Random Walk Theory of Elastic and Inelastic Time Dependent Collisional Processes in an Electric Field *

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Random walk theory is applied to the motion of electrons in the early stage of breakdown of helium in an electric field. Details of inelastic and elastic interactions are based on integral and differential cross section data. The concept of mean free time is extended to include the effect of acceleration between collisions due to the electric field.

The relaxation of electron energy distributions from initial delta functions to steady terminal distriubtions is studied. Relaxation time determined by the random walk is shown to be closely approximated by a simple energy exchange relation between electrons and the electric field.

Drift velocity and the first Townsend ionization coefficient are determined and compared with experimental results. Various simplifying assumptions which have been used in analytical studies are appraised by use of the random walk procedure.

Introduction

The time dependent motion of electrons in a relatively steady electric field is often of interest; for example, in the early stages of the breakdown of a gas between two parallel electrodes [1]. The time for an initial distribution to relax to a steady state distribution is important in determining the method of calculation as well as for the physical description it affords. The final steady state is independent of the initial distribution and has been the concern of numerous analytical investigations [2–7].

There are no adequate experimental techniques for directly measuring electron energy distribution [8]. There are, however, appreciable amounts of experimental differential and total cross section data available, especially for the rare gases. By use of a random walk (RW) procedure this data can, in principle, be used to determine electron energy distribution without the limiting restrictions imposed by analytical approaches to the problem. By such a procedure the trajectories of a representative sample of electrons are followed in detail as they undergo various types of collisions and as they are acted upon by the electric field in the time between collisions. The details of each collision are based on random selection of values from sets of numbers distributed in accordance with the cross section data.

A random walk method which incorporates a large amount of physical detail may however require large amounts of computer time. Studies of stochastic collisional processes, especially for weak interactions between particles, can well exceed allowable time limits. In the case of interest this depends on the number of collisions required for the electrons to relax to the terminal distribution.

In the gaseous discharge problem, the collisions between the electron and neutrals are predominantly the elastic type, except for very high energy electrons. Usually, therefore, only a small amount of energy, $\Delta\varepsilon$, of the order of $2\,\varepsilon\,m/M$ is exchanged during collisions. (The mass of the electron is denoted by m and that of the atom by M.) The time and number of collisions required for relaxation is estimated to be very large when the criterion is based on this energy exchange. Substituting $\Delta\varepsilon$ for elastic collisions into the energy exchange time expression of CHANDRASEKHAR [9, 10]

$$t_\varepsilon = \varepsilon^2/[\nu(\overline{\Delta\varepsilon})^2] \qquad (1)$$

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[1] H. E. WILHELM and B. ZAUDERER, Electricity from MHD, Vol. II, IAEC, Vienna (Austria) 1968.
[2] M. J. DRUYVESTEYN, Physica **X**, 69 [1930].
[3] J. A. SMIT, Physica **3**, 543 [1936].
[4] H. W. ALLEN, Phys. Rev. **52**, 707 [1937].
[5] F. H. REDER and S. C. BROWN, Phys. Rev. **95**, 885 [1954].
[6] A. E. D. HEYLEN and T. J. LEWIS, Proc. Roy. Soc. London **271**, 531 [1963].
[7] H. DREICER, Phys. Rev. **117**, 343 [1960].
[8] L. B. LOEB, Basic Prcesses of Gaseous Electronics, University of California Press, Berkeley, and Los Angeles 1961.
[9] S. CHANDRASEKHAR, Astrophys. J. **97**, 255 [1943].
[10] L. SPITZER, Physics of Fully Ionized Gases, Intersci. Publishers, New York 1946.

gives a number of collisions, νt_ε, of the order of 10^6 to 10^8 for light gases. (A bar over $\Delta\varepsilon$ is used to denote average per collision and ν is collision frequency.) With 10^3 to 10^4 test particles to comprise a minimum suitable statistical sample, the number of collisions for relaxation can be well beyond that permittting a reasonable computer time effort.

In the presence of an electric field, however, there there is an exchange of energy between electrons and the electric field, E, over the distance, l, traveled between collisions. It can be approximated by

$$\Delta\varepsilon \approx e\,E\,l\cos\theta \tag{2}$$

where θ is the angle between the electron velocity and the negative field direction. The rms average of $\cos\theta$ is equal to $1/\sqrt{3}$ for an isotropic distribution. The average number of collisions to exchange an amount of energy ε can then be expressed as

$$N_\varepsilon \equiv \nu t_\varepsilon = 3(\varepsilon\, n\, Q_a/e\,E)^2 \tag{3}$$

with l set equal to the reciprocal of the product of number density of background particles, n, times the total absorption cross section, Q_a. For helium, this expression gives a number of collisions of the order of 10^5 to 10 for an ε of 10 eV, for example, and E/p ranging from 1 to 100 eV/cm-Torr.

Since collisions with the background neutrals usually cause large angle deflections of the electron, the electric field force on the electron is frequently reversed in sign from one of acceleration to deceleration and vice versa. Thus, even though $\Delta\varepsilon$ is large in magnitude, the net field energy given the electron at steady state conditions merely balances the energy lost in collisions with the neutrals. The relaxation time of Eq. (3) is much shorter than that based on electron neutral interaction and hints that the gaseous discharge problem is well within solution by means of a straight forward random walk procedure. It is interesting to note that the manual effort of YARNOLD [11] required about 70 collisions for relaxation for $m/M = 100$. This is a much lower number than estimated for relaxation by elastic scattering.

The theory of electron interaction with an electric field and with neutral atoms is developed in the next sections for use in the RW. The usual concept of free time between collisions is revised for use in the RW at high E/p. The RW theory is then applied to the gaseous discharge problem with helium atoms comprising the background gas. In the early stages of breakdown considered herein, the interactions of electrons with the small amount of helium ions or excited neutrals are negligible [12].

Equilibrium energy distributions are determined and compared with previous analytical results. The consequences of assuming an isotropic distribution of scattering angle, of assuming a constant collision frequency, as well as the use of various inelastic energy loss assumptions are studied. Drift velocity, and Townsend ionization coefficients are obtained and compared with experimental measurements.

Dynamics of Electrons in Electric Fields

Spacial homogeneity of the electric field and of the particle distributions is assumed. As in the classical approach, the time during an encounter of an electron with a neutral is assumed negligible. Thus, the effect of the electric field on the electron motion is accounted for only during the free time between collisions.

The conservation of momentum of an electron is

$$m(\mathrm{d}\boldsymbol{v}/\mathrm{d}t) = -e\,\boldsymbol{E}\,,$$

where $e = 1.602 \times 10^{-19}$ Coulomb. The vectors are broken into components anti-parallel and perpendicular to $\boldsymbol{E}$ as

$$\boldsymbol{v} = (v_{\|}, v_\perp)$$

and

$$\boldsymbol{E} = (-E, 0)\,.$$

Integration then yields

$$v_\perp = v_i \sin\theta_i\,, \tag{4}$$

$$v_{\|} = v_i\cos\theta_i + \frac{e}{m}\,E\,t \tag{5}$$

where t is the free time between collisions and subscript i denotes conditions immediately after the preceding collision ($t = 0$).

The change in kinetic energy in time t is

$$\begin{aligned}\Delta\varepsilon &= \tfrac{1}{2}\,m(\boldsymbol{v}\cdot\boldsymbol{v} - \boldsymbol{v}_i\cdot\boldsymbol{v}_i)\\ &= \tfrac{1}{2}\,m(v_{\|}^2 - v_{\|,i}^2)\,.\end{aligned} \tag{6}$$

Using Eq. (5) this reduces to

$$\Delta\varepsilon = e\,E\,v_i\,t\cos\theta_i + \frac{1}{2\,m}\,(e\,E\,t)^2. \tag{7}$$

[11] G. D. YARNOLD, Phil. Mag. **36**, 185 [1945].

[12] R. J. SOVIE and J. V. DUGAN, NASA TN D-3121 [1965].

Thus the energy exchange with the electric field can be determined in terms of the initial magnitude and direction of the velocity vector at the start of the trajectory, the electric field strength, and the free time t.

The direction, θ, of the electron velocity vector can now be obtained by use of Eq. (6) in

$$\cos^2\theta = \tfrac{1}{2}\, m\, v_{\parallel}^2 / \tfrac{1}{2}\, m\, v^2$$

$$\text{as} \quad \cos\theta = \pm\sqrt{(\cos^2\theta_i + \Delta\varepsilon/\varepsilon_i)/(1+\Delta\varepsilon/\varepsilon_i)}\,. \tag{8}$$

When $\theta_i \leqq \pi/2$ the positive sign always applies. In cases where $\theta_i > \pi/2$ and free time reaches a value equal to $-m\, v_{\parallel,i}/e\, E$, the parallel component of electron momentum is reduced to zero, and $\cos\theta$ changes from a negative to a positive value.

Effect of Electric Field on Free Time Between Collisions

For each step of a RW a free time, t, is required for use in Eqs. (7) and (8) in order to determine energy and direction of the test electrons. In the computer simulation of electron behavior this free time is selected at random from a distribution of free times. Expressions for the distributions must be general enough to apply to particles having appreciable velocity changes during the time t due to the electric field force. A derivation of such a distribution of free time, as well as mean free time is given in the Appendix. The resulting distribution is

$$f(t) = n\, Q_a\, v \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big], \tag{9}$$

and the mean free time is

$$\tau = \int_0^\infty \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\, \mathrm{d}t\,. \tag{10}$$

For some species of neutrals, the total electron-neutral absorption cross section times the electron velocity is close to a constant [13]. That is

$$v\, Q_a = \text{constant}\,,$$

and then

$$v_i\, Q_{a,i} = v\, Q_a = \nu/n$$

where ν is the collision frequency. Eqs. (9) and (10) then reduce to the familiar expressions [14]

$$f(t) = n\, Q_{a,i}\, v_i \exp[-n\, Q_{a,i}\, v_i\, t],$$

$$\text{and} \qquad \tau = (n\, Q_{a,i}\, v_i)^{-1}\,. \tag{11}$$

For no electric field v is a constant between collisions and the last two equations apply again. For these two cases a distribution function can be written as

$$F_t(t/\tau) = \exp(-t/\tau)\,. \tag{12}$$

The total absorption cross section times the electron velocity, $Q_a\, v$, for electron-helium interaction is shown in Fig. 1 as a function of electron energy, ε. The

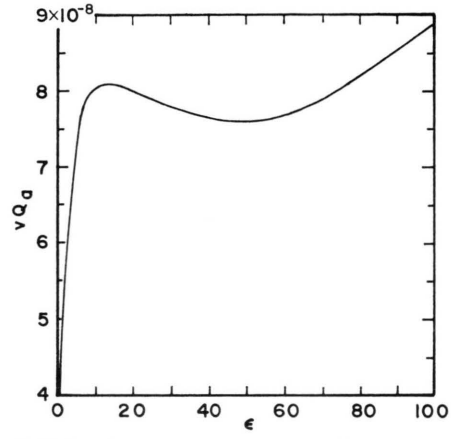

Fig. 1. Collision frequency parameter, $v\, Q_a$, versus electron energy, ε, in eV; v is electron velocity in cm/sec, and Q_a is total absorption cross section of helium in cm^2.

cross section Q_a was obtained from the experimental results of RAMSAUER and KOLLATH [15] over the range of ε available (from 2 to 20 eV). For higher energies a curve parallel to the data of NORMAND [16] was used but raised 25 percent to bring it up to the level of the data of Ramsauer and Kollath. The parameter $v\, Q_a$ varied less than 5 percent from a value of 7.8×10^{-8} cm^3 per second over a distance of $5 \leqq \varepsilon \leqq 80$ eV. Thus, collision frequency, ν, is constant within 5 percent in this energy range.

The variation of $v\, Q_a$ with ε in Eqs. (9) and (10) can be accounted for by a numerical procedure.

Let: $\qquad \gamma \equiv n\, Q_{a,i}\, v_i\, \tau\,,$

$$T \equiv n\, Q_{a,i}\, v_i\, t\,,$$

[13] G. H. WANNIER, Statistical Physics, John Wiley & Sons, New York 1966.

[14] A. F. BROWN, Statistical Physics, Elsevier Publ. Co., New York 1968.

[15] C. RAMSAUER and R. KOLLATH, Ann. Physik **12**, 529 [1932].

[16] C. E. NORMAND, Phys. Rev. **35**, 1217 [1930].

and $$V = v/v_i .$$

Eqs. (9) and (10) can then be written as

$$F_t\left(\frac{t}{\tau}\right) = \left(\frac{V\gamma Q_a}{Q_{a,i}}\right) \exp\left[-\int_0^{t/\tau} \left(\frac{V\gamma Q_a}{Q_{a,i}}\right) \mathrm{d}\left(\frac{t'}{\tau}\right)\right] \quad (13)$$

and $$\gamma = \int_0^{\infty} \exp\left[-\int_0^{T} \left(\frac{V Q_a}{Q_{a,i}}\right) \mathrm{d}T'\right] \mathrm{d}T . \quad (14)$$

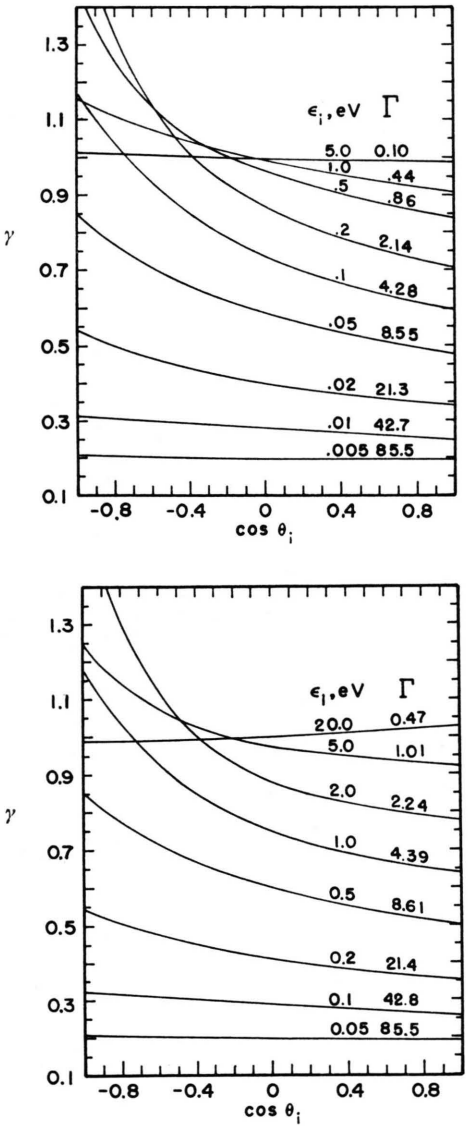

Fig. 2. Effect of electron initial energy, ε_i, and angle θ_i on free time between collisions, τ. γ is the ratio of τ to the mean free time for no electric field, $(n\,Q_{a,i}\,v_i)^{-1}$. Γ is an energy ratio parameter equal to $e\,E/(n\,Q_{a,i}\,\varepsilon_i)$.
a) E/p=10 eV/cm-Torr; b) E/p=100 eV/cm-Torr.

Velocity ratio, V, can be determined as a function of ε_i, $\cos\theta_i$, E/n, $Q_{a,i}$, and T by use of Eqs. (5) and (7) as

$$V = \left\{1 + \frac{e(E/n)\,T\cos\theta_i}{Q_{a,i}\,\varepsilon_i} + \left[\frac{e(E/n)\,T}{2\,Q_{a,i}\,\varepsilon_i}\right]^2\right\}^{1/2} . \quad (15)$$

Use of Eqs. (13) through (15) and an empirical fit to the total cross section curve (Q_a vs. ε) permits evaluation of the distribution of free times, and mean free time as functions of ε_i, $\cos\theta_i$, and E/n. Some results for helium are given in Figs. 2 and 3. To conform with convention, E/p is reported in place of E/n, with $n/p = 3.54\times10^{16}$ cm^{-3}-Torr^{-1} at 0 °C.

Mean free time, τ, differs little from $(n\,Q_{a,i}\,v_i)^{-1}$ at low E/p and high ε_i where the energy ratio parameter $[\Gamma \equiv e\,E/(n\,Q_{a,i}\,\varepsilon_i)]$ is less than 0.1. The variation of γ with $\cos\theta_i$ is almost linear here. Thus, τ is increased when the electron motion initially opposes the electric field, and is decreased at high values of $\cos\theta_i$ where the electron is being accelerated over its entire trajectory. As Γ is increased to values near unity, γ increases sharply as $\cos\theta_i$ approaches -1. At an E/p of 100 and an ε_i of 2 eV, for example, the electrons are decelerated so much

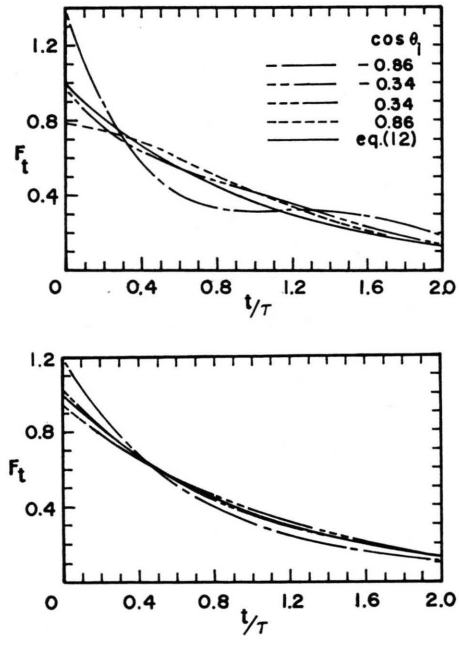

Fig. 3. Distribution, F_t, of free time, t, about mean free time for various initial electron energies, ε_i, and angles, θ_i.
a) E/p=100 eV/cm-Torr, ε_i=2 eV, Γ=2.24;
b) E/p= 30 eV/cm-Torr, ε_i=2 eV, Γ=0.67.

that τ is 50 percent greater than $(n\,Q_{a,i}\,v_i)^{-1}$. As Γ is increased much beyond 3, the entire curve of γ versus $\cos\theta_i$ drops and eventually approaches zero as Γ approaches infinity. At very high Γ, $Q_a \approx Q_{a,i}$, and γ is a function of Γ only.

The distribution, F_t, of free times, t, about the mean free time is illustrated in Fig. 3. Comparison is made with the exponential distribution of Eq. (12). Only at the higher values of Γ and lower ε_i and $\cos\theta_i$ do the distributions differ much from that of Eq. (12).

Empirical relations were fit to the results of Figs. 2 and 3 for use in the random walk. When the distributions, $F_t(t/\tau)$, were close to that of Eq. (12) a simplification in computer programming results. The usual computer library contains only a means of generating uniformly distributed random numbers, R, in the interval $0 \leqq R \leqq 1$. The relation between R_t and the free time is [17]

$$R_t = \int_0^{t/\tau} \exp(-t'/\tau)\, \mathrm{d}(t'/\tau).$$

Using the fact that $1-R$ has the same distribution as R and solving for t results in

$$t = \tau \ln(1/R_t). \tag{16}$$

Interaction of Electrons with Helium Background Atoms

To determine the type of encounter at each collision a random number R_Q was drawn from a set of numbers uniformly distributed over the interval from 0 to 1. If R_Q were less than Q_{el}/Q_a the calculations for an elastic collision were performed. If

$$Q_{el}/Q_a \leqq R_Q \leqq (Q_{el}+Q_{ex})/Q_a,$$

the calculations for an excitation were made, and if

$$(Q_{el}+Q_{ex})/Q_a \leqq R_Q$$

the calculation for an ionization was made. Here, Q_{el}, Q_{ex}, and Q_a are the integral elastic, electronic excitation, and total absorption cross sections respectively.

The integral cross section used in the analysis are shown in Fig. 4. The excitation cross section is that obtained by SOVIE [18]. It is the sum of the cross sections for excitation from the ground state, 1^1S, to the next seven energy levels in each of the ^1S, ^1P, ^1D, ^3S, ^3P, and ^3D spectral series. That is

$$Q_{ex} = \sum_{n=2}^{8} (Q_{1^1S}^{n^1S} + Q_{1^1S}^{n^1P} + Q_{1^1S}^{n^1D} + Q_{1^1S}^{n^3S} + Q_{1^1S}^{n^3P} + Q_{1^1S}^{n^3D}).$$

The ionization cross section, Q_{ion}, of Fig. 4 is from the experimental results of SMITH [19]. These data agree favorably with the data of MAIER-LEIBNITZ [20] over the limited energy range available. The cross section for elastic collisions was obtained by subtracting Q_{ex} and Q_{ion} from Q_a. Absorption cross section as previously discussed is from the experimental results of Refs. [15] and [16].

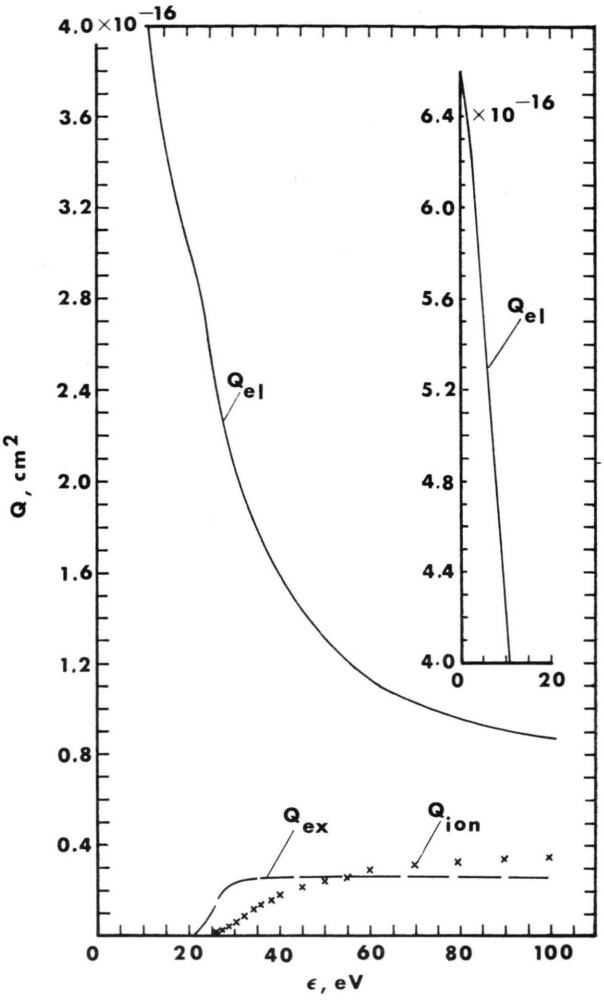

Fig. 4. Integral cross sections for electrons in helium.

[17] Y. A. SCHREIDER, Method of Statistical Testing, Elsevier Publ. Co., New York 1964.
[18] R. J. SOVIE, NASA TN D-2324 [1964].
[19] P. T. SMITH, Phys. Rev. **36**, 1293 [1930].
[20] H. MAIER-LEIBNITZ, Z. Physik **95**, 499 [1935].

Differential cross section data were used in the determination of scattering angles of the test particles at each collision. For elastic encounters the data of MOHR and NICHOLL [21], RAMSAUER and KOLLATH [15] and MASSEY and BURHOP [22] were used (Fig. 5). For excitations the data of NICHOLL and MOHR [23] and MOHR and NICHOLL [21] were used (Fig. 6). Most of the excitation data is for transitions from the ground state to the 2^1P state, which is by far the most probable transition [18]. Additional justification for this is provided by the data of MOTT and MASSEY [24], which indicate that excitations to the 2^1P, 3^1P, and 4^1P levels yield similar curves of cross sections versus scattering angle. When normalized the curves lie very close to one another. It was further assumed that the differential excitation cross sections are suitable for representing the scattering angle during transitions to ionization energy level. It was later found that the final results (energy distribution, and electron transport coefficients) were quite insensitive to distribution of scattering angle. Thus the data of Figs. 5 and 6 appear to be adequate for purposes herein.

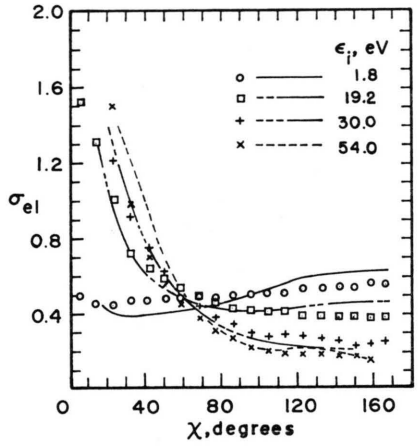

Fig. 5. Elastic differential scattering cross section, σ_{el}, for helium versus scattering angle χ. Lines are experimental data obtained from Ref. [15], [21], and [22], and normalized. Symbols are tallies of distributions of random numbers, R_χ, obtained by use of Eq. (17).

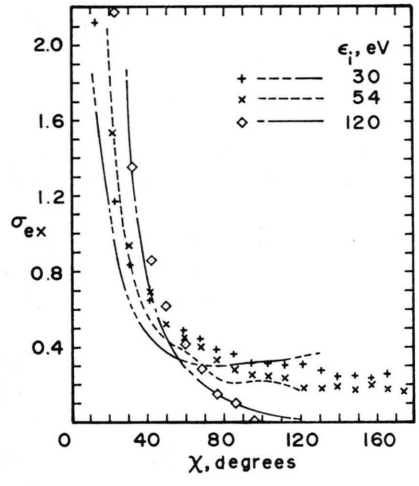

Fig. 6. Excitation differential scattering cross section, σ_{ex}, for helium versus scattering angle, χ. Lines are experimental data from Refs. [21] and [23], and normalized. Symbols are tallies of distributions of random numbers, R_χ, obtained by use of Eqs. (17) and (18).

In the computer simulation of the scattering process a random number R_χ was drawn at each collision. The relation between R_χ and differential scattering angle, χ, is

$$R_\chi = \int_0^\chi \sigma(\chi') \sin\chi' \, d\chi' / \int_0^\pi \sigma(\chi') \sin\chi' \, d\chi'.$$

Empirical curves were fit to the cross section data of Figs. 5 and 6, the above integration performed, and χ determined as a function of R_χ by the Newton-Raphson root finding method. The final relations were kept as simple as possible for computing expediency. The relations used for elastic encounters are

$$\begin{aligned} &\chi = \arccos(1 - 2R_\chi^y) \\ \text{where} \quad &y = 1 + (\varepsilon/30)^a \\ \text{and} \quad &a = 1.7\,. \end{aligned} \tag{17}$$

For inelastic encounters and $\varepsilon \leqq 60$ eV, Eq. (17) remained suitable with $a = 1$; however for $\varepsilon > 60$ eV the formula

$$\chi = 120[\arcsin(R_\chi^{1.55})]/\varepsilon \tag{18}$$

was used. A comparison of these results with the experimental data is shown on Figs. 5 and 6.

The relation between scattering angle and angles θ and θ_i is

$$\cos\theta_i = \cos\theta\cos\chi + \sin\theta\sin\chi\sin\alpha\,, \tag{19}$$

[21] C. B. O. MOHR and F. H. NICHOLL, Proc. Roy. Soc. London **138**, 229 [1932].
[22] H. S. W. MASSEY and E. H. S. BURHOP, Electronic and Ionic Impact Phenomena, At the Clarendon Press, Oxford 1969.
[23] F. H. NICHOLL and C. B. O. MOHR, Proc. Roy. Soc. London **142**, 320 [1933].
[24] N. F. MOTT and H. S. W. MASSEY, The Theory of Atomic Collisions, At the Clarendon Press, Oxford 1965.

simply from spherical trigonometry. Here θ and θ_i are the angles between the electron velocity and the negative direction of the electric field before and after the collision respectively. The azimuthal angle, α, between the orbital plane of the collision and the plane determined by the vectors $\boldsymbol{v}$ and $\boldsymbol{E}$ has an isotropic distribution. It can thus be set equal to a uniformly distributed random number R_α, to be selected each collision. Since R_α varies from 0 to 1, and α varies from 0 to 2π radians, the constant of proportionality is 2π and

$$\alpha = 2\pi R_\alpha . \tag{20}$$

The energy loss for an elastic collision is given by [8]

$$\Delta\varepsilon = \frac{2m}{M}\varepsilon(1-\cos\chi). \tag{21}$$

For an ionizing event, the minimum energy lost by the test particle is the ionization potential, equal to 24.46 eV for helium. It is possible however, for the test electron to lose much more or even all of its energy in such a collision. Unless otherwise stated it is assumed that, on the average, half of the kinetic energy remaining after the collision is kept by the test electron, the other half being given to the liberated electron. Thus

$$\varepsilon_i = (\varepsilon - 24.46)/2 \tag{22}$$

This assumption appears quite plausible since the test electron is unidentifiable from the liberated electron.

For an excitation event the energy loss of the test electron is calculated from

$$\Delta\varepsilon_{ex} = \sum_{n=2}^{8} (Q_{1^1S}^{n^1S}\,\Delta\varepsilon_{1^1S}^{n^1S} + Q_{1^1S}^{n^1P}\,\Delta\varepsilon_{1^1S}^{n^1P} + Q_{1^1S}^{n^1D}\,\Delta\varepsilon_{1^1S}^{n^1D} + Q_{1^1S}^{n^3S}\,\Delta\varepsilon_{1^1S}^{n^3S} + Q_{1^1S}^{n^3P}\,\Delta\varepsilon_{1^1S}^{n^3P} + Q_{1^1S}^{n^3D}\,\Delta\varepsilon_{1^1S}^{n^3D})/Q_{ex} \tag{23}$$

where $\Delta\varepsilon_{1^1S}^{n^1S}$ are the energy differences between the $n\,^1S$ state and $1\,^1S$ or ground state for example. The transition cross sections are given in Ref. [18]. The resulting energy loss, $\Delta\varepsilon_{el}$ is equal to 21.9 ± 0.1 over the test particle energy range of 25 to 100 eV.

In summary, to perform a random walk for this weakly ionized plasma, four random numbers are drawn each collision. The first, R_t, to determine the ratio of free time to mean free time, then R_Q to determine the type of encounter. Finally R_χ and R_α to determine the scattering and azimuthal angles. The change of energy and angle due to the electric field force between collisions is given by Eqs. (7) and (8), whereas the energy loss by collisions is given by Eq. (21) for elastic events, Eq. (22) for ionization, and (23) for excitations.

As an initial condition, at the start of the very first free path for each test electron, an isotropic distribution in angle θ_i was assumed. To simulate this distribution, random numbers R_θ were related to θ_i by

$$\theta_i = \arccos(1 - 2R_\theta) . \tag{24}$$

The electron energy at the start of each walk was arbitrarily set equal to a constant value close to the expected average energy at steady state. The values selected were 2, 3, 3, 10, 20, and 20 eV for values of E/p of 1, 3, 10, 30, 60, and 100, respectively. The steady state, or terminal conditions were found to be independent of the initial condition selected.

Application to a Gaseous Discharge

The trajectories of 10,000 electrons were determined for each E/p and physical model of particle behavior considered. Computer time for each case was usually less than 30 minutes. At the beginning of each set of calculations, a reference mean free time, τ_{ref}, was determined from Eq. (11).

Multiples N_1, N_2, ..., N_i, ... of τ_{ref} provide convenient criterial for selecting time intervals for recording test particle data.

The accumulative walk time of each test particle was monitored by summing its free time between collisions as the walk progressed. When this accumulative time reached a $N_i\tau_{ref}$ value, its location, its total number of collisions as well as the number of ionizing events experienced, its energy, and its angle with respect to the electric field direction were all recorded. It was found that appreciable amounts of relaxation of the energy distribution (from the initial delta function distribution) are usually experienced within $N_i = 3$, 10, 30, 100, 300, ... multiples of τ_{ref}. This data recording process was continued (for the 10,000 electrons) to higher and higher N_i until the energy distribution no longer changed with further increase of N_i. The calculations were then terminated.

Electron energy distributions were obtained by dividing the energy range of interest into 20 or more increments. The number of test electrons which were located in each increment were tallied at each N_i.

Drift velocity, v_D, was determined at each N_i from

$$v_D = \sum \Delta z / \sum t$$

where $$\Delta z = \Delta\varepsilon / e E$$

and $\Delta\varepsilon$ was determined from Eq. (7). Summation is over all distances Δz between collisions and free times, t, in the time interval between $N_i \tau_{\text{ref}}$ and $N_{i-1} \tau_{\text{ref}}$ for all the test electrons. In like manner, Townsend ionization coefficient was obtained from

$$\alpha_T = \sum \text{no. of ionizing events} / \sum \Delta z .$$

Diffusion coefficient, $D = D_{\parallel} + D_{\perp}$, was obtained by use of Eqs. (4), (5), and (7) with

$$D_{\parallel} = \sum (\Delta z)^2 / 6 \sum t = \sum (\Delta\varepsilon / e E)^2 / 6 \sum t ,$$

and
$$D_{\perp} = \sum [(\Delta x)^2 + (\Delta y)^2] / 6 \sum t$$
$$= \sum (2 \varepsilon_i t^2 \sin^2 \theta_i / m) / 6 \sum t .$$

Relaxation of Electron Energy Distribution

The relaxation of distributions of random energy from initial delta functions to steady terminal conditions are shown on Fig. 7 (a) through (e) for a wide range of E/p values. Random energy, ε_r, differs from total energy, ε, by drift energy, which varied from 0.5×10^{-3} to 5.6 eV as E/p varies from 1 to 100 eV/cm-Torr. Values of the mean total energy determined from

$$\bar{\varepsilon} = \int_0^{\infty} \varepsilon f(\varepsilon)\, d\varepsilon$$

at the terminal, or steady state, condition are given in the figure legends. Also given are the average number of collisions per walk, N_E, for relaxation predicted by use of Eq. (3) with ε set equal to $\bar{\varepsilon}$. To predict the time of relaxation, t_ε, the collision frequency was approximately by

$$\nu = \frac{v}{l} \approx n Q_a(\bar{\varepsilon}) \sqrt{2 \bar{\varepsilon}/m} .$$

Substituting this into Eq. (3) gives

$$t_\varepsilon p = 0.18 \times 10^{10} Q_a(\bar{\varepsilon})\, \bar{\varepsilon}^{3/2} / (e E/p)^2 . \qquad (25)$$

Equations (3) and (25) are appraised by comparing their estimates with RW results.

Data points are omitted on the energy distributions, and only faired lines presented, as the large number of closely spaced and overlapping points tend to obscure trends where results change little with change of curve parameter. Data scatter was normally less than 2 percent for the 10,000 test particle sample size.

At an E/p of 1 eV/cm-Torr the energy distributions determined by the RW method relaxed to a terminal distribution in the order of 2000 collisions per test electron and within a tp of 10^{-6} second-

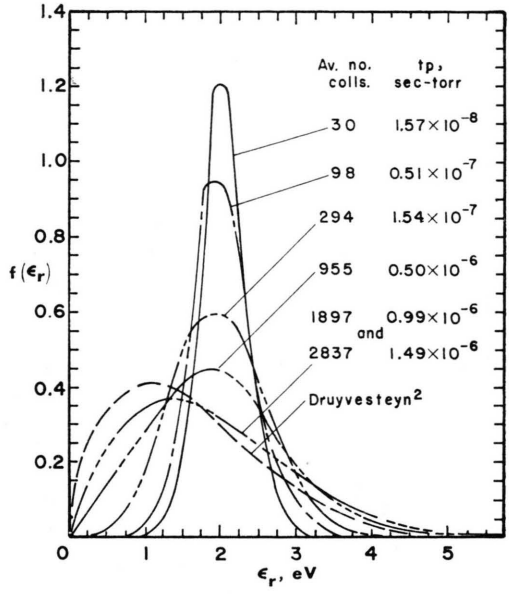

Fig. 7 a.

Torr. The N_ε and $t_\varepsilon p$ values of Eqs. (3) and (25) are higher than those indicated by the energy distributions, however, they are well within the accuracy expected for relaxation studies. The terminal distribution of Fig. 7 (a) is compared to the classical DRUYVESTEYN [2] distribution which is based on a constant cross section. A value of Q_a of 6.3×10^{-16} cm^2 was used (see Fig. 4). This comparison shows essentially the same amount of agreement as obtained in the RW studies of YARNOLD [11]. Both RW investigations give values of distribution function less than those of Druyvensteyn at low ε_r, but show a greater $f(\varepsilon_r)$ at high ε_r.

At an E/p of 3 the energy distribution was relaxed in about 1000 collisions per electron which is again slightly less than that predicted by Eq. (3). The terminal distribution compared well with the results of SMIT [3].

Considerably less than 1000 collisions per electron were sufficient to relax the energy distribution at an E/p of 10. This result is very close to that of Eq. (3). The results of Smit were only in fair agreement with those of the RW here.

As E/p is increased to 30 and 100 eV/cm-Torr the relaxation times are again consecutively reduced.

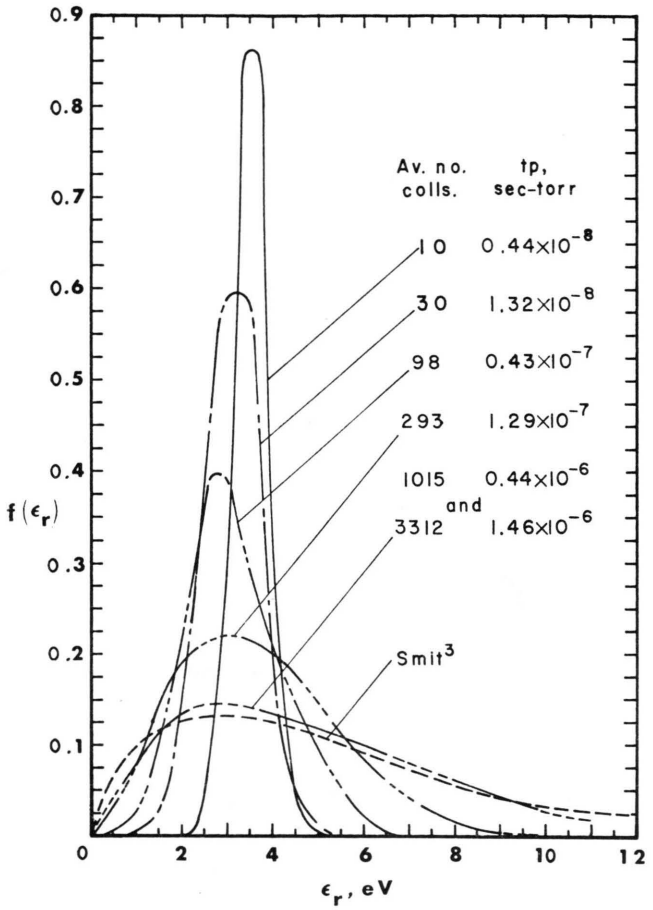

Fig. 7 b.

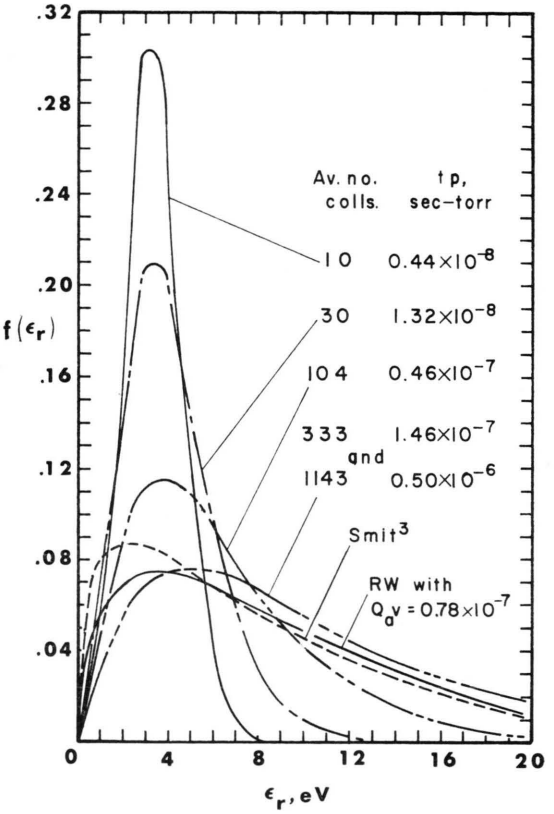

Fig. 7 c.

At an E/p value of 30 predictions of Eqs. (3) and (25) are in very good agreement with the RW results. At an E/p of 100 these equations may predict values slightly lower than obtained by the RW.

In general, the results of Fig. 7 are sufficiently close to those obtained from Eqs. (3) and (25) to show that relaxation time is governed by the process of energy exchange between the electrons and the electric field. Relaxation by electron energy exchange with the atoms would have required an estimated order of at least 10^3 more collisions per electron than that required in the RW results of Fig. 7 at even the lowest E/p values.

The calculations of Smit only cover the range of E/p from 3 to 10. In the higher E/p range some comparison of the terminal RW results can be made with the analytical results of REDER and BROWN [5] (who calculated energy distributions at E/p values of 6, 10, 20, 60, and 80 eV/cm-Torr) and HEYLEN and LEWIS [6] (who calculated distributions at E/p of 5, 20, 50, 100, and 200). In general, the results of these two analyses are in only fair agreement with the RW results.

The result of omitting the effect of electric field on mean free time between collisions in the energy distribution calculations was studied for most of the E/p values of Fig. 7. To determine this effect, mean free time, τ, was determined by Eq. (11) in place of (10). The resulting energy distributions were than compared with those of Fig. 7. At E/p values of 30 eV/cm-Torr or less the effect of electric field on τ was not discernible within an estimated 2 percent scatter in the energy distribution data. Drift velocity and diffusion coefficient were however found to be appreciably influenced even at an E/p of 10.

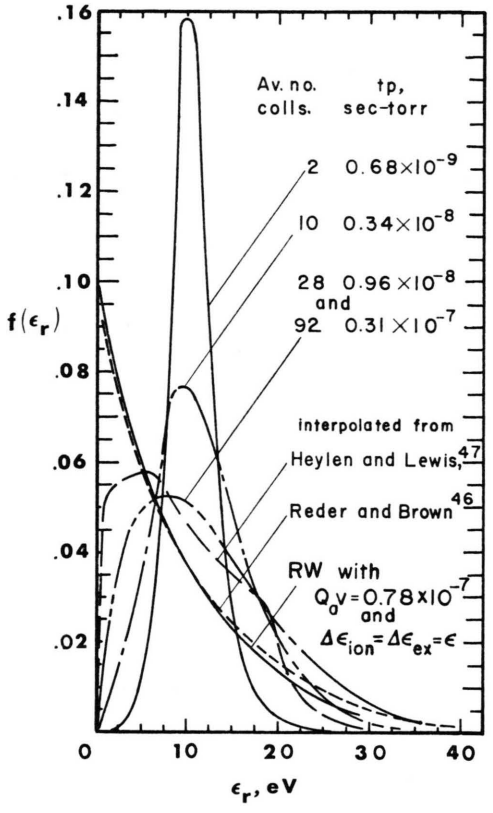

Fig. 7 d.

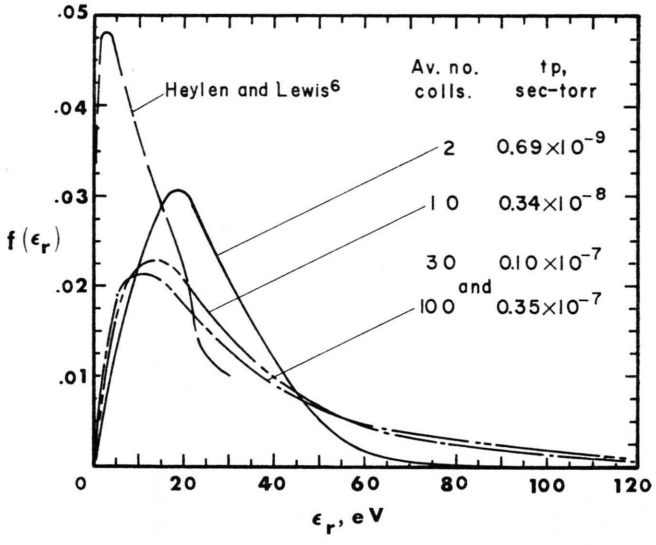

Fig. 7 e.

Fig. 7. Electron energy distribution, $f(\varepsilon_r)$, versus random energy, ε_r, at various times of relaxation from an initial delta function distribution. Time, t, is multiplied by background pressure, p, of helium referenced to 0 °C.

a) $E/p=$ 1 eV/cm-Torr, $\bar{\varepsilon}=$ 2.0 eV, $N_\varepsilon=6000$, $t_\varepsilon p=0.32\cdot10^{-5}$ sec-Torr.

b) $E/p=$ 3 eV/cm-Torr, $\bar{\varepsilon}=$ 5.0 eV, $N_\varepsilon=3300$, $t_\varepsilon p=0.13\cdot10^{-5}$ sec-Torr.

c) $E/p=$ 10 eV/cm-Torr, $\bar{\varepsilon}=$ 8.4 eV, $N_\varepsilon=$ 613, $t_\varepsilon p=0.21\cdot10^{-6}$ sec-Torr.

d) $E/p=$ 30 eV/cm-Torr, $\bar{\varepsilon}=$12.5 eV, $N_\varepsilon=$ 93, $t_\varepsilon p=0.34\cdot10^{-7}$ sec-Torr.

e) $E/p=$100 eV/cm-Torr, $\bar{\varepsilon}=$35.8 eV, $N_\varepsilon=$ 16, $t_\varepsilon p=0.73\cdot10^{-8}$ sec-Torr.

Drift Velocity, Townsend Ionization Coefficient, Mean Energy, and Diffusion Coefficient

Drift velocity and diffusion coefficient for the terminal steady state conditions of Fig. 7 are plotted on Fig. 8 versus E/p. Good agreement with the experimental drift velocities of HORNBECK [25], PHELPS, PACK, and FROST [26], and ANDERSON [27] is shown.

Diffusion coefficient is generalized independent of helium density by multiplying D by the pressure p (referenced to 0 °C). Fair agreement with the theoretical results of Heylen and Lewis is shown.

The first Townsend ionization coefficient is given on Fig. 9 plotted against E/p. The average number of ionizations per net distance the electrons travel in the z direction has been divided by p. These RW results are in good agreement with the experimental results of TOWNSEND and MACCALLUM [28].

The average random energy (equal to the total average energy, $\bar{\varepsilon}$, minus the drift energy) is also plotted on Fig. 9. As expected from Fig. 7, the results of Refs. [5] and [6] are lower than the RW values.

The drift velocities, first Townsend ionization coefficients and diffusion coefficients obtained from this microscopic random walk study provide the coefficients for the electron transport equation [29].

Appraisal of Assumptions Used in Previous Theories

The effects of a number of simplifying assumptions which have been used in various analytical studies [8] can be easily appraised by the RW procedure. A listing of the resulting coefficients and mean random energies are given in Table 1.

[25] J. A. HORNBECK, Phys. Rev. **83**, 374 [1951].
[26] A. V. PHELPS, J. L. PACK, and L. S. FROST, Phys. Rev. **117**, 470 [1960].
[27] J. M. ANDERSON, Phys. Fluids **7**, 1517 [1964].
[28] J. S. TOWNSEND and S. P. MACCALLUM, Phil. Mag. **17**, 678 [1934].
[29] H. E. WILHELM, Phys. Rev. **187**, 382 [1969].

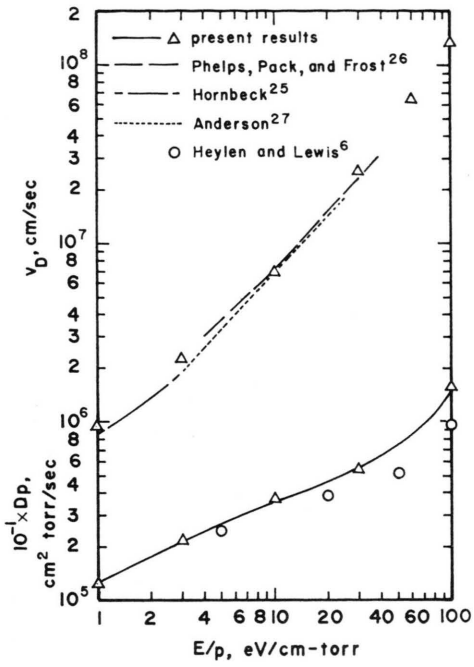

Fig. 8. Diffusion coefficient, D, times background pressure, p, and drift velocity, v_D, of electrons in helium.

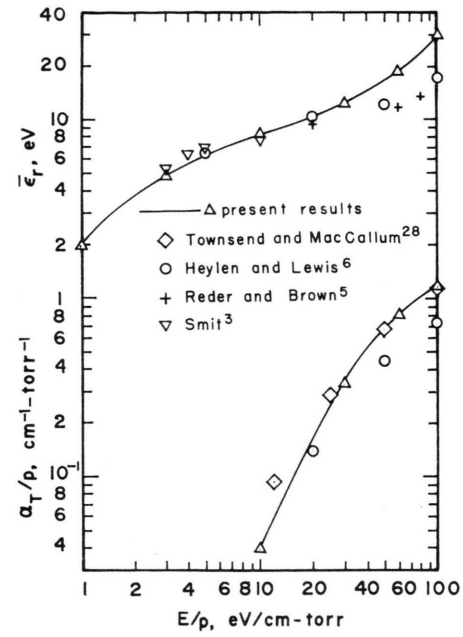

Fig. 9. First Townsend ionization coefficient, α_T, divided by helium pressure; also illustrated is average random energy of electrons, $\bar{\varepsilon}_r$.

Table 1. Appraisal of various simplifying assumptions.

	E/p eV/cm-Torr	v_D cm/sec	$D_{\parallel} p$ cm²-Torr/sec	$D_{\perp} p$ cm²-Torr/sec	$\bar{\varepsilon}_r$ eV	α_T/p cm⁻¹-Torr⁻¹
Basic calculation	10	$6.9 \cdot 10^6$	$1.3 \cdot 10^6$	$2.5 \cdot 10^6$	8.4	0.04
	30	$2.5 \cdot 10^7$	$2.0 \cdot 10^6$	$3.5 \cdot 10^6$	12.3	0.33
	100	$1.4 \cdot 10^8$	$8.5 \cdot 10^6$	$7.4 \cdot 10^6$	30.3	1.18
Constant mean free time, $Q_a v = 0.78 \cdot 10^{-7}$ cm³/sec	10	$7.4 \cdot 10^6$	$1.2 \cdot 10^6$	$2.4 \cdot 10^6$	8.4	0.04
	30	$2.6 \cdot 10^7$	$2.0 \cdot 10^6$	$3.4 \cdot 10^6$	11.8	0.34
	100	$1.6 \cdot 10^8$	$1.3 \cdot 10^7$	$8.4 \cdot 10^6$	28.4	1.04
Minimum energy loss during ionization, $\Delta\varepsilon_{ion} = 24.46$ eV	30	$2.5 \cdot 10^7$	$2.0 \cdot 10^6$	$3.6 \cdot 10^6$	12.9	0.33
	100	$4.2 \cdot 10^8$	$2.6 \cdot 10^7$	$1.4 \cdot 10^7$	70.8	1.59
Maximum energy loss during ionization, $\Delta\varepsilon_{ion} = \varepsilon$	30	$2.5 \cdot 10^7$	$2.0 \cdot 10^6$	$3.4 \cdot 10^6$	12.3	0.31
	100	$1.1 \cdot 10^8$	$6.9 \cdot 10^6$	$5.3 \cdot 10^6$	22.4	0.85
Isotropic distribution of scattering angle, χ	30	$2.0 \cdot 10^7$	$1.9 \cdot 10^6$	$3.4 \cdot 10^6$	12.1	0.31
	100	$6.2 \cdot 10^7$	$4.6 \cdot 10^6$	$6.4 \cdot 10^6$	22.4	1.36

It is often assumed[5, 13] that collision frequency is constant over the entire energy range of the electrons. This assumption can be incorporated into the RW by setting the product of absorption cross section times the magnitude of electron velocity equal to a constant. For helium, a value of $Q_a v$ equal to 0.78×10^{-7} cm³ per sec was selected from Fig. 1. At ε less than 5 eV this assumption far underestimates the free time between collisions [Eq. (11)]. This in turn permits less transfer of energy between the electric field and the electrons [Eq. (7)] causing the peak of the energy distribution to shift toward lower ε_r as shown on Fig. 7 c. Mean energy was significantly effected, however, only for E/p of 30 and greater. Except for the component of diffusion coefficient parallel to the electric field, the electron transport coefficients changed at most 15 percent over the range of E/p studied.

Another assumption of interest involves the amount of energy loss per inelastic collision. The recent results of Ref. [18] permit determination of an average energy loss, $\Delta\varepsilon_{ex}$, for excitation events in helium from cross section data. The energy loss in ionization events is less certain as it depends on the amount of energy transferred to the liberated electron. To study the magnitude of this effect, RW calculations were made with the limiting amounts of test electron energy loss, $\Delta\varepsilon_{ion}$, per ionizing event, in addition to that of Eq. (22); that is,

$$\Delta\varepsilon_{ion} = 24.46 \text{ eV} \quad \text{and} \quad \Delta\varepsilon_{ion} = \varepsilon .$$

As expected, the greater the energy loss per ionizing event, the more the energy distribution was shifted toward lower ε_r values. The properties listed in Table 1 show little dependence on $\Delta\varepsilon_{ion}$ at an E/p of 30, but become very sensitive to ionization loss as E/p is increased to 100.

An isotropic distribution of scattering angle was used in the RW procedure to study the effect of a large deviation from the distributions of Figs. 5 and 6. Results were anticipated to be quite insensitive to such a change since the uniform distribution of azimuthal angle, α, normally tends to randomize the distribution of θ_i and thus offset the effect of persistence of velocity in local scattering coordinates [Eq. (19)].

Results show, however, that the isotropic distribution of χ tends to reduce $v_{\|}$ and thus v_D and $D_{\|}$ as well (Table 1). This reduction is slight at an E/p of 30 or less, but considerable at a value of 100. At an E/p of 100 (Fig. 7 e) a large percent of the electrons are in a high energy range where the distributions of Figs. 5 and 6 deviate extremely from the isotropic assumption.

Finally, both the assumption of a constant collision frequency plus the assumption that

$$\Delta\varepsilon_{ion} = \Delta\varepsilon_{ex} = \varepsilon$$

were used in the RW procedure. Both of these assumptions are used in Ref. [5]. The RW results were now very close to the results in Ref. [5], as shown on Fig. 7 d. Considerable contrast with the basic unsimplified RW results is observed.

Conclusions

The random walk provides a means of determining detailed behavior of a gaseous discharge with a reasonabe expenditure of computer time.

The characteristic time of relaxation of the electron energy distribution depends primarily on the energy exchange between the electrons and the electric field. The background atoms serve mainly to randomize the electron motion with respect to the electric field direction. This relaxation time is closely approximated by a simple energy exchange relation.

The values of drift velocity and Townsend first ionization coefficient determined by the random walk compare well with experimental results. Various inelastic energy loss assumptions, as well as the simplifying assumptions of constant collision frequency and isotropic scattering angle were appraised. Electron energy distributions and transport coefficients were found to be especially sensitive to these assumptions at high values of E/p.

Acknowledgments

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Appendix

Distribution of Free Time between Collisions for Charged Particles in the Presence of an Electric Field

An expression for the free time, t, is derived which allows velocity changes during t and in turn permits inclusion of the influence of the electric field on charged test particles. From this distribution a mean free time is determined, which is a function of the energy and direction of the test particle at the start of the free trajectory between collisions, and of the ratio of electric field to background density, E/n.

Let $N(t)$ be the number of test particles (electrons) which have survived without a collision at time t, out of an original number $N_i = N(0)$. The fraction of free times between t and $t+dt$ is

$$f(t)\, dt = [N(t) - N(t+dt)]/N_i . \qquad \text{(A 1)}$$

Expanding $N(t+dt)$:

$$N(t+dt) = N(t) + \frac{dN}{dt}\, dt$$

and substituting the result into (A 1) gives

$$f(t)\, dt = -\frac{1}{N_i}\frac{dN}{dt}\, dt \qquad \text{(A 2)}$$

The number of collisions, dN, that an electron suffers can in a differential time element dt be expressed as $n\, Q_a\, v$ where n is the density of field particles, $Q_a(v)$

is the total collisional cross section area, and $v(t)$ is the speed of the electron. Thus

$$(\mathrm{d}N/\mathrm{d}t) = -N\, n\, Q_a\, v \qquad \text{(A 3)}$$

is the rate at which free paths are being terminated. Substituting Eq. (A 3) into (A 2) gives the distribution of free times to be

$$f(t) = \frac{N}{N_i}\, n\, Q_a\, v\,. \qquad \text{(A 4)}$$

Integrating Eq. (A 3) gives

$$\frac{N}{N_i} = \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]$$

and substituting the result into Eq. (A 4) gives

$$f(t) = n\, Q_a\, v \cdot \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\,. \qquad (9)$$

Let τ be the average time between collisions, that is

$$\tau = \frac{\int_0^\infty t\, f(t)\, \mathrm{d}t}{\int_0^\infty f(t)\, \mathrm{d}t} = \frac{\int_0^\infty t\, n\, Q_a\, v \cdot \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\, \mathrm{d}t}{\int_0^\infty n\, Q_a\, v \cdot \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\, \mathrm{d}t}\,. \qquad \text{(A 5)}$$

Consider first the denominator of Eq. (A 5). Let

$$u \equiv \int_0^t n\, Q_a\, v\, \mathrm{d}t',$$

then

$$\mathrm{d}u = n\, Q_a\, v\, \mathrm{d}t$$

and the denominator reduces to $\int e^{-u}\, \mathrm{d}u = 1$.

Next consider the numerator of Eq. (A 5). Let

$$g(t) = \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\,,$$

then

$$\mathrm{d}[g(t)] = -n\, Q_T\, v \cdot \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\, \mathrm{d}t$$

and the numerator becomes

$$-\int_0^\infty t\, \mathrm{d}[g(t)] = -[\mathrm{tg}(t)]_0^\infty + \int_0^\infty g(t)\, \mathrm{d}t = \int_0^\infty g(t)\, \mathrm{d}t\,,$$

using integration by parts and L'Hospital's rule. Finally Eq. (A 5) reduces to

$$\tau = \int_0^\infty \exp\Big[-\int_0^t n\, Q_a\, v\, \mathrm{d}t'\Big]\, \mathrm{d}t\,. \qquad (10)$$

Equation (10) can be placed in convenient dimensionless form by letting

$$\gamma \equiv n\, Q_{a,i}\, v_i\, \tau\,, \qquad T \equiv n\, Q_{a,i}\, v_i\, t\,,$$

and

$$V \equiv v/v_i\,.$$

Then

$$\gamma = \int_0^\infty \exp\Big[-\int_0^T \Big(\frac{Q_a}{Q_{a,i}}\Big)\, V\, \mathrm{d}T'\Big]\, \mathrm{d}T\,. \qquad \text{(A 6)}$$

Next let

$$U = \int_0^T \frac{Q_a}{Q_{a,i}}\, V\, \mathrm{d}T', \qquad \text{(A 7)}$$

and Eq. (A 6) becomes

$$\gamma = \int_0^\infty \exp(-U)\, \frac{Q_{a,i}}{Q_a}\, V\, \mathrm{d}U \qquad \text{(A 8)}$$

which is a form especially suited for Laguerre numerical integrations.

Equations (A 7), (A 8), and (15) permit numerical determination of γ as a function of ε_i, $\cos\theta_i$, and E/n for total cross section $Q_a(V)$.