

The two term expansion is

$$f = f_0 + \cos(\theta) * f_1 \quad (22),$$

where θ is the angle between the electron velocity vector and the field. Coordinate x is aligned with the field, which is noted by a subscript x on E , and v_r is the relative electron-molecule velocity. $S_I(v)$ is the inelastic collision term, shown in equation (21) as a function of energy.

The f_0 term of the expansion describes the bulk heating of the electrons by the electric field in an environment dominated by collisions, while the f_1 term describes the net drift of this electronic swarm along the field and represents the macroscopic current.

The recoil and thermal agitation collision terms transmit a small fraction of an electron's energy to a molecule, this fraction being given by the ratio of the electron to molecule masses. The inelastic term involves the transfer of sufficient energy to initiate rotational, vibrational, electronic, dissociation, and ionization phenomena.

The zeroth and first order velocity distribution equations are transformed to a dependence on electron kinetic energy in units of eV. During this change of parameters the relative velocity between electrons and molecules is ascribed entirely to electron speed. Specifically:

$$\epsilon = mv^2/2e,$$

$$f_0(\epsilon, x, t) = [4\pi\sqrt{2}/(m/e)^{3/2}] * f_0(v, x, t), \quad (23).$$

Equations (19), (20), and (21) are combined into a single expression for f_0 , hence that subscript is eventually dropped. This equation is divided by N and integrated over energy from 0 to ϵ .

The analysis beyond this point is completely analogous to that of Ref. (1), only now additional terms appear because of the inclusion of the $\partial/\partial x$ terms in equations (19) and (20). A quadratic equation for $B(\epsilon, x, t)$ results given the following two conditions:

$$(\epsilon / 2 v_m) * \partial B / \partial t \rightarrow 0$$

$$(\epsilon \lambda_m) * \partial B / \partial x \rightarrow 0 \quad (24),$$

essentially, changes in B are negligible over a collision time and mean free path. The positive solution of this quadratic is given by equation (4), with terms as described by (5) through (18), but with this important exception:

function $\Phi(\epsilon, x, t)$, which appears in equations (5), (6), and (7), does not appear, it is an *ad hoc* modification.

The addition of factor $\Phi(\epsilon, x, t)$ is justified on the following grounds. The B of equation (4) becomes infinite when $(U + \mu kT/e)$ goes to zero, f becoming infinitely steep. This occurs when ϵ equals ϵ_m which is defined in (7). Electrons in the neighborhood of (x, t) with energy higher than $\epsilon_m(\epsilon, x, t)$ simply do not sense the electric field, they gain less energy from the field between collisions than they do by purely thermal effects. As a result electrons above $\epsilon_m(\epsilon, x, t)$ are distributed in what would be a Maxwellian at the gas temperature (kT/e in eV) if Q_i were absent. The factor Φ effects this transition. Note that for a uniform field $1/\lambda_e = 0$, $\epsilon_m = \infty$, $\Phi = 1$.

Examples in a Model Gas

Examples are shown for a model gas with molecular weight $Z = 29$ (like air), a constant $Q_m = 10^{-15} \text{ cm}^2$, at temperature $T = 300^\circ \text{ K}$, and at number density $N = 3.54 \times 10^{16} \text{ cm}^{-3}$ (1 Torr). An inelastic cross section similar to vibrational excitation in N_2 and with a peak of $Q_i(1.7) = 3 \times 10^{-16} \text{ cm}^2$ was chosen and is shown below.

Figure 1: Model Inelastic Cross Section

The following examples have electric fields that decay exponentially with scaled distance x/λ_E , where coordinate x and parameter λ_E are expressed in cm. The first two examples have λ_E equal to 0.0282 and 0.282 cm. respectively. The electron-molecule mean-free-path, λ_m , is 0.0282 cm. Both examples display results for a total distance of $3 \times \lambda_E$.

The first example has $\lambda_E = \lambda_m$ and exhibits a strong gradient effect, which is negligible in the second case. For each case the results are calculated twice: with $E(x,t)$ and its gradients, and then again for $E(x,t)$ but with its spatial and temporal derivatives (equations (9) and (11)) set to zero. The "zero gradient" results are labeled by a letter z in their names. Figures 2 through 8 show the first example, Figures 9 through 15 are for the second.

$B(\epsilon, x)$

$B(\epsilon, x) @ 1/\lambda_e = \omega = 0 \Rightarrow B_z$

Figure 2: B and B_z for $\lambda_E = 0.0282$, example 1

Figure 3: $f(\varepsilon, x = \text{selected space steps})$, $\Delta x = 0.0021$, example 1

$f(\epsilon, x)$

$\log(f)$

Figure 4: $f(\epsilon, x)$ to $(\epsilon, x) = (4 \text{ eV}, 0.0846 \text{ cm.})$, example 1

Figure 5: Variation with x for $\lambda_E = 0.0282$, example 1

Figure 6: $\varepsilon_m(x)$, maximum energy sensing $E(x)$, example 1

Figure 7: Comparison of ε and ε_z shows the field gradient effect, example 1

$$f(\epsilon, x) @ 1/\lambda_e = \omega = 0 \Rightarrow fz$$

$$\log(fz)$$

Figure 8: $fz(\epsilon, x)$ to $(\epsilon, x) = (4 \text{ eV}, 0.0846 \text{ cm.})$, example 1

B

B_z

**Figure 9: B and B_z for $\lambda_E = 0.282$, example 2,
(compare to Figure 2)**

Figure 10: $f(\epsilon, x = \text{selected space steps})$, $\Delta x = 0.0212$, example 2, (compare to Figure 3)

f

$\log(f)$

Figure 11: $f(\epsilon, x)$ to $(\epsilon, x) = (4 \text{ eV}, 0.846 \text{ cm.})$, (compare to Figure 4)

Figure 12: Variation with x for $\lambda_E = 0.282$, (compare to Figure 5)

Figure 13: $\epsilon_m(x)$, maximum energy sensing $E(x)$, example 2, (compare to Figure 6)

Figure 14: Negligible field gradient effect, $\lambda_E = 0.282$, example 2, (compare to Figure 7)

fz

$\log(fz)$

Figure 15: fz for $\lambda_E = 0.282$, (compare to Figures 11, 8, and 4)

The last example is for E/N a 100 Td (1 Td = Townsend = 10^{-17} Volt- cm^2) sine wave in time, at 500 kHz with phase angle $\phi = \pi/4$, and with an exponential decay along x/λ_E for $\lambda_E = 0.0282$. Figures 16 through 23 show various features of this example.

$E/N(x, t)$

$\lambda_m(kT/e)/\lambda_e(x, t)$

Figure 16a: E/N and the functions dependent on it, for example 3

$$\omega (x, t) / 2 v_m (kT/e)$$

$$A(\text{djusted})\epsilon_m (x, t)$$

Figure 16b: E/N and the functions dependent on it, for example 3
 ($A\epsilon_m$ is ϵ_m adjusted by removing large values at node lines of temporal sine, see Figure 17)

Figure 17: ϵ_m for example 3

Figure 18: ϵ and ϵ_z (eV) over time at selected $\Delta x (= 0.0021)$ steps

The large excursions that occur in ϵ and other functions for large $\omega/2v_m$ at low E/N (as in the sine nodes) arise from the basic discrepancy between the actual form of $B(\epsilon, x, t)$ and the very approximate form for B utilized within the normalization integral (equation (19) in Ref. 1) during the derivation of equation (4). Basically, the relationship between ω and E/N embodied in equations (11) and (12) is not sufficiently accurate for E/N comparable to $Q_m * kT/e$. In physical terms, the time dependent model breaks down when the energy gained per mean free path from the field becomes comparable to thermal energy.

Figure 19: ϵ and ϵ_z at time 0 along coordinate x (compare to Figure 7)

Figure 20: ratio ϵ/ϵ_z along t at selected space steps ($\Delta x = 0.0021$)

$\epsilon(x, t)$

$A\epsilon(x, t)$, (adjustment along node lines)

Figure 21: $\epsilon(x, t)$ to $(x, t) = (0.0846 \text{ cm.}, 2.5 \mu\text{s})$ for example 3

$\epsilon_z (x, t)$

Figure 22: $\epsilon_z (x, t)$ (compare to Figure 21)

Figure 23: ϵ/ϵ_z to $(x, t) = (0.0846 \text{ cm}, 2.5 \text{ } \mu\text{s})$ for example 3

Ratio $\epsilon/\epsilon_z (x, t)$, using ϵ adjusted along the node lines

Conclusion

This analytical model of inelastic electron kinetics with space and time dependent external electric fields is centered on $B(\epsilon, x, t)$ as defined in equation (4). The model distribution function collapses to appropriate limiting behavior, as shown in Ref. (1) for both uniform and uniform-static electric fields. In addition, the model distribution function along with its velocity and energy moments compare very favorably with calculated and measured properties of real gases in the uniform-static limit, as demonstrated in Ref. (3).

This model is convenient in that B is an explicit analytical form in which the influence of the field magnitude along with its spatial and temporal gradients at (x, t) are individually accounted for in separate parameters. As few assumptions were made about the nature of $E(x, t)$ and the cross sections, a wide variety of electrically excited gases can be modeled.

Finally, this analytical result could be useful as the electron kinetics component of a much larger electrically excited gas model, such as for an RF plasma-chemical sheath.

References

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