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Computer calculation of positron diffusion and annihilation in atomic hydrogen

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Abstract. We have performed a computer-aided analysis of position behaviour in atomic hydrogen. Effect of electric, magnetic and temperature fields on the diffusion and annihilation of positrons has been studied. Electric field is varied over a wide range of 0–200 V cm^{-1} amagat^{-1}, magnetic field over 0–30 kG while the temperature range considered is 300–10,000°K. The positron decay rate decreases with electric and temperature fields but increases with magnetic fields. However, the effect of these fields is reversed on the diffusion coefficient.

Keywords. Positron diffusion; annihilation; atomic hydrogen.

1. Introduction

Annihilation of positrons in noble gases has been studied fairly well both theoretically (Ghosh *et al* 1982 and references therein) and experimentally (Grifith and Heyland 1978 and references therein).

It is comparatively easy to study the behaviour of positrons in noble gases, molecular gases and their mixtures, but very difficult to study positron annihilation in atomic hydrogen due to difficulty in obtaining atomic hydrogen in the laboratory. However, in solar atmosphere large quantities of hydrogen in atomic form are available. Positron-electron annihilation line (0·51 MeV) has been observed in solar flares and employed to infer the properties of flare and solar atmosphere. Thus, it is of interest to investigate the life-time and other properties in atomic hydrogen. We have done computer-based analysis of positron interaction in atomic hydrogen and the results are reported in this paper. It is hoped that the present results will generate interest in $e^+ - H$ study and help to understand the interaction of positrons with atomic hydrogen.

We have determined positron annihilation decay rate, average energy and diffusion coefficient as a function of electric, magnetic and temperature fields. The values of annihilation decay rate, average energy and diffusion coefficient at zero electric and magnetic fields and 300°K are 8·281, 0·038 eV, and 0·049 10^4 cm^2 s^{-1} whereas at 10,000°K, the values are 5·824, 1·31 eV and 3·390 10^4 cm^2 s^{-1} respectively. These parameters are quite sensitive to the fields.

2. Basic equations and computations

We restrict our analysis to positrons whose energies are less than the positronium formation threshold (6·7 eV for hydrogen). In this energy region, only elastic scattering and annihilation take place which enable us to determine the behaviour of slow positrons in hydrogen. Assuming that the gas assembly is spatially homogeneous and the electric and magnetic fields are perpendicular to each other, the velocity distribution function of positrons in gases is given by the Boltzman equation (Grover 1977).

$$\left(\frac{a^2v^2}{3\nu_m(1+\omega^2/\nu_m^2)}+\frac{kTv^2\nu_m}{M}\right)\frac{\partial f}{\partial v}+\mu\nu_m v^3 f(v)=\int_0^\infty(\nu_a-\lambda)v^2 f(v)\,\mathrm{d}v \tag{1}$$

where v and $f(v)$ are positron velocity and velocity distribution function respectively, a is the acceleration of positrons $= eE/m$, e is the positron charge, m the mass and E, the applied external electric field. ν_a and ν_m are positron annihilation and scattering rates respectively. $\mu = m/M$ ratio of positron mass (m) and gas atom mass (M). The presence of the term kT (T is the temperature of the gas and k the Boltzman constant) in equation (1) accounts for the thermal motion of the gas atoms of mass M. This term is quite important when the energy of the positrons is comparable to thermal energies. ω = cyclotron frequency $= \mu_p H_e/mc$ (μ_p is the magnetic permeability and is unity for gases) where H is the applied external magnetic field and c, the velocity of light.

The annihilation decay constant (λ) is given by

$$\lambda=\left[\textstyle\int_0^\infty \nu_a(v)v^2 f(v)\,\mathrm{d}v\right]\left[\textstyle\int_0^\infty v^2 f(v)\,\mathrm{d}v\right]^{-1}, \tag{2}$$

while the average energy of the positron is

$$\bar{\varepsilon}=\tfrac{1}{2}\left[\int_0^\infty v^4 f(v)\,\mathrm{d}v\right]\left[\int_0^\infty v^2 f(v)\,\mathrm{d}v\right]^{-1} \tag{3}$$

in units of k T_0, $T_0 = 300°$K is the room temperature.

The diffusion coefficient of positrons is given by

$$D=\frac{4\pi}{3n}\int_0^\infty \frac{v^4}{3\nu_m}f(v)\,\mathrm{d}v, \tag{4}$$

where n is the positron density:

$$n=4\pi\int_0^\infty v^2 f(v)\,\mathrm{d}v. \tag{5}$$

D is also referred to isotropic diffusion coefficient.

In the presence of the magnetic field, the diffusion coefficient has two components, one parallel to the direction of the magnetic field called transverse diffusion coefficient (D_T) and the other transverse to the direction of the magnetic field, called perpendicular diffusion coefficient (D_p). They are related to the distribution function as

$$D_p=\frac{4\pi}{3n}\omega\int_0^\infty \frac{v^4}{(v^2+\omega^2)}f(v)\,\mathrm{d}v, \tag{6}$$

and

$$D_T=\frac{4\pi}{3n}\int_0^\infty \frac{\nu v^4}{(v^2+\omega^2)}f(v)\,\mathrm{d}v, \tag{7}$$

Here

$$\nu=\nu_m+\nu_a\approx\nu_m \quad \text{as} \quad \nu_a\ll\nu_m$$

These relations can be readily obtained by following the treatment of Gilardani (1972).

Thus, we see that the annihilation decay constant (λ), the average energy ($\bar{\varepsilon}$), the transverse diffusion coefficient (D_T) and the perpendicular diffusion coefficient (D_p) can be obtained provided the positron velocity function is known. This function can be obtained by solving the Boltzman equation (1). To do this, it is essential that ν_a and ν_m are known. These quantities have complicated dependence on velocity and the Boltzman equation cannot be solved analytically. So, we have solved it numerically and obtained the distribution function by performing extensive computer calculations.

Bhatia *et al* (1977) calculated $\nu_a(v)$ and $\nu_m(v)$ using Feshbach formalism in atomic hydrogen. They studied the variation of life-time of positrons with temperature only. Their results of $\nu_a(v)$ and $\nu_m(v)$ are reported in figure 1 for reference. Figure 1 represents the variation of annihilation decay rate $Z_{\text{eff}}(k)$ and momentum transfer cross-section $\sigma_m(k)$ with the wave number of positron (k). Both of them decrease upto $k = 0{\cdot}3(a_0^{-1})$ (a_0 = Bohr radius) and then become nearly constant. Further, it is observed that decrease in σ_m is faster as compared to that in $Z_{\text{eff}}(k)$.

No study of effect of electric and magnetic field on the positron life-time, average energy and diffusion coefficient appears to have been performed by using this model. Because of their importance in the study of e^+-atom interactions, we have performed a computer-based study of these parameters.

We define dimensionless annihilation decay rate $\bar{Z}_{\text{eff}} = \lambda/\pi r_0^2 cn$ where $r_0^2 = e^2/mc^2$, is the classical electron radius. We shall take gas density n to be one amagat. $\bar{Z}_{\text{eff}}$ also refers to the number of electrons per atoms with which positrons can annihilate.

3. Results and discussion

Figure 2 shows the dependence of annihilation decay constant ($\bar{Z}_{\text{eff}}$) on temperature. The temperature is varied from 300°K to 10,000°K. Curves 1, 2, 3 are for $E = 0$, 25 and

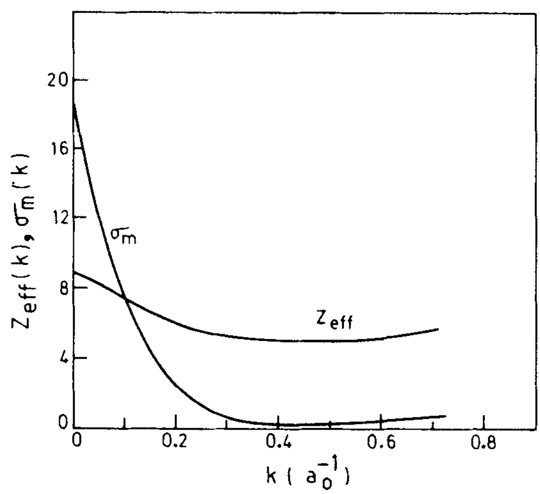

Figure 1. Variation of Z_{eff} and σ_m with $k(a_0^{-1})$.

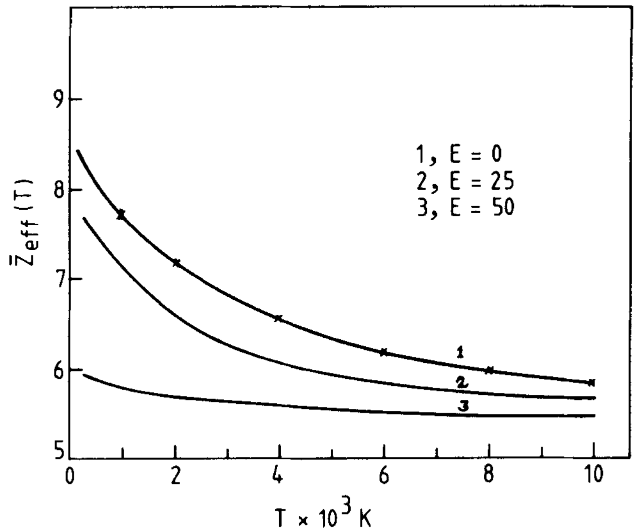

Figure 2. Dependence of annihilation decay constant on temperature. Curves 1, 2, 3 are for $E = 0$, 25 and 50 V cm^{-1} amagat^{-1} respectively.

Table 1. Value of $\bar{Z}_{eff}$, average energy and diffusion coefficient at zero electric, magnetic field and various temperatures.

Temperature (K)	300	1000	2000	4000	6000	10,000
Decay constant	8·2815	7·6832	7·1543	6·5355	6·1818	5·8241
Average energy (eV)	0·0388	0·129	0·258	0·517	0·762	1·131
Diffusion coefficient (cm^2 s^{-1})	0·049	0·145	0·348	1·10	2·140	3·390

50 V cm^{-1} amagat^{-1} and zero magnetic field respectively. $\bar{Z}_{eff}$ decreases with increasing temperature for all the electric fields. But the temperature has more effect at lower electric fields. At high fields $\gtrsim$ 50 V cm^{-1} amagat^{-1}, $\bar{Z}_{eff}$ becomes almost independent of temperature beyond 6000°K. The values of $\bar{Z}_{eff}$ at different temperature and zero electric and magnetic fields are given in table 1. It is found that at weaker electric fields, the effect of temperature is much greater than at higher electric fields. The asterisks (*) in figure 1 (curve 1) indicate the points of Bhatia *et al* (1977). At $E = 0$, our results are in complete agreement with their results. These workers calculated $\bar{Z}_{eff}$ by Maxwellian function average method but we have computed the decay constant by the perturbation iteration technique. The agreement of the results by the two methods shows the accuracy of our computer codes and the method of calculation.

In figures 3 to 5 we have shown the variation of annihilation decay constant with electric fields for temperatures 300, 1000 and 10,000°K respectively. The electric field is varied over the range 0–200 V cm^{-1} amagat^{-1}. The values of magnetic field taken are $H = 0$, 10, 20 and 30 kG and indicated in the figures.

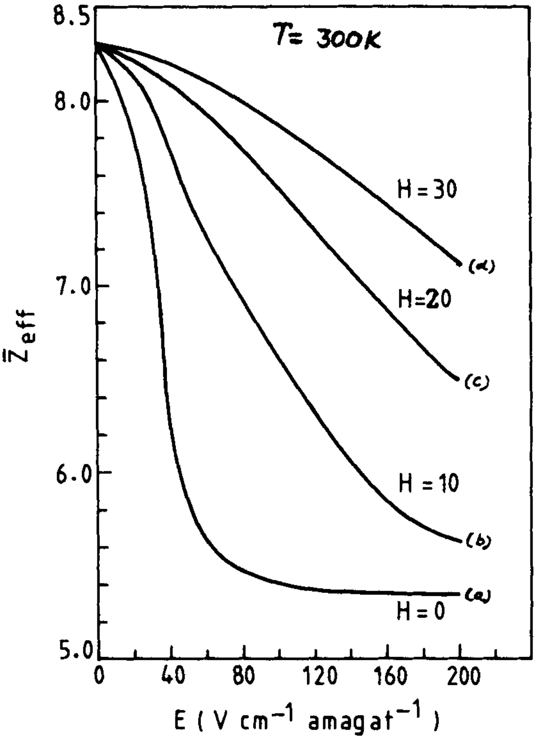

Figure 3. Variation of annihilation decay constant with electric field at $T = 300$ K, curves a, b, c, d are for magnetic field $H = 0$, 10, 20 and 30 kG respectively.

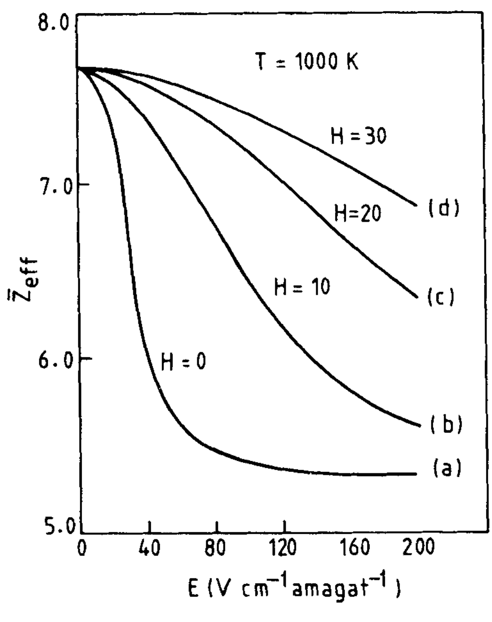

Figure 4. Variation of annihilation decay constant with electric field at $T = 1000$ K, curves a, b, c, d are for magnetic fields $H = 0$, 10, 20 and 30 kG respectively.

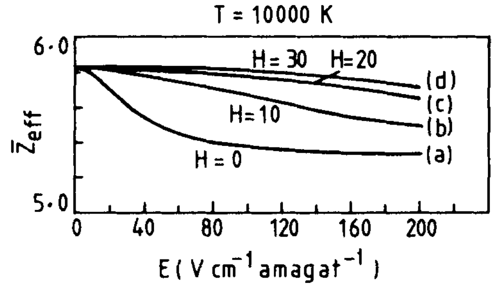

Figure 5. Variation of annihilation decay constant with electric field at $T = 10{,}000$ K, Curves a, b, c, d are for magnetic field $H = 0$, 10, 20 and 30 kG respectively.

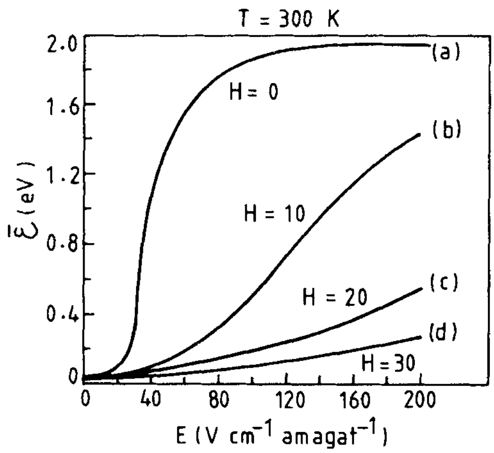

Figure 6. Variation of average energy with electric field at $T = 300$ K. Curves a, b, c, d are for magnetic field $H = 0$, 10, 20 and 30 kG respectively.

It is observed that $\bar{Z}_{eff}$ decreases rapidly upto $E \approx 100$ V cm^{-1} amagat^{-1} and then becomes almost constant (curve (a) of figure 3.) For $H = 10$ kG, $\bar{Z}_{eff}$ again decreases with increasing electric fields but the decrease in this case is different from the previous case (curve (b)). In the former, $\bar{Z}_{eff}$ becomes almost constant beyond $E \approx 100$ V cm^{-1} amagat^{-1} but in the latter, $\bar{Z}_{eff}$ goes on decreasing with electric field even upto 200 V cm^{-1} amagat^{-1}. Again for $H = 20$ kG and 30 kG we find that $\bar{Z}_{eff}$ decreases with electric field but the decrease in $\bar{Z}_{eff}$ becomes lower and lower (curve c, curve d). Even the slope of the curve changes continuously as the magnetic field is increased.

We observe that $\bar{Z}_{eff}$ decreases rapidly upto $E \approx 100$ V cm^{-1} amagat^{-1} and then becomes almost constant when the magnetic field is zero. But when the magnetic field is increased, $\bar{Z}_{eff}$ goes on decreasing with electric field even upto $E = 200$ V cm^{-1} amagat^{-1}. Even the slope of the curve changes continuously as the magnetic field is increased. But at very high temperatures, about 10,000°K, and higher magnetic fields, $\bar{Z}_{eff}$ decreases very smoothly with electric field, figure 5.

Figure 6 represents the variation of average energy with electric fields at 300°K and at different magnetic fields. It is evident that at zero magnetic field, the average energy changes most rapidly in certain range of electric field (curve a). This range is

$\approx$ 20–100 V cm^{-1} amagat^{-1}. At higher electric field, the average energy becomes almost constant when the magnetic field is zero. At $H = 10$ kG, the average energy increases slowly at lower electric fields. The average energy does not remain constant even at higher electric fields but increases (curve b). The variation of average energy with electric field becomes almost linear at high magnetic fields (curve c, d).

This type of behaviour of average energy with electric and magnetic fields is found even at very high temperatures.

The electric and magnetic fields have opposite effect on the decay constant and average energy. This can be explained as follows:

After integration of equation (1) we get

$$f(v) = \int_0^\infty \alpha^{-1}\left[v^2 \int_0^v (v_a - \lambda)v^2 f(v)\,dv - \mu v_m v f(v)\right] dv \tag{8}$$

where

$$\alpha = x + y.$$

Here

$$x = \frac{a^2}{3v_m(1+\omega^2/v_m^2)} \quad \text{and} \quad y = \frac{kTv_m}{M}.$$

x involves the electric and magnetic fields and y the temperature only. The distribution function is lowered (eq. 8) and broadened (Grover 1977) as α (or E) is increased, while the effect of magnetic field is opposite. This leads to increase in average energy with electric field and decrease with magnetic field. Alternatively, we can understand this as follows: in the absence of fields, for a uniform distribution of positrons, about as many positrons enter a small volume after being scattered in the backward direction. These are decelerated by the electric field and thus have a lower energy. Those which are scattered forward are accelerated and have higher energy. There are fewer positrons scattered backward than forwards, and the net effect is an increase in the average energy with respect to electric field.

The variation of $\overline{Z}_{\text{eff}}$ can be explained by keeping in view the variation of $\bar{\varepsilon}$. In the electric field region where the average energy undergoes maximum changes, the annihilation decay constant also changes rapidly. This electric field region is 20–100 V cm^{-1} amagat^{-1} (curve a of figures 3 and 6). Thus we observe that when the positron life-time undergoes rapid variations, this corresponds to a rapid gain of energy.

The average energy at room temperature and zero electric and magnetic fields as calculated by us is 0·0388 eV while the actual value is 0·039 eV. Thus the agreement between the calculated and actual values is very good.

Figures 7 and 8 show the dependence of diffusion coefficient on electric field at 300°K and $H = 10$ kG and 30 kG respectively. D_T is the transverse diffusion coefficient and D_p is the perpendicular diffusion coefficient. Both the diffusion coefficient increase with electric field (figure 8). At lower electric fields, D_p and D_T remain almost constant upto $E = 40$ V cm^{-1} amagat^{-1}. But beyond this D_T increases slowly while D_p increases rapidly with electric fields. This is because the positron tends to diffuse more in the perpendicular direction of the electric field. Hence D_p increase rapidly than D_T. We also observe that diffusion coefficient remains constant in the lower electric field region and then increases. It implies that positrons do not diffuse appreciably at lower electric

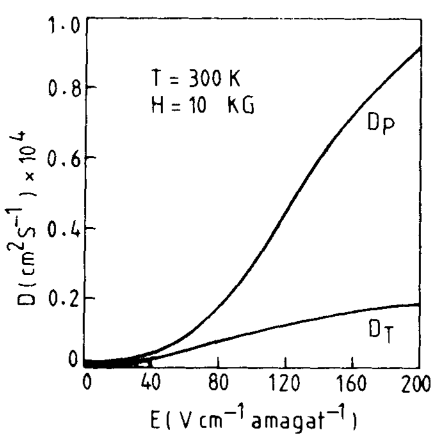

Figure 7. Effect of electric field on diffusion coefficient at $T = 300$ K at magnetic field $H = 10$ kG.

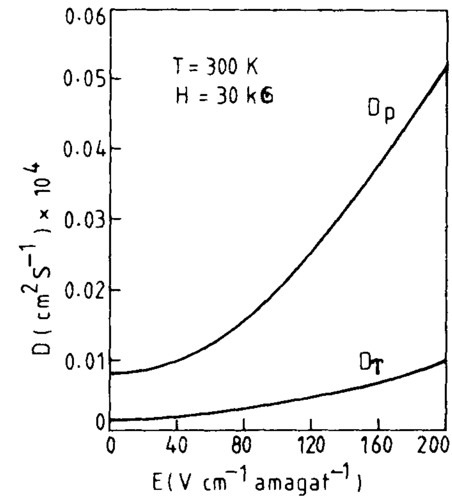

Figure 8. Effect of electric field on diffusion coefficient at $T = 300$ K and magnetic field $H = 30$ kG.

fields. At higher fields, the positron diffusion is greater in the perpendicular direction of the electric field. D_T at $E = 200\ \text{V cm}^{-1}$ amagat^{-1}; $T = 300°\text{K}$ and $H = 10$ kG and 30 kG are $0{\cdot}180 \times 10^4\ \text{cm}^2\ \text{s}^{-1}$ and $0{\cdot}010 \times 10^4\ \text{cm}^2\ \text{s}^{-1}$ respectively. D_p at $E = 300\ \text{V cm}^{-1}$ amagat^{-1} 300°K and $H = 10$ kG and 30 kG are $0{\cdot}911 \times 10^4\ \text{cm}^2\ \text{s}^{-1}$ and $0{\cdot}057 \times 10^4\ \text{cm}^2\ \text{s}^{-1}$ respectively.

4. Conclusions

At present, no experimental results are available on positron diffusion and annihilation in atomic hydrogen gas. We are therefore unable to compare our computer calculations with any other data.

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