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POSDIF – A PROGRAM TO COMPUTE POSITRON DIFFUSION AND ANNIHILATION IN RARE GASES

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PROGRAM SUMMARY

Title of program: POSDIF

Catalogue number: AAHN

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application from in this issue)

Computer: IBM-360 at York University, Toronto and also CDC 7600 at ULCC, University of London and Felix C-256 at University of Cluj Computer Centre.

Programming language used: FORTRAN IV

Storage required: 26 kwords in double precision

Number of bits in a word: 32

Overlay structure: none

Peripherals used: card reader, line printer

Number of cards in the program and the test deck: 917

Keywords: positron, diffusion equation, lifetime spectrum, Crank–Nicolson method, finite differences, momentum transfer, effective charge

Nature of the physical problem
Calculates positron lifetime spectrum in a gas being given the gas pressure and temperature, the value of the external electric field strength and the fits to momentum dependence of the positron–atom momentum transfer cross section and of the effective charge number [1].

Method of solution
The parabolic equation, representing positron diffusion and annihilation in the gas, is solved using the Crank–Nicholson method and other standard finite difference methods [2]. At each timestep the velocity distribution is used to calculate the averaged effective charge number and the averaged positron momentum.

Typical running time
About 300 s CPU time on the IBM-360.

References

[1] R.I. Câmpeanu and J.W. Humberston, J, Phys. B 10 (1977) 239.
[2] Harwell Subroutine Library, Report AERE-R9185, HMSO London (September 1980).

LONG WRITE-UP

1. Introduction

The positron lifetime experiments measure the annihilation rate averaged over the velocity distribution of the positrons and it is therefore necessary to calculate the time-dependent velocity distribution as well as the velocity dependence of the annihilation rate before comparison of the experimental and theoretical results can be made. Most of the experimental spectrum corresponds to the positrons scattered elastically before annihilation. In the past years extensive theoretical investigations have been made on various positron–rare gas atoms elastic scattering and today we have reliable results to be employed in this type of comparison. For a detailed account of the status of agreement between theory and experiment see refs. [1–3].

2. Summary of the theory

The velocity distribution of the elastically scattered positrons in a gas of absolute temperature T, subject to a uniform electric field of strength E, is governed by the diffusion equation:

$$\frac{\partial y(v,t)}{\partial t}=\frac{\partial}{\partial v}\left\{\left(\frac{e^2E^2}{3m^2vN\sigma_{\mathrm{mt}}(v)}+\frac{vN\sigma_{\mathrm{mt}}(v)\,kT}{M}\right)\times\frac{\partial y(v,t)}{\partial v}+\left(\frac{mv^2N\sigma_{\mathrm{mt}}(v)}{M}-\frac{2e^2E^2}{3m^2v^2N\sigma_{\mathrm{mt}}(v)}-\frac{2N\sigma_{\mathrm{mt}}(v)\,kT}{M}\right)\times y(v,t)\right\}-\pi r_0cNZ_{\mathrm{eff}}(v), \quad (1)$$

where e and m are the charge and mass, respectively, of the positron, N is the number density of the gas atoms each of mass M; k is the Boltzman's constant, r_0 is the classical electron radius, c is the velocity of light, σ_{mt} is the momentum transfer cross section and Z_{eff} is the effective number of electrons per target atom with which a positron can annihilate.

The number density of positrons in the velocity interval v to $v+\mathrm{d}v$ at time t is $y(v,t)\,\mathrm{d}v$. With the boundary conditions $y(0,t)=y(\infty,t)=0$ for all t and a given initial velocity distribution $y(v,t=0)$ the diffusion equation can be solved to obtain the velocity distribution $y(v,t)$ for all subsequent times.

The velocity average of $Z_{\mathrm{eff}}(v)$, which can be obtained from the experimental annihilation rate, is then given by:

$$\bar{Z}_{\mathrm{eff}}(t)=\int_0^\infty y(v,t)\,Z_{\mathrm{eff}}(v)\,\mathrm{d}v\Big/\int_0^\infty y(v,t)\,\mathrm{d}v. \quad (2)$$

Similarly one can obtain the averaged values of the positron momentum:

$$\bar{k}(t)=\int_0^\infty y(v,t)\frac{mv}{\hbar}\mathrm{d}v\Big/\int_0^\infty y(v,t)\,\mathrm{d}v. \quad (3)$$

2.1. The initial velocity distribution

We assumed that initially no free positrons exist with energies greater than the threshold energy for positronium formation E_{ps}. The reason for this assumption is the following: a high-energy positron will lose energy very rapidly by inelastic collisions until its energy has fallen below the lowest inelastic threshold; its energy will be either below E_{ps} or in the Ore gap (the region between E_{ps} and the lowest excitation threshold), where it has a high probability of forming positronium. It was actually proven [1] that the extension of the initial velocity region to the first excitation threshold does not modify significantly the theoretical results. The eqs. (2) and (3) will employ the velocity corresponding to E_{ps} as upper limit in the integrations.

Several forms of the initial velocity distribution were considered in ref. [1] but their choice was found not very important. The present program uses the uniform distribution in momentum space:

$$y(v,t=0)=v^2. \quad (4)$$

2.2. Momentum transfer cross sections and effective charge numbers

The diffusion equation (1) requires $\sigma_{mt}(v)$ and $Z_{eff}(v)$ in an analytic form. It was found [1,2] that the appropriate forms to fit the He, Ne, Ar data are:

$$\sigma_{mt}(k) = a_0 + a_1 k + a_2 k^2 \ln k + a_3 k^2 + a_4 k^3 + a_5 k^4,$$
$$Z_{eff}(k) = b_0 + b_1 k + b_2 k^2 + b_3 k^3, \quad (5)$$

while for Kr and Xe the forms used in ref. [3] were:

$$\left.\begin{array}{l}\sigma_{mt}(k)\\ Z_{eff}(k)\end{array}\right\} = \sum_{i=0}^{4} c_i \exp(-\alpha_i k), \quad (6)$$

where k is the positron momentum and α_i are positive integers chosen by trial and error. Both forms (5) and (6) can be employed in the present program by using the appropriate value of the input parameter IFIT. For any other analytic forms one has to change the functions FZE(X), FQM(X) and FDQ(X).

3. Program structure

A block diagram is shown in fig. 1. The main program is:

POSDIF where the input requirements are described and the input data are read and written. The initial and the boundary conditions are then defined and for each step in time the eqs. (2) and (3) are calculated by using the Simpson integration formula.

FZE, FQM and FDQ are functions calculating the values of Z_{eff}, σ_{mt} and $d\sigma_{mt}/dk$, respectively for a given value of the positron momentum k.

HISTO is used to represent graphically $y(v)$ at different times; if the step in time is chosen too large the velocity distribution $y(v)$ shows oscillations which are amplified in time [5]; therefore HISTO can be switched on with an appropriate value of IGRAF to check on the correctness of the timestep.

DP01A finds the solution at time $t+\delta t$ of a parabolic equation, such as (1), given the solution at time t. The coefficients in the standard form are defined by subroutine FUNCTS and the derivatives are calculated by TD01A. DP01A uses the Crank–Nicholson method to bring the parabolic equation to a 2-point boundary value second order differential equation.

DD01A solves the second order differential equation by using up to 4th central differences (calculated by TA03A) to yield a system of linear equations solved by MA07A. The third and the fourth differences are applied iteratively until subroutine TD01B decides that the accuracy was achieved; the vector S in POSDIF contains at each timestep the effect of the 3rd and 4th order corrections. For other details see ref. [4].

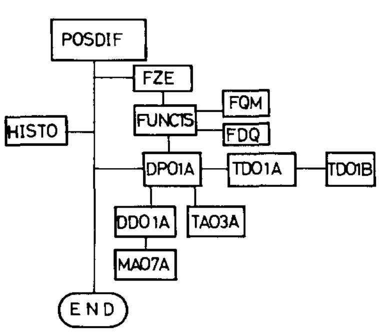

Fig. 1. Block diagram of the program POSDIF.

4. Arrangement of common

W(20 × NPT) is working space, NPT being the number of mesh points on the velocity axis.

DN, SAM, TEMP, E, B0,... B4, A0,... A4, V1,... V5, W1,... W5, are variables, put in the common block after the working space, which contain input data.

5. Numerical accuracy

A typical number of points is NPT = 199 on the velocity axis and a timestep of order of 0.1 ns. An inappropriate mesh would give an incorrect shape of $y(v)$, and the use of HISTO is therefore

Table 1
Input data to be punched

Card no.	Variables	Format	Comments
1	DN, SAM, TEMP, E	5F15.1	
2	IGRAF, IFIT	2I5	
3	MM, DT, ICLIM	I5, D15.5, I5	
4	NPT, XN	I5, D15.5	
5	A0, A1, A2, A3, A4	5F15.8	
6	B0, B1, B2, B3, B4	5F15.8	
7	W1, W2, W3, W4, W5	5F5.1	cards 7 and 8 are read only for IFIT =1
8	V1, V2, V3, V4, V5	5F5.1	

DN	number density given in amagats,
SAM	atomic mass given in electron masses,
TEMP	gas temperature in kelvin,
E	electric field strength given in V cm^{-1} $amagats^{-1}$,
IGRAF=0	if only $\bar{Z}_{eff}$ and $\bar{k}$ are required,
=1	at each timestep a plot of $y(v)$ is added to Z_{eff} and $\bar{k}$,
=2	the plot of $y(v)$ is given only at the last timestep,
IFIT=0	$\sigma_{mt}(k)$ and $Z_{eff}(k)$ are fitted with the analytical forms (5),
=1	$\sigma_{mt}(k)$ and $Z_{eff}(k)$ are fitted with the analytical forms (6),
MM	number of timesteps after which the results are printed,
DT	timestep length δt,
ICLIM	number of steps in time for which the results are printed,
NPT	number of steps on the velocity axis,
XN	positron wave number corresponding to E_{ps},
A0,... A4	linear parameters in the fit to $\sigma_{mt}(k)$,
B0,... B4	linear parameters in the fit to $Z_{eff}(k)$,
W1,... W5	nonlinear parameters in (6) when fitting $\sigma_{mt}(k)$,
V1,... V5	nonlinear parameters in (6) when fitting $Z_{eff}(k)$.

necessary as a check on the numerical accuracy.

The calculations were performed in single precision on the CDC7600 and the Felix C-256 and in double precision on the IBM-360. It was found that the use of single precision on IBM or Felix gives values of $\bar{Z}_{eff}$ different by less than 1% from the double precision values.

6. Input

The input data have to be punched as shown in table 1.

7. Test run

The test run is given for positron diffusion in krypton. All the input data are printed at the beginning of the test run output.

Acknowledgements

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References

[1] R.I. Câmpeanu and J.W. Humberston, J. Phys. B 10 (1977) 239.
[2] R.I. Câmpeanu, J. Phys. B 14 (1981) L157.
[3] R.I. Câmpeanu, Can. J. Phys. to appear.
[4] Harwell Subroutine Library, Report AERE-R9185, HMSO London (September 1980).
[5] R.I. Câmpeanu, PhD Thesis, University of London (1977).