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Computer Simulation of an Electron Swarm at low E/p in Helium

A. I. McIntosh

Department of Physics, University of New England, Armidale, N.S.W. 2351.

Abstract

A computer simulated electron swarm at $E/p_{293} = 1{\cdot}0\ \mathrm{V\,cm^{-1}\,torr^{-1}}$ in a model gas has been used to examine the validity of a recent theory of electron drift and diffusion. The computed results are in agreement with well-established theories for the electron energy distribution function, drift velocity and transverse diffusion coefficient, and confirm that, for a constant momentum transfer cross section, the longitudinal diffusion coefficient is approximately half the transverse coefficient. However, significant differences have been found between the computed swarm and the predictions of the theory of Huxley (1972). In particular, over the time scale considered, the electron swarm is not symmetric about its centroid but is spatially anisotropic in such a way that it could appropriately be described as 'pear shaped'.

1. Introduction

Monte Carlo techniques have been used to study the motion of electrons through gases subjected to an external d.c. electric field by a number of previous authors (Yarnold 1945; Itoh and Musha 1960; Bell and Kostin 1968; Skullerud 1968; Thomas and Thomas 1969; Folkard and Haydon 1970; Kline and Siambis 1971; Sakai *et al.* 1972). With the exceptions of Yarnold (1945) and Bell and Kostin (1968), these authors have considered simulations which were principally directed at studying the growth of ionization in electron avalanches and electron swarms with high mean energy. Both elastic and inelastic collisions were considered although, in each case, use was made of the justifiable simplifying assumption that, in an elastic encounter, the direction but not the energy of the electron was changed.

The early work of Yarnold (1945) was restricted by the extent of manual computation required. Bell and Kostin (1968) considered low values of E/p (where E is the electric field strength and p the gas pressure) in helium, hydrogen and nitrogen, where the fraction of the power being dissipated in elastic collisions is a significant fraction of the total. This fraction is 1·0 in helium when the mean electron energy is well below the threshold for the first inelastic collision process and is $\sim 0{\cdot}2$ for $0{\cdot}5 \leqslant E/p_{293} \leqslant 10\ \mathrm{V\,cm^{-1}\,torr^{-1}}$ in hydrogen (Crompton *et al.* 1969). Bell and Kostin included in their comprehensive study the variation with energy of the scattering cross sections, the anisotropy of the scattering angles, and the thermal velocity of the gas molecules. In the case of helium, they reported good agreement between their computed energy distribution and that predicted by the Davydov formula and satisfactory agreement between their calculated values of the electron drift velocity and the experimental data of Pack and Phelps (1961).

Despite this earlier work there remain a number of reasons for carrying out a Monte Carlo investigation of an electron swarm for the simpler case of a model gas in which only isotropic elastic scattering occurs. These reasons include:

(i) Huxley (1972) has developed a mathematical model to describe the behaviour of a group of electrons drifting and diffusing through a gas under the influence of an electric field. He obtained an expression for the electron number density as a function of position and time which differs significantly from that used in the past (see e.g. Huxley and Crompton 1962) but which can be tested only indirectly and with low sensitivity in a conventional experiment. A sensitive test of the Huxley theory can be provided by a computer simulation in which the electron number density is sampled for direct comparison with the theoretical predictions. At the same time, a broad view of the 'shape' of an electron swarm as it drifts and diffuses through the gas should allow greater insight into the fundamental processes which are occurring. Information about the shape of the electron swarm is also of interest in the light of the theory developed by Kumar and Robson (1973) who predict that a group of electrons released from the origin at zero time should develop a 'pear shape' which then decays with time as the electrons drift and diffuse in the electric field.

(ii) In recent years the effect of electron density gradients has been recognized (Parker and Lowke 1969; Lowke and Parker 1969; Skullerud 1969; Huxley 1972; Robson 1972; Kumar and Robson 1973) and the influence of this on the measured transport coefficients, such as drift velocity W and parallel and transverse diffusion coefficients D_L and D_T, has been examined in detail by Parker and Lowke. Robertson and Rees (1972) have questioned the validity of the theory of Parker and Lowke when applied to argon, in which the momentum transfer cross section changes rapidly with energy. It is thus of interest to examine the situation for a case (namely, constant elastic scattering cross section) in which the theory of Lowke and Parker may be applied analytically.

(iii) As described by Huxley (1972), the existence of anisotropic diffusion requires the energy distribution function to be spatially anisotropic, so that at any time the most energetic electrons are at the front of the swarm (have travelled further in the field direction) and the least energetic electrons are at the tail. It should be possible to test this hypothesis directly as well as indirectly through the computed values of the transverse and longitudinal diffusion coefficients.

(iv) Previous computer simulations carried out at the University of New England, Armidale, by Folkard and Haydon (1970) have been useful in the study of the non-equilibrium growth of ionization in hydrogen. These authors used a number of artifices to overcome computer restrictions and, although there is little doubt that their results are satisfactory in general terms, the use of the artifices has made it impossible to include surface processes such as the ejection of secondary electrons by positive ion, photon or metastable atom impact in their simulation. The present work is the first step in a continuing project to develop a comprehensive computer program, which is capable of including all relevant processes and whose accuracy and validity will be established at each stage of development.

2. Model and Expected Properties

The chosen model is one in which only isotropic elastic scattering occurs. The gas molecules are assumed stationary before each encounter, they are assigned a

molecular weight of four, and the cross section for elastic scattering by the gas molecules has the energy independent value of $7{\cdot}0\times10^{-16}$ cm^2.

For $E/p_{293} = 1{\cdot}0$ V cm^{-1} torr^{-1} these conditions closely approximate those obtaining in helium. The assumptions that only elastic scattering occurs and that this scattering is isotropic are justified because at low E/p in helium virtually no electrons have energies in excess of 5 eV. Between 0·002 and 6 eV the momentum transfer cross section (which is identical to the elastic scattering cross section under the assumption of isotropic scattering) lies between 5×10^{-16} and 7×10^{-16} cm^2 (Crompton *et al.* 1967) so that selecting the constant value of $7{\cdot}0\times10^{-16}$ cm^2 not only provides a situation that can be handled analytically but also one that is not too different from that applicable to the real gas. Since for $E/p_{293} = 1{\cdot}0$ V cm^{-1} torr^{-1} the mean energy of the electrons is very much greater than that of the gas molecules, the approximation that the gas molecules are stationary before a collision is a good one.

For a model gas having the above-mentioned properties, the distribution of electron energies is expected to be Druyvesteynian (Huxley and Crompton 1962), in which case, the formulae for drift velocity W and the ratio of transverse diffusion coefficient D_T to the mobility μ $(= W/E)$ reduce to (Crompton *et al.* 1967)

$$W = 4{\cdot}07\times10^6\,(E/Nq_m)^{\frac{1}{2}} \text{ cm s}^{-1} \qquad \text{and} \qquad D_T/\mu = 27{\cdot}8\,(E/Nq_m) \text{ volts},$$

where E is expressed in V cm^{-1}, N is the gas number density and the momentum transfer cross section q_m is expressed in cm^2. The mean electron energy is given by (see e.g. Massey *et al.* 1971, p. 48)

$$\bar{\varepsilon} = 0{\cdot}427\,(M/m)^{\frac{1}{2}}\,Ee\lambda,$$

where e and m are the electronic charge and mass and λ is the mean free path. Parker and Lowke (1969) predict that, for a constant cross section and $E/p_{293} \gtrsim 0{\cdot}3$ V cm^{-1} torr^{-1}, the ratio of the longitudinal to the transverse diffusion coefficient is given by

$$D_L/D_T = 0{\cdot}495.$$

Skullerud (1969) has shown that a more accurate value is $D_L/D_T = 0{\cdot}491$, which is independent of the value of E/p for the conditions used in the present simulation, namely, constant cross section and zero gas temperature. Inserting the numerical values appropriate to $E/p_{293} = 1{\cdot}0$ V cm^{-1} torr^{-1}, we find that the swarm should have a Druyvesteyn distribution of electron energies with a mean value of 1·58 eV, the drift velocity should be $8{\cdot}47\times10^5$ cm s^{-1}, while the transverse and longitudinal diffusion coefficients are expected to be $2{\cdot}55\times10^4$ cm^2 s^{-1} and $1{\cdot}26\times10^4$ cm^2 s^{-1} respectively.

3. Theory

The basic Monte Carlo method has been summarized by Cashwell and Everett (1959) and its application to gaseous electronics has been described in the references cited in Section 1. Previous authors have moved the sample electron along linear paths of one-tenth the length of the mean free path and tested for a collision at the end of each such step, thereby requiring the generation of a sequence of random numbers to determine at what point a collision occurs. However, in the present work

the assumption of an energy-independent scattering cross section allows the exact calculation of the complete trajectory while, by use of the known mean free path λ and the relation (Cashwell and Everett 1959, p. 28)

$$l = -\lambda \log(r),$$

the generation of a single random number r allows the selection of a free path l at the end of which a collision is known to occur. A considerable saving in computer time results from this simplification.

Trajectory

Consider the motion of an electron in a rectangular coordinate frame in which the electric field lies along the $-z$ axis. If an electron of initial velocity V_0 begins a free path of length l with direction cosines u, v, w then a rotation of the coordinate axes according to

$$x = x' \cos\phi, \qquad y = x' \sin\phi, \qquad \tan\phi = v/u$$

will produce the $x'z$ plane on which the trajectory lies. The equation of the trajectory is

$$z = \tfrac{1}{2}a(x')^2 + bx', \tag{1}$$

where

$$a = eE/(mV_0^2 u'), \qquad b = w/u, \qquad u' = (1-w^2)^{\frac{1}{2}}.$$

The special cases corresponding to $V_0 = 0$, $w = \pm 1$ are trivial. In general the free path will be given by

$$l = \int \mathrm{d}s = \int \{(\mathrm{d}z/\mathrm{d}x')^2 + 1\}^{\frac{1}{2}} \, \mathrm{d}x'.$$

Substituting from equation (1) and solving, we obtain

$$2al = (ax'+b)\{1+(ax'+b)^2\}^{\frac{1}{2}} + \sinh^{-1}(ax'+b) - b(1+b^2)^{\frac{1}{2}} - \sinh^{-1}(b). \tag{2}$$

Equation (2) may be solved for x' from a knowledge of a, b and l. This enables us to calculate z according to equation (1), the time t for the free path from $t = x'/(u'V_0)$ and the distances moved in the x and y directions by transforming back to the original coordinate system. At the end of the trajectory, i.e. before the collision, the velocity of the electron is given by

$$V_{BC} = \{V_0^2 + 2V_0 eEwt/m + (eEt/m)^2\}^{\frac{1}{2}} \tag{3}$$

and its direction cosines by

$$u_{BC} = uV_0/V_{BC}, \qquad v_{BC} = vV_0/V_{BC}, \qquad w_{BC} = (wV_0 + eEt/m)/V_{BC}. \tag{4}$$

Collision

After a collision with a stationary gas molecule of mass M a new set of direction cosines u_{AC}, v_{AC}, w_{AC} are chosen at random from an isotropic distribution. The angle by which the electron changes its direction is

$$\alpha = \cos^{-1}(u_{BC}u_{AC} + v_{BC}v_{AC} + w_{BC}w_{AC}). \tag{5}$$

In an elastic collision the velocity V_{AC} of m after the collision is given by

$$V_{AC}^2 = V_{BC}^2\{1-(4\mu^2/mM)\cos^2\beta\}, \tag{6}$$

where μ is the reduced mass and β is the scattering angle of M in the laboratory frame. The angle β is related to the scattering angle γ in the centre of mass frame by

$$\beta = \tfrac{1}{2}(\pi-\gamma) \tag{7}$$

and, for $m \ll M$, we have*

$$\alpha \approx \gamma. \tag{8}$$

Thus, knowing α from equation (5), we may use equations (6), (7) and (8) to calculate the velocity of the electron after the collision.

4. Simulation

A group of 150 electrons were released from the origin at time $t = 0$ into 40 torr of 'helium' subjected to a d.c. electric field of 40 V cm^{-1}. The initial distribution of angles was assumed to be isotropic. Since the energy relaxation time $\tau \approx M/(2mNqv)$ (where q is the elastic scattering cross section and v the electron velocity) is $\sim 10^{-7}$ s, corresponding to a drift distance approaching 1 mm for a 1 eV electron, meaningful information about the swarm may be obtained after a short drift distance only if the initial distribution of electron energies is as close as possible to the equilibrium distribution. Accordingly, the group of electrons was released with the expected Druyvesteyn distribution of energies. No boundaries or electrodes were imposed on the simulation.

After a suitable time interval, information about the number of collisions experienced by an electron since its release, its x, y and z coordinates, the total distance traversed and its energy at that instant were recorded. Corrections were made for the fact that the sampling time did not in general correspond to the completion of an integral number of free paths. Each electron in the ensemble was sampled at regular time intervals up to a maximum elapsed time of $1{\cdot}0\ \mu$s, which corresponded to the completion of about $6{\cdot}6\times10^4$ collisions and a drift distance in the field direction of about 9 mm.

When this information is gathered for the group of electrons, the following quantities may be calculated at each sampling time: the distribution of energies $f(\varepsilon)$, the mean energy $\bar{\varepsilon}$, the position of the centroid $(\bar{x},\bar{y},\bar{z})$, the average of the square of the longitudinal displacements from the centroid $\langle(z-\bar{z})^2\rangle$ and the average of the square of the off-axis radial distance $\langle\rho^2\rangle$.

5. Results

Program Checks

Before the present results can be considered to provide a reliable test of any analytic formula, it is essential to have confidence that the program is working correctly. In essence, only two things happen in the simulation: (i) the electron

* Strictly $\gamma = \alpha+\sin^{-1}((m/M)\sin\alpha)$. However, it may be shown that, when V_{AC}^2 is averaged over a large number of collisions, the effect of making the approximation (8) is to produce an error in V_{AC}^2 of the order of $\frac{1}{3}m/M$, which is negligible.

moves along a free path and its kinetic energy is changed by the field, and (ii) the electron loses some fraction of its energy at the collision which terminates the free path.

As outlined in Section 3, the calculation of both the distance Δz moved in the field direction between successive collisions and the velocity V_{BC} at the end of the trajectory relies on the solution of equation (2). If the positions at which successive collisions occur are recorded, we can compare the gain in energy computed by the program (as represented by the difference between V_0 and V_{BC}) with that expected by multiplying Δz by the field strength. These two calculated energy changes were identical to 8 significant figures.

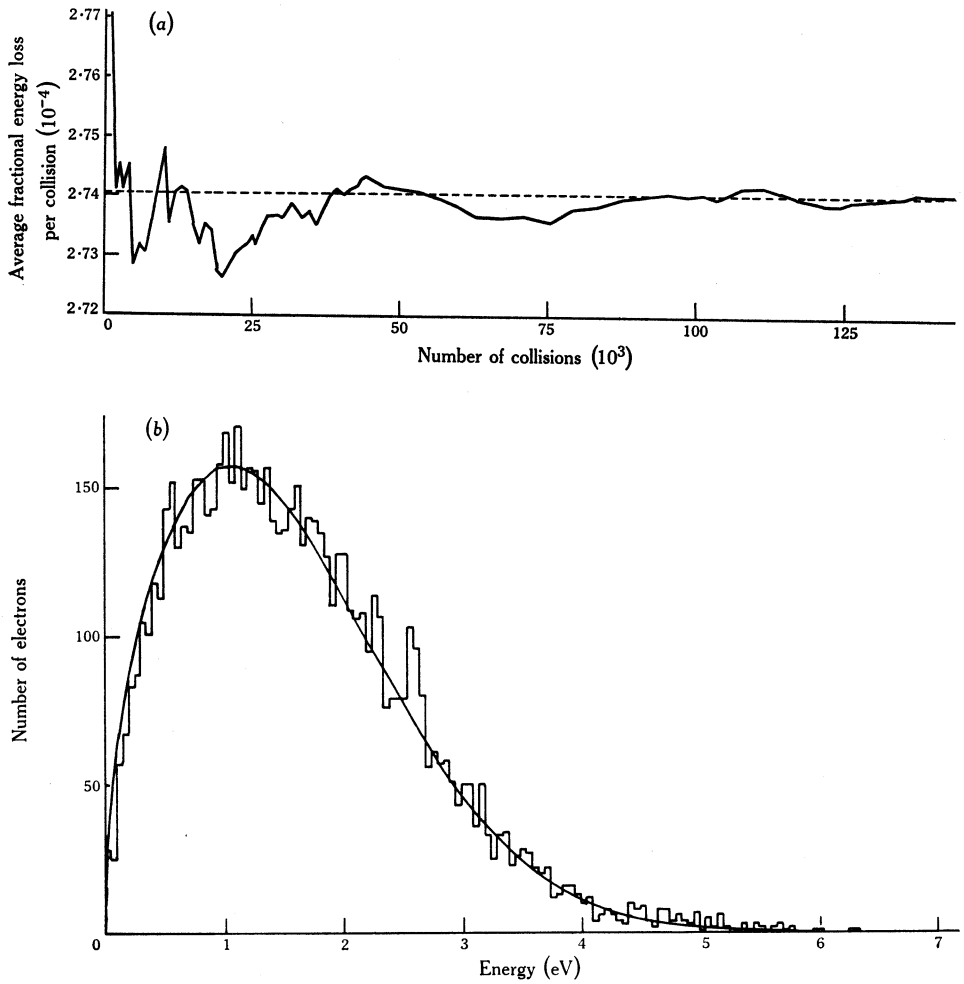


Fig. 1. (*a*) Average fractional energy loss per collision as a function of the number of collisions experienced by a single electron. The horizontal dashed line represents the expected analytic value of $2mM/(m+M)^2$. (*b*) Comparison between the expected Druyvesteynian electron energy distribution (smooth curve) and that obtained by sampling the computer-simulated electron swarm (histogram).

The average fractional energy loss per collision may also be computed and compared with the expected analytic value of $2mM/(m+M)^2 = 2{\cdot}7404 \times 10^{-4}$. Fig. 1*a*, which shows such a comparison, was obtained by studying one electron for a large

number of collisions and reveals that after $\sim 10^5$ collisions the average fractional energy loss computed directly by the program converges to the expected value. The irregularities in this curve have no significance. The convergence is not affected by the order in which the collisions are considered.

Energy Distribution

The energy distribution function may be obtained by sampling one electron at regular time intervals over a long period of time, by sampling the whole ensemble at one instant of time, or by sampling a group of electrons over a period of time. All three methods were tried and in each case good agreement with the expected Druyvesteyn distribution of mean energy 1·58 eV was obtained. Fig. 1*b* shows a comparison between the Druyvesteyn distribution and that obtained by sampling the entire group of electrons every 10^{-9} s between elapsed times of 0·30 and 0·35 μs.

Drift Velocity and Diffusion Coefficients

As shown by Parker and Lowke (1969), when the electrons are released from the origin with zero energy, the drift velocity W and transverse and longitudinal diffusion coefficients D_T and D_L are related to the position of the centroid $\bar{z}$, the average of the square of the displacements about the centroid $\langle(z-\bar{z})^2\rangle$ and the average of the square of the off-axis radial distance $\langle\rho^2\rangle$ by the equations

$$\bar{z} = Wt - A_{10}, \qquad \langle(z-\bar{z})^2\rangle = 2D_L t - A_{10}^2 + 2A_{20}, \qquad \langle\rho^2\rangle = 4D_T t - 4A_{01}.$$

Here t is the time, A_{10} is a constant proportional to N^{-1}, where N is the gas number density, and A_{01} and A_{20} are constants proportional to N^{-2}. Parker and Lowke show that, when q_m is constant, $A_{10}\mu E = 2{\cdot}1\, D_T$ for electrons released from the origin with zero energy. Substitution of numerical values shows that $A_{10} = 0{\cdot}06$ cm for $E/p_{293} = 1{\cdot}0$ V cm^{-1} torr^{-1} and 40 torr of helium. In fact, the electrons in the simulation were released with the equilibrium distribution of energies rather than zero energy and for these conditions the appropriate value of A_{10} is zero.

Fig. 2*a* shows $\bar{z}$ plotted as a function of time. A least squares fit to the data points is a straight line of slope $(8{\cdot}6 \pm 0{\cdot}1) \times 10^5$ cm s^{-1}, which is in excellent agreement with the expected value of $W = 8{\cdot}47 \times 10^5$ cm s^{-1}. The value of the vertical intercept is $0{\cdot}002 \pm 0{\cdot}004$ cm, thus confirming that the coefficient A_{10} is zero for the conditions of the simulation.

Figs 2*b* and 2*c* respectively show $\langle(z-\bar{z})^2\rangle$ and $\langle\rho^2\rangle$, averaged over the computed positions of the 150 electrons at each time, plotted as functions of the time since the swarm was released from the origin. The least squares lines of best fit to the computed data points are consistent with the analytic values of D_L and D_T to within 4%, this discrepancy being attributable to statistical fluctuations in the small group of electrons considered. There are insufficient data to determine values of the coefficients A_{20} and A_{01} but the evidence suggests that these quantities are smaller than the values predicted by Parker and Lowke (1969).

Spatial Dependence of Energy Distribution Function

Parker and Lowke (1969) have argued that the existence of anisotropic diffusion is due to spatial variations in the electron energy distribution function. At any instant those electrons which have travelled further in the field direction (at the front of the

swarm) should, on the average, be of higher energy than those at the back of the swarm. The energy distribution shown in Fig. 3*a* appears to confirm this argument, the same trend being apparent when data points at other sampling times are examined. The correlation coefficient between energy and position is about 0·7–0·9 for sampling times soon after the release of the swarm but decreases to and apparently stabilizes at 0·2–0·5 for times greater than 0·3 μs.

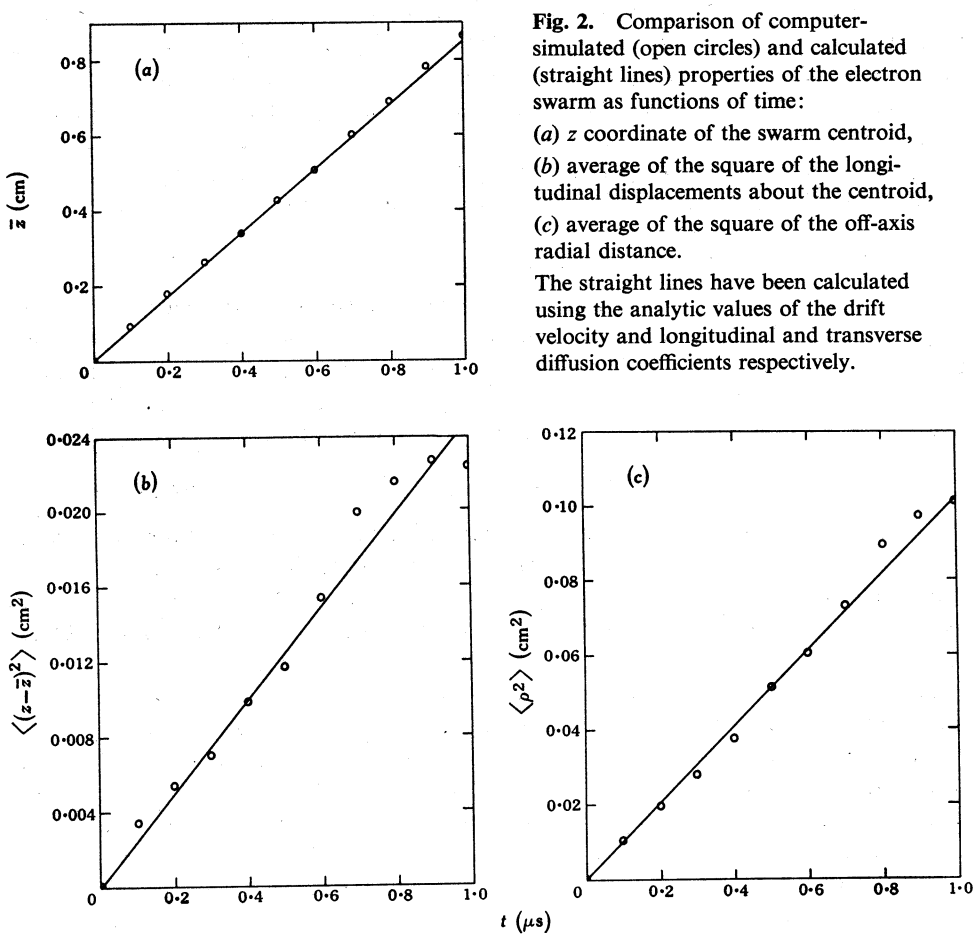


Fig. 2. Comparison of computer-simulated (open circles) and calculated (straight lines) properties of the electron swarm as functions of time:
(*a*) *z* coordinate of the swarm centroid,
(*b*) average of the square of the longitudinal displacements about the centroid,
(*c*) average of the square of the off-axis radial distance.
The straight lines have been calculated using the analytic values of the drift velocity and longitudinal and transverse diffusion coefficients respectively.

Shape of Electron Swarm

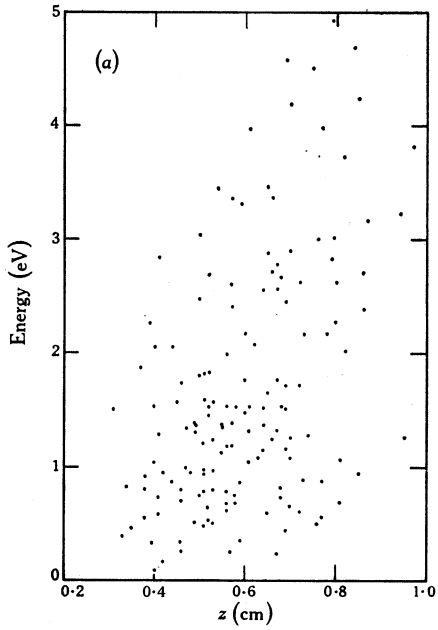
Huxley (1972) has written the continuity equation describing the drift in the *z* direction and the diffusion of a group of n_0 electrons released from the origin at time $t = 0$ in the form

$$-\frac{\mathrm{d}n}{\mathrm{d}t}+D_{\mathrm{T}}\left(\frac{\partial^2 n}{\partial x^2}+\frac{\partial^2 n}{\partial y^2}\right)+D_{\mathrm{L}}\frac{\partial^2 n}{\partial z^2}-W\frac{\partial n}{\partial z}=0, \tag{9}$$

which has the unique solution

$$n=\frac{n_0}{4\pi D_{\mathrm{T}}t(4\pi D_{\mathrm{L}}t)^{\frac{1}{2}}}\exp\left(-\frac{\rho^2}{4D_{\mathrm{T}}t}\right)\exp\left(-\frac{(z-Wt)^2}{4D_{\mathrm{L}}t}\right). \tag{10}$$

Since at any time t the z coordinate of the swarm centroid will be Wt, equation (10) shows that the contours of equal electron number density should be symmetric about the centroid.



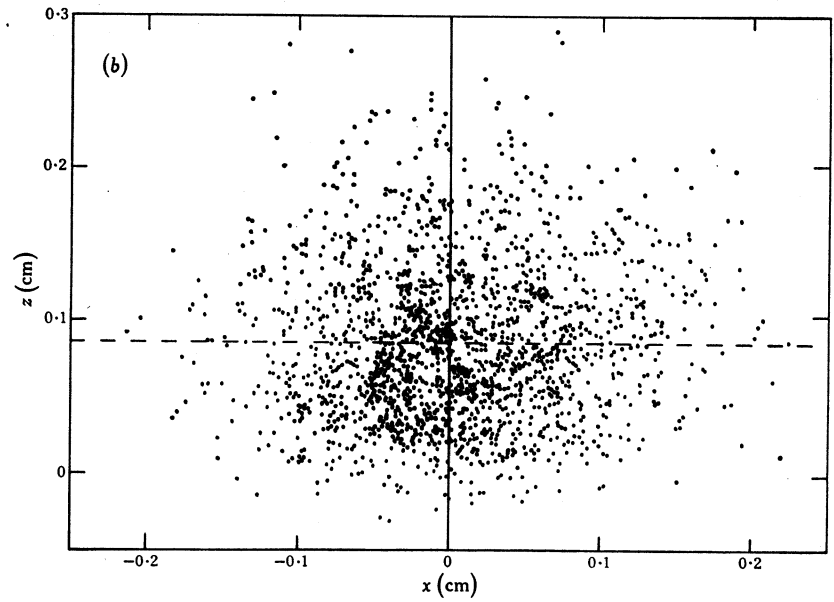


Fig. 3. (*a*) Energy of the electrons as a function of their z coordinate 0·7 μs after release from the origin.
(*b*) Shape of the electron swarm 0·1 μs after release from the origin.
Each point represents the computed x and corresponding z coordinates of an electron. The horizontal line indicates the position of the swarm centroid.

When the computed positions of the electrons in the swarm are examined at any time, results of the type shown in Fig. 3*b* are obtained. This diagram was plotted

by superimposing data for the increments in x and z coordinates at time increments of $0{\cdot}1\ \mu$s.* The features shown in Fig. 3*b* are confirmed when the positions of the 150 electrons are analysed mathematically at every sampling time. Thus, rather than being symmetric about the centroid, the swarm has the following properties:

(i) there are more electrons behind the centroid than in front,
(ii) the electrons behind the centroid are distributed over a smaller range of z values than those in front,
(iii) the peak value of the electron concentration is not coincident with the position of the centroid but is located slightly behind it.

Since the data shown in Fig. 3*b* were obtained at $t = 0{\cdot}1\ \mu$s, that is, relatively soon after the release of the swarm from the origin, it was thought possible that the asymmetries may have been due to the existence of large concentration gradients when the whole group of electrons was released from the origin. To test this hypothesis, the positions of the original 150 electrons were examined at $t = 0{\cdot}2\ \mu$s, which corresponded to a drift in the field direction of ~ 2 mm, a total free path of ~ 15 cm and an average of $\sim 1{\cdot}4 \times 10^4$ collisions, at which stage the swarm was so diffuse that the effects of the concentration gradients should have been negligible. The 100 electrons most symmetrically situated with respect to the centroid were selected and this same subgroup examined again at a time of $0{\cdot}7\ \mu$s. It was found that the symmetric group of electrons had re-established themselves in the asymmetric way described above. About 30 of the symmetric group had moved to extreme positions in the front, rear and wings of the swarm. When the 50 electrons rejected as being in extreme positions at the earlier time of $0{\cdot}2\ \mu$s were examined at $0{\cdot}7\ \mu$s and added to the group of 100, it was found that ~ 30 of these had moved from extreme positions to positions in the essentially symmetric core of the swarm. Thus it appears that the proportion of the swarm in the core is essentially unchanging but that particular electrons interchange between central and extreme positions during their lifetime between cathode and anode.

Further insight into this interchange is obtained by examining the position of one electron with respect to the bulk of the swarm as a function of time. If we select, for example, an electron in an extreme position at the rear of the swarm, it is found that this electron occupies its extreme position with respect to the swarm for a comparatively large number of sampling times and then moves rapidly to a new position in the swarm and continues in this new position over a relatively large number of sampling times and so on. Such behaviour can be explained by noting that, for most of its lifetime, each electron should behave like a 'typical' electron and that there are no electron–electron interactions. Thus, for most of its lifetime, an electron proceeds with the average characteristics of the swarm and its 'drift velocity' is essentially the same as that of the swarm as a whole; it is unaware of the presence of the other electrons and proceeds as the 'centroid' of its own swarm. During the short periods of time when its behaviour differs from the average behaviour (i.e. when its energy is substantially different from the mean energy), the electron has a 'drift velocity' higher or lower than that of the swarm as a whole and moves

* This procedure may be justified by noting that at any time the 150 electrons have a distribution of energies approximating the actual equilibrium distribution. Thus plotting increments in spatial coordinates at equal time intervals is equivalent to commencing the initial simulation with a set of different approximations to the equilibrium energy distribution. In this way the number of electrons in the simulation at early times is effectively increased.

rapidly to a new position within the swarm after which it again settles into average behaviour with the same 'drift velocity' as that of the swarm.

These same asymmetries are observed if the times at which the electrons cross a given plane for the first time are examined. A smaller number of electrons arrive ahead of the mean time than after it, the most common arrival time is slightly longer than the mean and there is a greater spread of times shorter than the mean than of times longer.

Table 1. Distribution of electron number density at 0·1 μs

The computed number density is given for cells of size $2\pi\rho\,d\rho\,dz$ with $d\rho = dz = 0{\cdot}05$ cm. The mid-point of each cell is expressed relative to the position of the swarm centroid, and the entry for the cell containing the centroid is given in bold type

$z-\bar{z}$ (cm)	$\rho-\bar{\rho}=0{\cdot}00$	0·05	0·10	0·15	0·20	0·25 cm
0·20	3·8	0·5	0·3	0·1		
0·15	16·4	6·4	1·9	0·6		
0·10	51·5	25·4	10·2	1·9	0·3	
0·05	99·1	65·4	26·5	8·2	1·3	0·1
0·00	**173·6**	120·7	50·4	11·5	1·3	0·2
−0·05	188·9	112·6	40·4	7·2	0·5	
−0·10	36·7	17·7	5·8	1·4	0·1	
−0·15	0·5	0·2	0·1			

Examination of Fig. 3*b* suggests that the electrons ahead of the centroid are not as far off axis as those the corresponding distance behind the centroid. Table 1 shows the spatial variations of electron density obtained by analysing the positions of 4650 electrons at $t = 0{\cdot}1$ μs. Each cell in the table represents a volume of $2\pi\rho\,d\rho\,dz$, with $\rho = (x^2+y^2)^{\frac{1}{2}}$ and $d\rho = dz = 0{\cdot}05$ cm. The table was constructed in such a way that the centroid occurs in the middle of the fourth cell representing the z direction. As well as illustrating the fore–aft asymmetry described above, this table allows us to calculate the average off-axis radial distance at eight positions from front to back of the swarm. The average off-axis radial distances (cm) through the swarm at 0·1 μs are:

Front				Centroid			Rear
0·068	0·077	0·084	0·094	0·091	0·083	0·080	0·075

Similar behaviour is observed for data at other sampling times.

6. Discussion and Conclusions

The present results for the electron energy distribution, the drift velocity and transverse diffusion coefficient are consistent with the well-known analytic formulae applicable to the model gas studied. The ratio of longitudinal to transverse diffusion was found to be approximately 0·5, which is in agreement with the theory of Lowke and Parker (1969). Direct support was obtained for the contention that, at any instant, the most energetic electrons should be at the front of the swarm.

The continuity equation (9) and its solution (10) as used by Huxley (1972) are supported only indirectly by experimental measurements of the transverse and longitudinal diffusion coefficients. It has been shown (Crompton 1972) that, under widely used experimental conditions, the measured values of D_T are insensitive to the assumption

of isotropic diffusion, and thus the experimental D_T values do not indicate that equation (9) is necessarily the correct continuity equation in all circumstances. There have been relatively few experimental determinations of the longitudinal diffusion coefficient while the method and theory of deducing D_L from the experimental data have not yet been exhaustively tested over a wide range of the experimental parameters. The most recent data (R. W. Crompton, personal communication) suggest that anomalous values of D_L may be obtained in some circumstances when theories based on equation (9) are used to analyse the experimental data.

The values of electron concentration computed in the present investigation do not substantiate equation (10). The electron swarm was not found to be symmetric in space: the maximum electron concentration was not coincident with the centroid, electrons were found in smaller numbers and over larger distances in front of the centroid than behind it, and the variation of the average off-axis radial distance was such as to lead to the description of the swarm as 'pear shaped'. It was shown that these anisotropies cannot be explained by invoking effects due to the high concentration gradients set up when the group of electrons is released from the origin. These observations lead to the conclusion that the continuity equation (9) as used by Huxley (1972) is not a completely adequate description of the drift and diffusion of the electron swarm.

The continuity equation used by Huxley (1972) and others is based on the assumption that the macroscopic motion of drift is superimposed on the symmetric random microscopic motion of the electron. It is also inherently assumed that the motions of drift and of transverse and longitudinal diffusion can be uncoupled and treated by scalar coefficients. In fact, at any instant, an electron having a certain kinetic energy has the potential to move an arbitrarily large distance in the field direction but can move no further against the field direction than its original kinetic energy allows. If the free path is large, the electron will either move a large distance in the field direction or its direction along the free path will be reversed and its position virtually unchanged. The microscopic motion is asymmetric in this fundamental way. A sequence of such events will allow some electrons to be spread well ahead of the centroid and others to be bunched behind it. Since the electron concentration is greatest on the axis, the spreading in the forward direction will be most noticeable here and thus give rise to the 'neck' of the pear shape. Such behaviour was observed in the present simulation.

According to the theory of mobility and diffusion developed extensively by Kumar and Robson (1973), a delta function pulse of electrons released from the origin should expand into a form which has pear-shaped components but the pear-shaped deformation should decay with time, perhaps as fast as t^{-2}. The present results confirm the establishment of the pear-shaped swarm at early times but, as far as can be determined within the limits imposed by the small number of electrons considered, this distortion does not appear to decay as rapidly with time as the argument of Kumar and Robson suggests. Comparison of the approximately 2000 data points shown in Fig. 3*b* which describe the shape of the swarm $0{\cdot}1$ μs after its release from the origin with a similar number of data points corresponding to an elapsed time of $0{\cdot}2$ μs does not reveal any marked changes in the degree of asymmetry of the swarm. There are insufficient data points to establish significant details of the shape of the swarm at considerably longer times, but the evidence suggests that the pear shape

persists at least for as long as it takes the swarm to move through a potential difference corresponding to five times the mean electron energy.

Although the simulation has been carried out for a simple ideal gas, there is no reason to expect qualitatively different behaviour in more realistic cases. Consequently, the asymmetries disclosed by the present work may provide a possible explanation for the discrepancies which occur between the 'luminous flux' method of determining electron transport coefficients (Buursen *et al.* 1972) and the older approaches which make no assumptions about the spatial variation of the electron pulse. Further insight into this problem should be obtained when the present program is extended to include the effects of energy-dependent elastic and inelastic collisions.

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