

Novel computer simulation of electron swarm motion

L. Friedland

Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem, Israel
(Received 10 November 1976; final manuscript received 24 March 1977)

A novel computer simulation technique for the study of properties of electron swarms in gases is presented. As an example, the method is applied to nitrogen at E/N values of 10^{-16} – 10^{-15} V cm². A strong directional anisotropy in the electron velocity distribution function is observed. The anisotropy is especially strong at electron energies for which the inelastic collision cross section is large relative to the total collision cross section. The first asymmetric term in the expansion of the distribution function in spherical harmonics can be as high as 70% of the value of the symmetric part of the distribution. A comparison with the computer simulation shows, however, that in spite of such strong anisotropy in nitrogen at these values of E/N , the solution of the Boltzmann equation based on the first two terms of the spherical harmonic expansion, gives correct values of electron drift velocity, average electron energy, and average vibrational excitation frequency.

I. INTRODUCTION

Knowledge of the electron velocity distribution function is necessary to understand the processes occurring in electrical gas discharges. The distribution function, however, is an elusive entity which cannot easily be obtained by the experimental methods, even in the case of a uniform electric field.

The theoretical method, most commonly used, to determine the electron velocity distribution function $f(\mathbf{v})$ in a gas discharge in a uniform electric field is based on the solution of the Boltzmann equation, using an approximate description of the dependence of $f(\mathbf{v})$ on the angle θ between electron velocity \mathbf{v} and the direction of the electric field. To accomplish this the electron velocity distribution function is usually expanded in spherical harmonics

$$f(\mathbf{v}) = f(v, \theta) = f_0(v) + \cos\theta f_1(v) + \frac{1}{2}(3\cos^2\theta - 1)f_2(v) + \dots \quad (1)$$

using only the first two terms of the expansion.¹ It is expected that as the deviation of the distribution function from spherical symmetry depends on the ratio E/N between the strength of the electric field and the gas number density, the deviation will be small at least for small enough values of E/N .

For many years the two-term expansion was used to calculate the electron velocity distribution and various electron transport coefficients in a large number of electrical gas discharges.²⁻⁷ Although this approach is quite successful, the justification and validity for neglecting the higher terms in expansion (1) is being presently questioned,^{8,9} for certain gases even at small values of E/N . Such a situation appears in gases like nitrogen or carbon monoxide having high inelastic collision cross section at low electron energies.

The problem is emphasized if one looks into the relation between the symmetrical part of the distribution $f_0(v)$ that defines the electron energy distribution function and the asymmetric part $f_1(v)$. This relation is given by Nighan⁵ as

$$f_1(v) = -\frac{eE}{mN} \frac{1}{v\sigma_m(v)} \frac{df_0(v)}{dv}, \quad (2)$$

where e and m are electric charge and mass of the electron, respectively, and $\sigma_m(v)$ is the momentum transfer cross section. As a result of large vibrational excitation cross sections in gases like nitrogen or carbon monoxide, the electron energy distribution function [and therefore, the function $f_0(v)$] decreases drastically in the electron energy region of 2–3 eV. Therefore, as a result of (2), in this energy region the values of the function $f_1(v)$ can be large even for small of E/N . This fact poses the question of whether it is justified to ignore the high order terms in the expansion (1) for such gases. It should be pointed out that for the electron energies for which the cross section of the inelastic excitation of the molecules is not so large, the two-term approximation is apparently quite good. Even so, changes in the distribution function in a certain electron energy region certainly cause a change in the distribution function for all electron energies as a result of the normalization condition.

In this paper we present a novel computer simulation method in which the distribution function can be obtained with minimum assumptions. The method will be applied to nitrogen for which various electron transport coefficients will be calculated and compared with those obtained by the two-term expansion method.

II. THE SIMULATION METHOD

A computer simulation method to calculate the electron transport coefficients in electrical discharges in gases was first introduced by Itoh and Musha¹⁰ in a helium discharge. Later, other investigators^{11,12} used the same simulation algorithm for argon and neon. The algorithm proposed by Itoh and Musha is based on dividing the parabolic trajectory of the electron between two successive collisions into a large number of small intervals in which the trajectory is considered straight. This stepwise process involves time consuming computations to simulate the electron motion between collisions.

Lately, a number of improved algorithms were suggested^{13,14} which reduce the amount of the calculations. In these papers, however, only atomic gases were considered. It should be emphasized that the use of simulation methods for atomic gases is restricted to relatively

large values of E/N . In fact, in these cases, after an inelastic collision with the atom, the electron must gain in the electric field energy of 10–20 eV so that the next inelastic collision can occur. The stabilization in time of the electron distribution function requires a large number of inelastic collisions with atoms and therefore, the calculations (which are limited by computer time) can be performed only for relatively large values of E/N . These values are much higher than those existing in the positive column of glow discharges in atomic gases.

Recently, a number of papers were published^{15,16} in which a computer simulation method was used to calculate transport coefficients in nitrogen. These publications, however, deal with large values of E/N ($\sim 2 \times 10^{-15} - 3 \times 10^{-14}$ V cm²). For such high values, the most important processes affecting the distribution function are electronic excitation of molecules and ionization. For example, one of the characteristic phenomena for these values of E/N is a meaningful decrease in the average energy of the electrons caused by the appearance in the discharge of a large number of slow secondary electrons due to increased ionization.¹⁷

In the present work a computer simulation method is developed which makes it possible to calculate various transport coefficients in nitrogen for E/N values smaller than 10^{-15} V cm², values that characterize the conditions in the positive column of the glow discharge in nitrogen. The electron motion is simulated by taking into account the real parabolic trajectory of the electrons between successive collisions with molecules. The possibility of successful simulation for such low values of E/N is due to the fact that the stabilization of the distribution function in nitrogen in these cases stems from collisions which excite the vibrational levels of the molecule. Therefore, the electron must gain only about 1 eV between two successive inelastic collisions.

The simulation algorithm is as follows: We consider a free electron that starts its motion in the gas with a velocity \mathbf{v}_0 and energy ϵ_0 at time t_0 . In the time interval dt which follows t_0 , the electron can collide elastically with a molecule of the gas or excite the molecule into one of the vibrational or electronic levels. Let $\nu_{e1}(\epsilon_0)dt$ and $\nu_{r1}(\epsilon_0)dt$ denote the probabilities that these processes occur, where the index i runs through all possible inelastic collisions. The quantities

$$\nu_{\mu}(\epsilon) = N \left(\frac{2\epsilon}{m} \right)^{1/2} \sigma_{\mu}(\epsilon) \quad (\mu = e1, r1) \quad (3)$$

are the frequencies of elastic and various inelastic collisions of an electron of energy ϵ with gas molecules. The energy of the electron changes during the time interval Δt_0 that passes until the first collision with a gas molecule and the change is given by

$$\Delta\epsilon(\Delta t_0) = 2(\epsilon B)^{1/2} \Delta t_0 s + B(\Delta t_0)^2, \quad (4)$$

where $B = e^2 E^2 / 2m$ and $s = \cos\theta_0$ (where θ_0 is the angle between the initial velocity \mathbf{v}_0 and the direction of the electric field). The time interval Δt_0 is a random value associated with random numbers γ , with a uniform distribution in the interval $[0, 1]$, by the following integral equation:

$$\int_0^{\Delta t_0} \nu[\epsilon_0 + \Delta\epsilon(t)] dt = -\ln\gamma, \quad (5)$$

where $\nu(\epsilon) = \nu_{e1}(\epsilon) + \sum_i \nu_{r1}(\epsilon)$ is the total collision frequency. Equation (5) enables us (at least, in principle) to simulate the free path time interval Δt_0 with the help of pseudo-random numbers γ that are generated by the computer. To facilitate the solution of (5) for Δt_0 , let the electron energy axis be divided into small intervals by the points ϵ_j such that $\epsilon_j - \epsilon_{j-1} = 0.1$ eV and assume that the total collision frequency $\nu(\epsilon)$ is constant in each of these intervals. By use of this approximate description of the function $\nu(\epsilon)$ Eq. (5) becomes a simple algebraic equation from which Δt_0 can easily be computed.

After the time interval, Δt_0 , the electron with the energy $\epsilon'_1 = \epsilon_0 + \Delta\epsilon(\Delta t_0)$ collides with a molecule and its energy becomes $\epsilon_1 = \epsilon'_1 - \xi_i$, where ξ_i is the electron energy loss depending on the collision type. We ignore energy loss in elastic collisions, assuming that for the values of E/N which will be considered here, the electrons transfer most of the energy gained in the electric field to the excitation of vibrational and electronic levels.

The type of the collision is simulated in the following manner: The next pseudo-random number γ is generated and is checked to see into which of the following intervals:

$$\left[0, \frac{\nu_{e1}}{\nu} \right]; \left[\frac{\nu_{e1} + \nu_{r1}}{\nu}, \frac{\nu_{e1} + \nu_{r1}}{\nu} \right]; \left[\frac{\nu_{e1} + \nu_{r1}}{\nu}, \frac{\nu_{e1} + \nu_{r1} + \nu_{r2}}{\nu} \right]; \dots$$

(which together form the interval $[0, 1]$) it fits, and accordingly, it is decided that the electron collides elastically or excites the molecule into one of the vibrational or electronic levels.

Once the type of collision is identified the scattering angle is simulated. For simplicity, we assume, that the scattering is isotropic so that the value $s = \cos\theta$ (θ is the angle between the direction of the electron velocity immediately following the scattering and the direction of the electric field) is uniformly distributed in the interval $[-1, 1]$. Therefore, the simulation formula for s , which is required for the calculation of the electron energy until the next collision [see (4)], is given by

$$s = 2\gamma - 1, \quad (6)$$

where γ are again pseudo-random numbers uniformly distributed in the interval $[0, 1]$.

At this stage of the computation there are enough data to proceed to the next collision. We simulate the new free path time interval Δt_1 , for the electron with initial energy ϵ_1 , find the type of the next collision, etc. The process is continued for a large number of vibrational excitations, which, for E/N values considered here, are the collisions that determine the stabilization of the distribution function. Then, according to the ergodic theorem, it is assumed that the average parameters of the test electron also represent the electron transport coefficients in the whole discharge. Calculation of these average parameters is performed by using a new method which is particularly suitable for use with the simulation process described.

At all the states of the simulation we have to know the

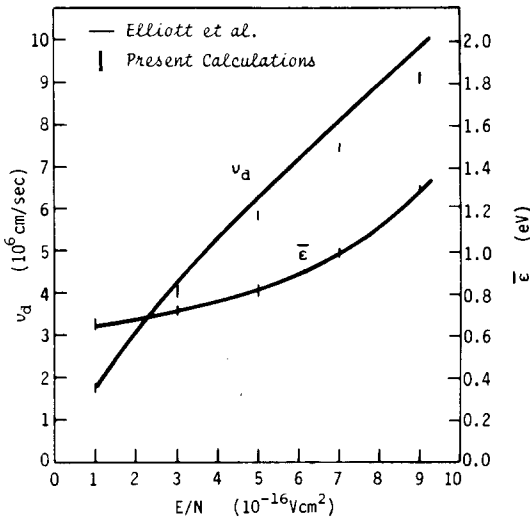


FIG. 1. The average electron energy $\bar{\epsilon}$ and electron drift velocity v_d in nitrogen vs E/N .

electron energy before each collision with a gas molecule. Thus, instead of using the regular electron distribution function $F(\epsilon)$, which is defined as the probability density of finding an electron with energy ϵ in the unit volume of the discharge in any given moment t , we will use a new distribution function $F^-(\epsilon)$ which is defined as follows: Let $F^-(\epsilon)$ be the probability density that the electron energy will be equal to ϵ just before it collides with a gas molecule.

It can now be proved that the two distribution functions are related by a simple formula. In order to do this consider the number of collisions per unit volume of the discharge between an electrons having energy in the interval $[\epsilon, \epsilon + d\epsilon]$, and gas molecules during a long time interval t , and denote this value as $M(\epsilon, t)$. $M(\epsilon, t)$ can be expressed in terms of $F(\epsilon)$ as

$$M(\epsilon, t) = N_e F(\epsilon) d\epsilon \nu(\epsilon) t, \quad (7)$$

where N_e is electron density and $\nu(\epsilon)$ is the total collision frequency. $M(\epsilon, t)$ can also be expressed in terms of $F^-(\epsilon)$. Let $\bar{\nu}$ be the average collision frequency between an electron in the discharge and gas molecules

$$\bar{\nu} = \int_0^\infty \nu(\epsilon) F(\epsilon) d\epsilon. \quad (8)$$

Therefore, since $F^-(\epsilon) d\epsilon$ is the probability that the electrons collide with a gas molecule when the electron energy is in the interval $[\epsilon, \epsilon + d\epsilon]$, we get

$$F^-(\epsilon) d\epsilon = M(\epsilon, t) / N_e \bar{\nu} t. \quad (9)$$

By comparing this expression with (7) the relation between $F^-(\epsilon)$ and $F(\epsilon)$ is obtained

$$F(\epsilon) = F^-(\epsilon) [\bar{\nu} / \nu(\epsilon)]. \quad (10)$$

This relation makes it possible to calculate various average electronic parameters using the simulation method proposed and for this it is enough to know the values of these parameters only just before each collision between an electron and a gas molecule. For example, if n is the total number of collisions and $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are the electron energies before each of the successive colli-

sions, then the average electron energy in the discharge is equal to

$$\bar{\epsilon} = \frac{1}{n} \sum_{i=1}^n \epsilon_i \frac{\bar{\nu}}{\nu(\epsilon_i)}. \quad (11)$$

The average collision frequency $\bar{\nu}$ in Eq. (11) is calculated after the completion of the simulation process and is equal to $\bar{\nu} = n/t$ (where t is the time interval in which the electron collides n times with the gas molecules).

Similar, to Eq. (11) the average value of any quantity $\alpha(\epsilon)$ which depends on electron energy can be calculated by using following formula

$$\bar{\alpha} = \frac{1}{t} \sum_{i=1}^n \frac{\alpha(\epsilon_i)}{\nu(\epsilon_i)}. \quad (12)$$

This method of finding average electron parameters in the discharge, in contrast with accepted methods, only requires knowledge of the electron energy just before each collision with a gas molecule, a value which has to be calculated, in any case, as a part of the simulation process. Furthermore, the proposed method provides for a smaller statistical error compared with existing simulation methods because of the large number of collisions (that also includes the elastic collisions) which are used to determine the average values using Eq. (12).

III. APPLICATION OF THE METHOD FOR NITROGEN

In this section we use the simulation method in the case of nitrogen for values of E/N in the range of 10^{-16} – 10^{-15} V cm². We will rely on the various cross sections for nitrogen given by Englehardt and Phelps.² In Fig. 1 the drift velocity v_d and the average electron energy $\bar{\epsilon}$, obtained using the simulation method, are compared with the results of Elliott *et al.*¹⁸ who use the two-term expansion for their calculations with the same set of cross sections. In Fig. 2 we also compare our results for average excitation frequencies of the first six vibrational levels of nitrogen with the results of Ref. 18. The simulation involved 10^5 collisions between the test electron and gas molecules. In order to determine the statistical error in the calculation of the average parameters, five values of these parameters were considered each after 2×10^4 collisions. All the calculations were performed on a CDC CYBER 70 computer and characteristic computer time for a given E/N was 30–50 sec. It should be pointed out that in the calculation of v_d and $\bar{\epsilon}$ the statistical error was less than 15% even when the total number of collisions was $n = 10^4$ and in this case the computing time was only about 5 sec.

The results described in Figs. 1 and 2 are in excellent agreement (but for a small deviation in values of v_d) with the results of calculations based on the two-term spherical harmonics expansion. This fact dispels the doubts described in the introduction as to the validity of the use of the two-term expansion in order to calculate the electron transport coefficients in nitrogen.

The agreement of our results with the results where the two-term expansion was used allows us to assume that the same electron energy distribution function is obtained by the two methods. We now use the simulation

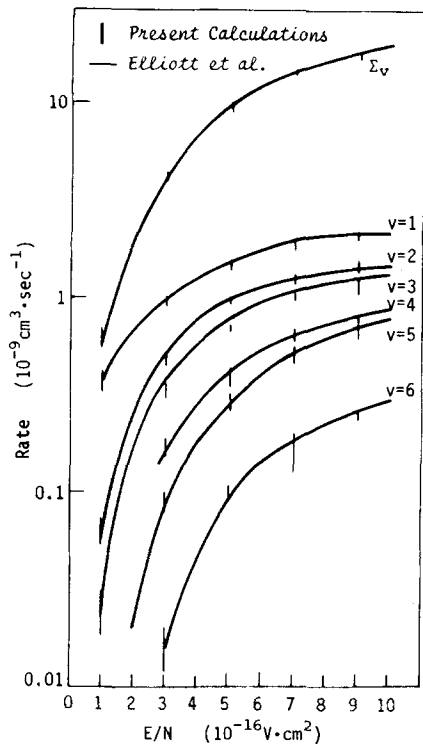


FIG. 2. The average vibrational excitation frequencies in nitrogen vs E/N .

method to test this assumption. The simulation procedure makes it possible to determine the electron energy distribution function $F^-(\epsilon)$. The dotted line in Fig. 3 describes the histogram of this distribution for $E/N = 5 \times 10^{-16} \text{ V cm}^2$. In the same figure we also show (the full line) the regular energy distribution function of the electrons $F(\epsilon)$ which is obtained from $F^-(\epsilon)$ by the relation (10). The criss-crossed areas in the figure describe the statistical error in determining $F^-(\epsilon)$ and $F(\epsilon)$. In order to increase the precision in calculating the distribution functions, the simulation proceeds until the test electron undergoes 5×10^5 collisions with gas molecules. In Fig. 4 the histograms of the symmetrical part, $f_0(\epsilon) = F(\epsilon)/\sqrt{\epsilon}$, of the expansion (1) for a number of values of E/N are shown. These distribution functions are in ex-

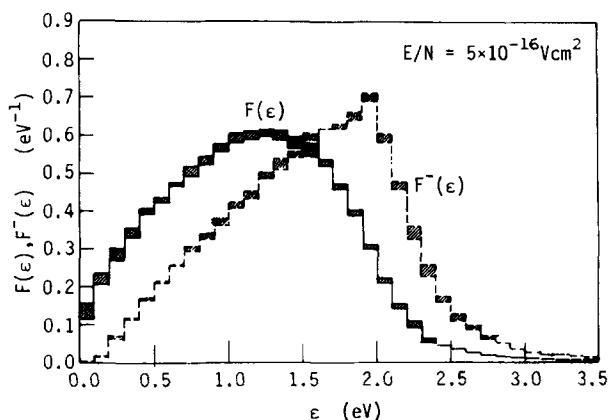


FIG. 3. The histograms of the electron energy distribution functions $F^-(\epsilon)$ and $F(\epsilon)$ in nitrogen at $E/N = 5 \times 10^{-16} \text{ V cm}^2$.

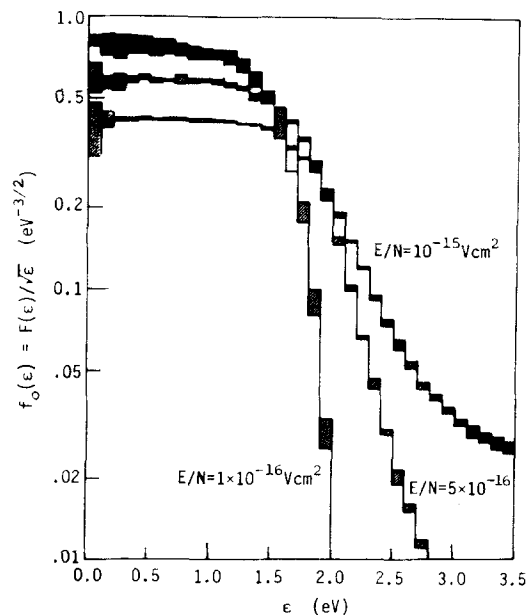


FIG. 4. The histograms of the symmetric part of the electron velocity distribution function in nitrogen.

cellent agreement with the results of Nighan⁵ based on the two-term expansion.

The proposed simulation method is suitable not only for the calculation of the electron energy distribution function, but can also be used to establish the angular dependence of the electron velocity distribution $f(\mathbf{v})$. For this, it should be pointed out that if $f^-(\mathbf{v})$ is defined as the electron velocity distribution function just before a collision with a gas molecule, then similar to (10) we have

$$f(\mathbf{v}) = f^-(\mathbf{v})[\bar{v}/v(\epsilon)] \quad (13)$$

Thus, in order to calculate $f(\mathbf{v})$ we can use the function $f^-(\mathbf{v})$ that is computed during the simulation process in a manner similar to $F^-(\epsilon)$.

The first asymmetric term f_1 in the expansion (1) can be calculated with the help of the velocity distribution function of electrons whose velocity vector is directed at angles $0 \leq \theta \leq \pi/2$ to the direction of the field. In fact, if we denote this distribution function by $\Phi(v, 0 \leq \theta \leq \pi/2)$, then the multiplication of (1) by the normalization factor $v^{2\frac{1}{2}} \sin \theta$ and integration between 0 and $\pi/2$ yields

$$\Phi(v, 0 \leq \theta \leq \pi/2) = \frac{1}{2} f_0(v) v^2 + \frac{1}{4} f_1(v) v^2 \quad (14)$$

The terms that include f_2, f_3, \dots become zero in this expression as a result of the integration. Equation (14) enables us to find $f_1(v)$ when the functions $f_0(v)$ and $\Phi(v, 0 \leq \theta \leq \pi/2)$ are determined using the simulation method. The ratio $k = f_1/f_0$ thus obtained, which describes the measure of directional anisotropy of the distribution function, is shown in Fig. 5 as a function of electron energy for a number of values of E/N . According to the dependence of the ratio k on E/N , the whole range of the electron energy can be divided into two parts. For $0 < \epsilon \leq 1.9 \text{ eV}$, the anisotropy factor k is strongly dependent on E/N and decreases as E/N increases. For $\epsilon \gtrsim 1.9 \text{ eV}$, the factor k does not depend on E/N , at least within the calculation errors. It is

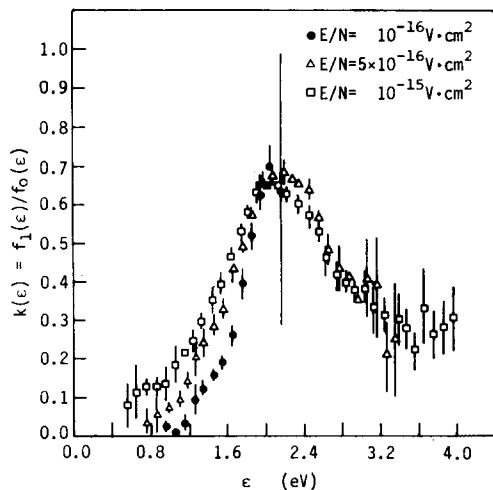


FIG. 5. The anisotropy factor $k = f_1/f_0$ in nitrogen.

noteworthy that this energy region is the range in which the cross section for inelastic collisions in nitrogen is particularly large relative to the total collision cross section.

IV. CONCLUSIONS

(i) A new computer simulation method is presented. It enables calculation of various average electronic parameters in electrical discharges in gases. The method is based on a small number of assumptions and competes with the fastest methods for the solution of the Boltzmann equation which usually use the two-term expansion.

(ii) The method was used for nitrogen. A strong anisotropy of the electron velocity distribution function in nitrogen for $E/N = 10^{-16} - 10^{-15}$ V cm² was found. The anisotropy factor $k = f_1/f_0$, which describes the ratio between the asymmetric and symmetric parts of the distribution, approaches, in the case of nitrogen, its maximum value of approximately 0.7 at an electron energy of 2 eV.

(iii) one of the interesting features of the anisotropy factor k is that in the electron energy range for which

the cross section of vibrational excitation in nitrogen is characterized by large values, k does not depend on E/N .

(iv) In spite of the strong anisotropy of the distribution function in nitrogen for $E/N = 10^{-16} - 10^{-15}$ V cm², the solution of the Boltzmann equation based on the two-term spherical harmonics expansion gives correct values for various electron transport coefficients. Furthermore, the distribution functions obtained by using the two-term expansion are in excellent agreement with the results of the simulation.

ACKNOWLEDGMENTS

The author would like to thank Professor P. Avivi and Professor F. Dothan for their helpful comments and suggestions in the preparation of this paper.

- ¹I. P. Shkarofsky, T. W. Johnston, and M. P. Bachynski, *The Particle Kinetics of Plasmas* (Addison-Wesley, Reading, Mass., 1966), p. 71.
- ²A. G. Engelhardt, A. V. Phelps, and C. G. Risk, *Phys. Rev.* **135**, A1566 (1964).
- ³R. D. Hake and A. V. Phelps, *Phys. Rev.* **158**, 70 (1967).
- ⁴A. V. Phelps, *Rev. Mod. Phys.* **40**, 399 (1968).
- ⁵W. L. Nighan, *Phys. Rev. A* **2**, 1989 (1970).
- ⁶W. L. Nighan, *Appl. Phys. Lett.* **20**, 96 (1972).
- ⁷W. L. Nighan and W. J. Wiegand, *Phys. Rev. A* **10**, 922 (1974).
- ⁸W. F. Bailey, presented at the 25th Gaseous Electronics Conference, London, Ontario (1972).
- ⁹A. V. Phelps (private communication).
- ¹⁰T. Itoh and T. Musha, *J. Phys. Soc. Jpn.* **15**, 1675 (1960).
- ¹¹R. W. L. Thomas and W. R. L. Thomas, *J. Phys. B* **2**, 562 (1969).
- ¹²Y. Sakai, U. Tagashira, and S. Sakamoto, *J. Phys. B* **5**, 1010 (1972).
- ¹³J. Lucas, *Int. J. Electron.* **32**, 393 (1972).
- ¹⁴J. Lucas and H. T. Saclee, *J. Phys. D* **8**, 640 (1975).
- ¹⁵L. E. Kline and J. G. Siambis, *Phys. Rev. A* **2**, 794 (1972).
- ¹⁶L. E. Kline and J. J. Lowke, in *Proceedings of the Twelfth International Conference on Phenomena in Ionized Gases* (University of Technology, Eindhoven, 1975), p. 9.
- ¹⁷L. Friedland, *J. Phys. D* **7**, 2246 (1974).
- ¹⁸C. J. Elliott, O. P. Judd, A. M. Lockett, and S. D. Rockwood, Los Alamos Scientific Laboratory, Report LA-5562-M5 (1974).