Aust. J. Phys., 1989, **42**, 187–196

Computer Simulation of Positron Annihilation and Diffusion Characteristics in Kr and Xe

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Abstract

Analysis of spectra, annihilation rates, and drift and diffusion characteristics of slow positrons is carried out in the heavy gases Kr and Xe. These properties are quite sensitive to the external electric and magnetic fields. Comparison with experiment is made where measurements are available.

1. Introduction

The lifetime of positrons emitted from a positron source and slowing down by collision with gas atoms has been the subject of many recent investigations (Jain *et al.* 1985). Studies have been mostly concerned with helium, neon and argon. Among these, helium and argon have been extensively studied by Singh and Grover (1986). Recently, attention has also been given to the study of the behaviour of slow positrons (with an energy less than the positronium formation threshold of 7·2 eV for Kr and 5·3 eV for Xe) in the heavy gases Kr and Xe. These gases have been studied experimentally by Canter (1972), Griffith *et al.* (1979), Heyland *et al.* (1982) and Charlton (1985), and theoretically by Schrader and Svetic (1982) and Campeanu (1982). Schrader and Svetic (1982) investigated the equilibrium behaviour of positrons as a function of temperature, while Campeanu (1982) calculated the time-dependent characteristics of positrons, but there has been no investigation of the effect of electric and magnetic fields on the annihilation of positrons in these gases, though it is well known that these fields appreciably influence the positron lifetime and other properties in gases, as investigated by Singh and Grover (1986).

In the present paper we analyse the effects of temperature and electric and magnetic fields on the drift, diffusion and annihilation of positrons. It is observed that the positron velocity distribution shifts to higher energies as the temperature and electric field are increased, and to lower energies with increasing magnetic field. The lifetime also increases with temperature and electric field, while it decreases with magnetic field. The positron diffusion coefficient and drift velocity are also sensitive to these fields.

0004-9506/89/020187$03.00

2. Method of Study

For slow positrons, interacting with the gas atoms, only elastic scattering and annihilation processes are important. It is assumed that the free positrons move in a homogeneous gas and that their behaviour is described adequately in terms of the single atom–positron interaction model. Let $F_0(v,t)$ be the time and velocity dependent isotropic distribution function which satisfies the boundary conditions $F_0(0,t)$ = finite and $F_0(\infty,t)=t$. When an electric field E and magnetic field B are applied to the gas assembly, the positron distribution function can be obtained from the Boltzmann equation, defined by Singh (1986),

$$\frac{\partial F_0(v,t)}{\partial t}=\frac{1}{v^2}\frac{\partial}{\partial v}\left\{\left(\frac{e^2E^2v^2}{3m^2[v_a(v)+v_m(v)+e^2B^2/m^2c^2\{v_a(v)+v_m(v)\}]}\right.\right.$$

$$\left.\left.-\frac{kTv_m(v)\,v^2}{M}\frac{\partial F_0(v,t)}{\partial v}\right)+\mu v_m(v)\,v^3F_0(v,t)\right\}-v_a(v)\,F_0(v,t), \quad (1)$$

where $v_a(v)$ and $v_m(v)$ are the annihilation and scattering rates respectively, e, m and v are the positron charge, mass and velocity, and c is the velocity of light.

After sufficient time, greater than the positron slowing down time, the velocity distribution tends to equilibrium. We are interested in finding the solution of equation (1) near equilibrium, that is, when the decay is nearly exponential. The exponential region can be characterised by the annihilation rate λ_a, and we assume that $F_0(v,t)=F(v)\,e^{-\lambda_a t}$. Using this assumption in equation (1) and after integrating over velocity, we get a linear integro-differential equation (see Singh and Grover 1987), the solution of which yields the equilibrium positron velocity distribution $y(v)$. After calculating $y(v)$, we obtain the annihilation rate

$$\bar{\lambda}_a=\int_0^\infty \lambda_a(v)\,y(v)\,dv\int_0^\infty y(v)\,dv.$$

Now we can also determine the drift and diffusion characteristics of positrons in the presence of electric and magnetic fields (Singh and Grover 1987). In the absence of a magnetic field, the diffusion and drift velocity of the positron can be evaluated as in Huxley and Crompton (1974):

$$D=\frac{4\pi}{3n_p}\int_0^\infty \frac{v^2}{v_m(v)}\,y(v)\,dv, \quad (2)$$

$$W=\frac{4\pi}{3n_p}\frac{eE}{m}\int_0^\infty \frac{v}{v_m(v)}\frac{\partial y(v)}{\partial v}\,dv, \quad (3)$$

where n_p is the positron density.

To perform the computer calculations and simulate the behaviour of various parameters in the heavy gases Kr and Xe, we need data on the annihilation and scattering cross sections. These parameters have been estimated by Schrader

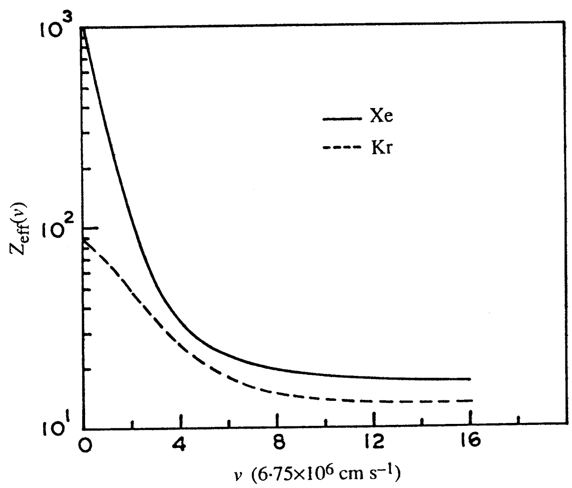

Fig. 1. Variation of decay rate $Z_{eff}(v)$ with velocity v for Kr and Xe.

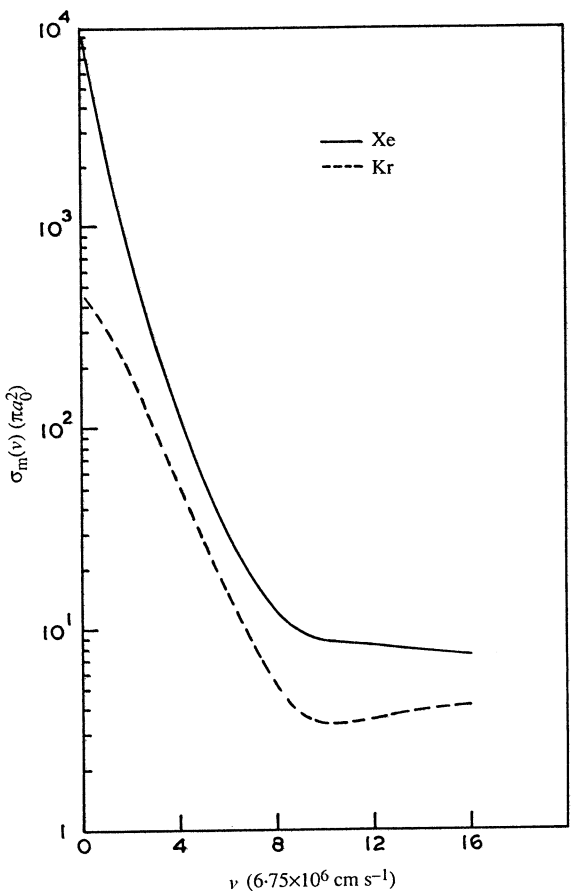

Fig. 2. Dependence of momentum transfer cross section $\sigma_m(v)$ on velocity for Kr and Xe.

(1979) and, more elaborately, by McEachran *et al.* (1980) for Kr and Xe. In our computer-aided analysis, we have used the data by McEachran *et al.* and performed extensive calculations to 'generate' positron behaviour numerically.

3. Results and Discussion

McEachran *et al.* (1980) computed the annihilation and momentum transfer rates in Kr and Xe using the frozen core orbital approximation; their results are shown in Figs 1 and 2. It can be observed that $Z_{\rm eff}(v)$ and $\sigma_{\rm m}(v)$ for Xe vary greatly at low velocity and then are nearly constant at higher velocity. For Kr, $Z_{\rm eff}(v)$ does not vary as rapidly, though $\sigma_{\rm m}(v)$ changes rapidly in the low velocity region. It is observed that a Ramsauer minimum is present in Kr, but not in Xe. This can effect positron diffusion and drift as these characteristics are more sensitive to the scattering properties of atoms.

We have obtained the positron distribution function $y(v)$ as a function of temperature, and electric and magnetic fields, for both gases. The electric field was varied over the range 0–200 $\rm V\,cm^{-1}$, while the magnetic field and temperature values are $10, 30, 50$ kG and $300, 1000, 3000$ K respectively. The distribution function $y(v)$ has been further normalised as $Y(v) = y(v)/\int_0^\infty y(v)\,dv$. Figs 3 and 4 present the variation of $Y(v)$ with velocity for various temperatures and electric and magnetic fields.

In Fig. 3 the curves a, b and c are for the normalised distribution function at $T = 300, 1000$ and 3000 K for $E = B = 0$; it is observed that the distribution shifts towards higher velocities and is broadened as the temperature is increased. In the absence of electric and magnetic fields, these distributions should be Maxwellian distributions. The dashed curves are the normalised theoretical positron Maxwellian distribution function $M(v) = Av^2\exp(-\frac{1}{2}mv^2/kT)$. We observe that the agreement between the equilibrium distribution and Maxwellian is very good, indicating the correctness of our computations and simulated distribution function.

For Kr, the positron distribution shifts towards higher velocities when the electric field is increased (curves d and e), due to the positrons gaining energy in the electric field, while it shifts to lower velocities in the presence of a magnetic field (curve f). Thus, the two fields have opposing effects (Huxley and Crompton 1974); the electric field 'heats' while the magnetic field 'cools' the distribution.

In Fig. 4 we give the curves for Xe and observe that the variation of the positron distribution function at different temperatures is quite similar, whereas the effect of the electric and magnetic fields is different (see curve 6 in Fig. 4).

The variation of the annihilation decay constant $\bar{Z}_{\rm eff} = \lambda_{\rm a}/\pi r_0^2 cn$ (where r_0 is the classical electron radius, c the velocity of light and n the gas density) with electric field is shown in Fig. 5, where curves a, b, c are for Kr while A, B, C are for Xe, corresponding to magnetic fields $0, 10, 50$ kG respectively. We observe that $\bar{Z}_{\rm eff}$ decreases sharply up to a certain electric field (say $E_{\rm c}$) and then is almost constant. When the magnetic field is applied to the gas assembly the value of $E_{\rm c}$ increases: $(E_{\rm c})_{\rm Kr} \approx 40\ \rm V\,cm^{-1}$ and $(E_{\rm c})_{\rm Xe} \approx 60\ \rm V\,cm^{-1}$ at $B = 10$ kG, whereas at $B = 50$ kG, $E_{\rm c}$ is $\approx 70\ \rm V\,cm^{-1}$ for Kr and $\approx 80\ \rm V\,cm^{-1}$ for Xe. The magnetic field has more effect in Kr than in

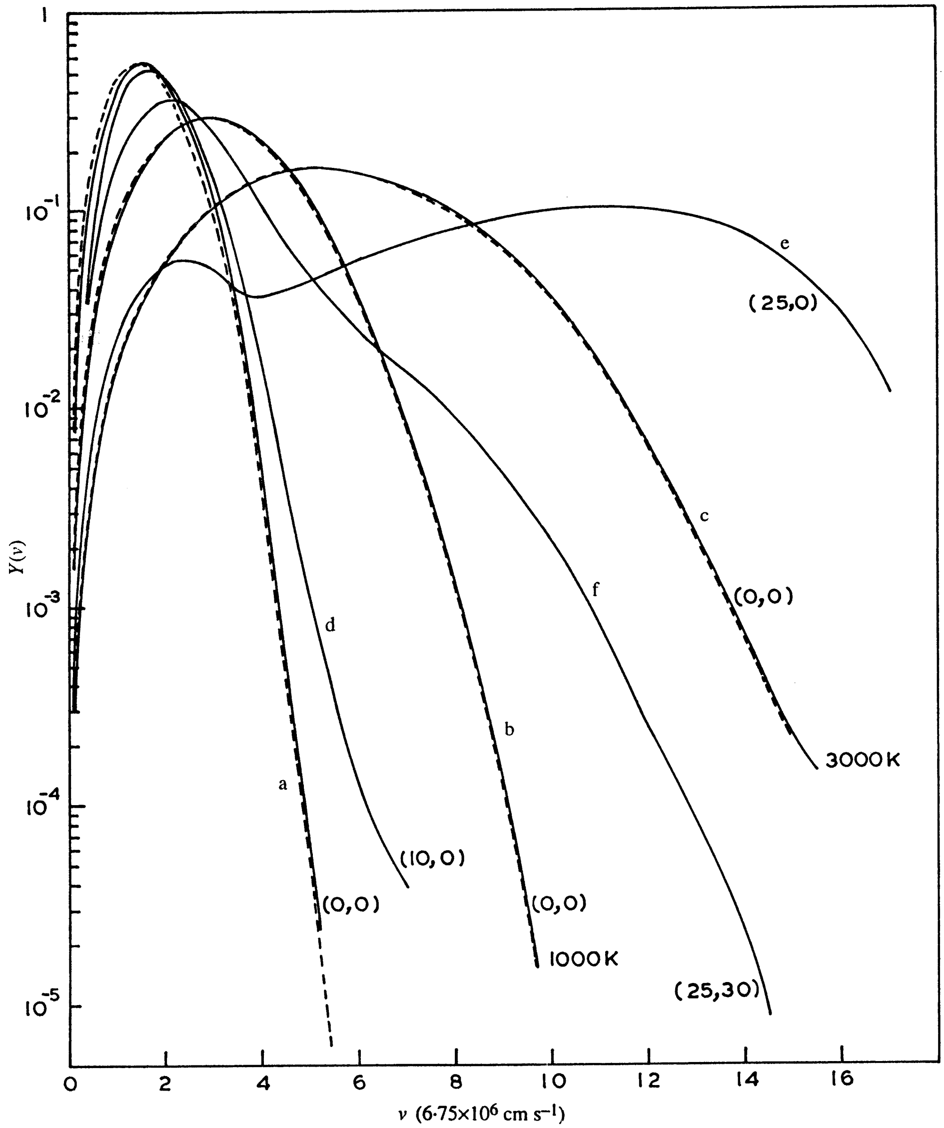

Fig. 3. Positron velocity distribution functions in Kr at various temperatures (see Section 3). The electric and magnetic fields (E,B) are shown on each curve. The dashed curves are Maxwellian distribution functions.

Xe because Kr is a lighter gas (see Singh and Grover 1986). The theoretical and experimental annihilation rates by different workers are presented in Table 1. It is seen that our results for Kr and Xe ($E = H = 0$, $T = 300$ K) are in good agreement with earlier theoretical results, but the discrepancy with the experimental results of Charlton (1985) and Heyland *et al.* (1982) are appreciable.

In Fig. 6 we have plotted the variation of the diffusion coefficient with electric and magnetic fields for Kr and Xe. At $B = 0$ the diffusion coefficient increases sharply in the low electric field region, i.e. $E \approx 35\ \mathrm{V\,cm^{-1}}$ for Kr and

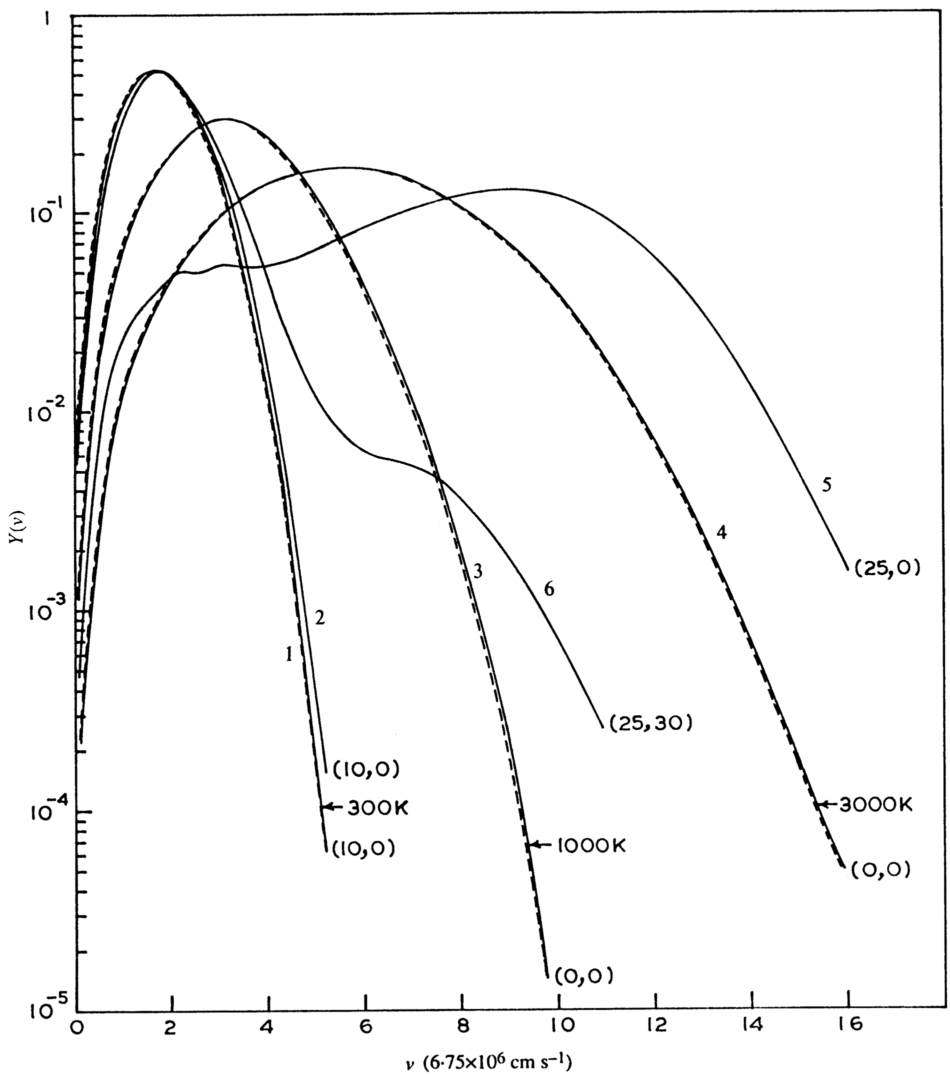

Fig. 4. Positron velocity distribution functions in Xe at various temperatures (see Section 3). The electric and magnetic fields (E, B) are shown on each curve. The dashed curves are Maxwellian distribution functions.

$\approx 50\,\mathrm{V\,cm^{-1}}$ for Xe. As the external magnetic field is applied, the diffusion coefficient splits into transverse and perpendicular components which decrease in strength as the magnetic field increases. The field has a greater effect on the perpendicular component (see Singh and Grover 1987). As can be seen also, the effect of the field is more pronounced in Kr.

The dependence of the drift velocity on the electric field for $B = 0, 10, 50$ kG is shown in Fig. 7. For $B = 0$ the velocity first increases with electric field and attains a maxima: $1 \cdot 27 \times 10^5\ \mathrm{cm\,s^{-1}}$ at $E = 25\ \mathrm{V\,cm^{-1}}$ for Kr and $1 \cdot 03 \times 10^5\ \mathrm{cm\,s^{-1}}$ for Xe. As a magnetic field is applied the drift velocity splits into the

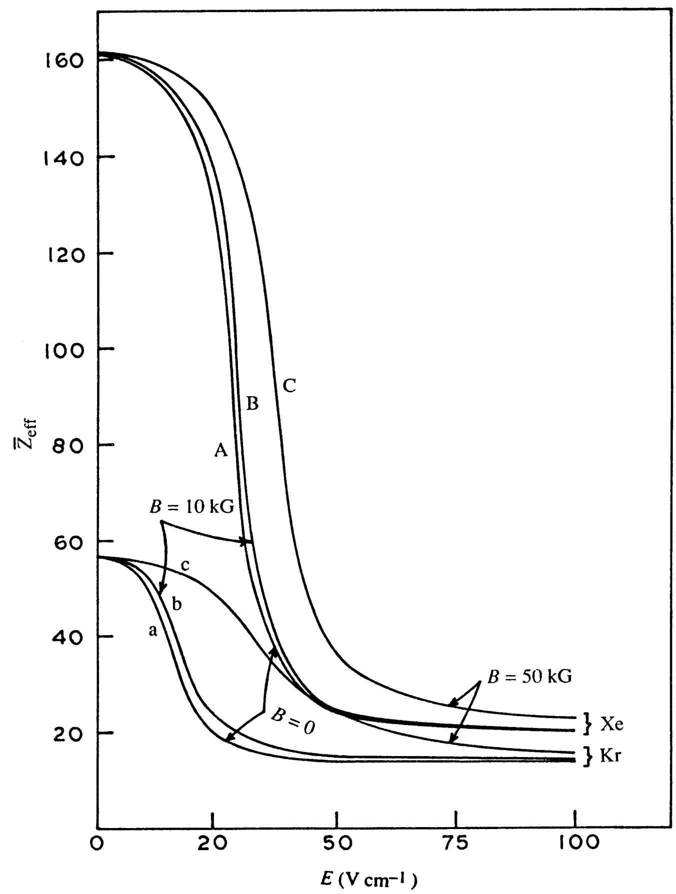

Fig. 5. Variation of $\bar{Z}_{eff}$ with electric field at $B = 0, 10, 50$ kG and $T = 300$ K for Kr and Xe. Each curve is discussed in Section 3.

Table 1. Annihilation decay constant $\bar{Z}_{eff}$ at $T = 300$ K and $E = B = 0$

Gas	$\bar{Z}_{eff}$(exp)	$\bar{Z}_{eff}$(theory)
Kr	66·8[A]	57·6±2·9[D]
	65·7±0·3[B,G]	57·11[E]
		55·9 [F]
Xe	320±1[A]	218±11[D]
	320±5[B,C,G]	159[E]
		161·32[F]

[A] Griffith (1979). [B] Heyland *et al.* (1982). [C] Wright *et al.* (1985).
[D] Schrader and Svetic (1982). [E] Campeanu (1982). [F] Present work.
[G] Charlton (1985).

transverse and perpendicular components shown. As the field increases, the maxima become broader and shift towards higher electric fields. Moreover, the transverse component, decreases with the field while the perpendicular component exhibits the reverse effect.

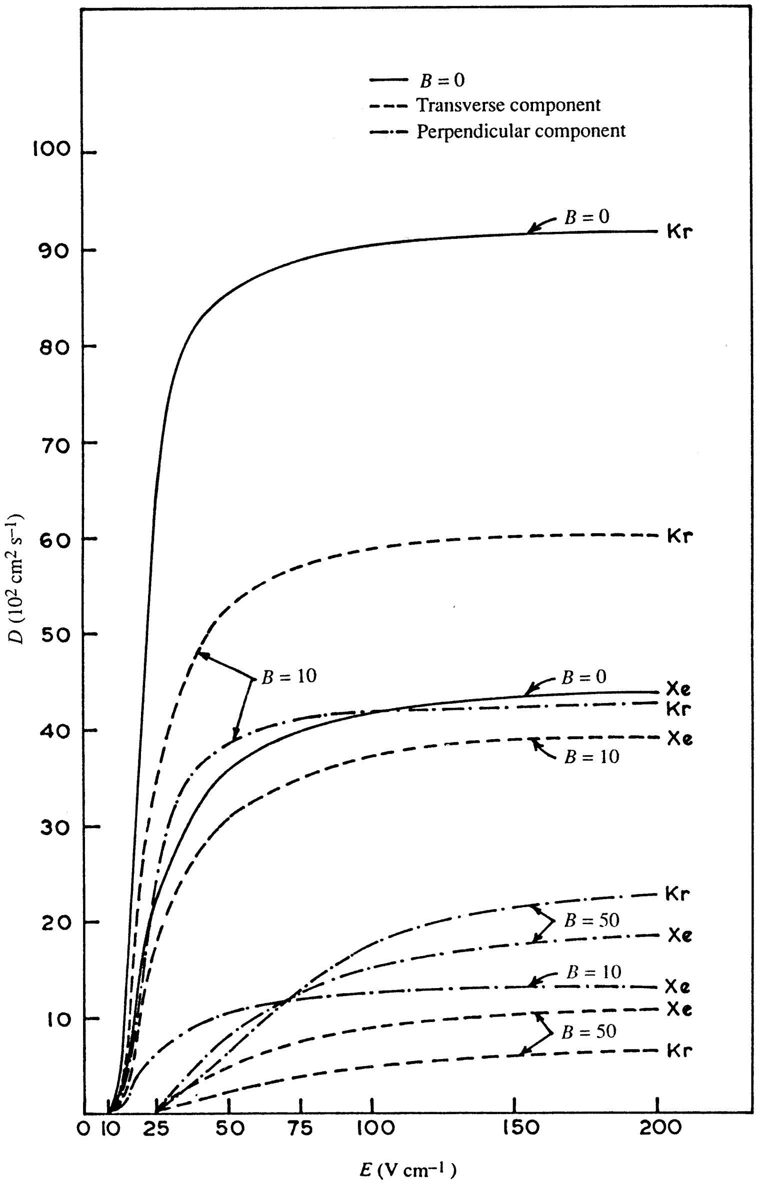

Fig. 6. Dependence of the diffusion coefficient on the electric field at $B = 0, 10, 50$ kG and $T = 300$ K for both gases.

4. Conclusions

We are not in a position to assess all our computer-based numerical results as no measurements of diffusion and drift characteristics have been made in heavy gases. However, for annihilation rates, the agreement with other computations is good. Agreement with measurements for $\bar{Z}_{\text{eff}}$ in Kr is also reasonable, though for the case of Xe the results disagree completely.

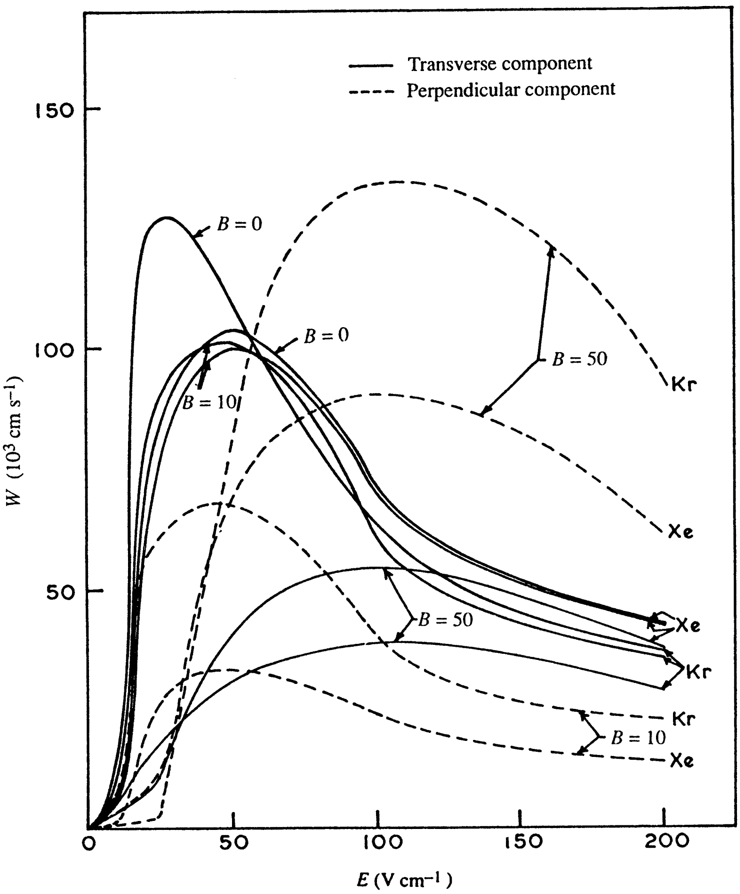

Fig. 7. Dependence of the drift velocity on the electric field at $B = 0, 10, 50$ kG and $T = 300$ K for both gases.

Comparison of the annihilation decay rate is only one 'contact' between theory and experiment. It will be of great interest if the drift and diffusion parameters are also measured as they are more sensitive to scattering properties of positrons. Our computer simulation studies suggest that such measurements are quite feasible. The numerical values depend on the positron–atom interaction model employed for the scattering and annihilation rates, but whatever the model the broad conclusions are expected to be similar.

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Manuscript received 21 July 1987, accepted 1 December 1988