J. Phys. B: At. Mol. Opt. Phys. **29** (1996) L465–L471. Printed in the UK

LETTER TO THE EDITOR

Annihilation in low-energy positron–helium scattering

P Van Reeth†, J W Humberston†, Koji Iwata‡, R G Greaves‡ and C M Surko‡

† Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

‡ Physics Department, University of California, San Diego, La Jolla, CA 92093, USA

Received 19 March 1996, in final form 24 April 1996

Abstract. Elaborate wavefunctions representing low-energy positron–helium elastic scattering, which were obtained in the course of calculating accurate values of the scattering phase shifts, are used to determine the electron–positron annihilation rate and the Doppler-broadened annihilation γ-ray spectrum. This spectrum is also measured using room-temperature positrons in a Penning trap and a non-Gaussian lineshape is observed for the first time. Excellent agreement is obtained between the theoretical spectrum and the present results.

An important and interesting feature of low-energy positron collisions with atoms and molecules is the possibility of annihilation of the positron with one of the electrons in the target. This has been the subject of extensive experimental (Iwata *et al* 1995, Heyland *et al* 1982, Coleman *et al* 1994) and theoretical (Drachman 1969, Humberston and Wallace 1972, McEachran *et al* 1977, Campeanu and Humberston 1977, Armour *et al* 1990) studies. Recent improvements in the scattering calculations (Van Reeth and Humberston 1995) and in the measurements obtained using positrons stored in a Penning trap, now enable us to make detailed comparisons between theoretical predictions and experimental measurements of positron annihilation in helium, the results of which are presented in this letter.

Experimentally, previous measurements in helium were performed in dense gases (Coleman *et al* 1975, 1994). Our measurements were performed in a Penning trap, where large numbers of positrons can be stored with well characterized energies. The system is ideal for studies of two-body interactions between a positron and an atom since it is operated at a low test gas pressure.

Annihilation into two γ-rays is far more probable than into three γ-rays. Assuming that the positrons are unpolarized, the annihilation rate in a gas is (Humberston 1979)

$$\lambda = \pi r_0^2 c n Z_{\mathrm{eff}} \qquad (1)$$

where $r_0 = e^2/(mc^2)$ is the classical radius of the electron, c the speed of light, n the number density of atoms and Z_{eff} the effective number of electrons in the target system. The value of Z_{eff}, which varies with the speed of the positron, is a measure of the probability of the positron being at the same position as one of the target electrons and is calculated from the elastic scattering wavefunction for the positron–target system as follows:

$$Z_{\mathrm{eff}} = N \int |\Psi(\boldsymbol{r}_1 = \boldsymbol{r}_2, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots, \boldsymbol{r}_{N+1})|^2 \, \mathrm{d}\boldsymbol{r}_2 \, \mathrm{d}\boldsymbol{r}_3 \ldots \mathrm{d}\boldsymbol{r}_{N+1} \qquad (2)$$

where $\boldsymbol{r}_1$ is the coordinate of the positron, $\boldsymbol{r}_2$, $\boldsymbol{r}_3, \ldots, \boldsymbol{r}_{N+1}$ are the coordinates of the N electrons in the target and Ψ is the wavefunction, normalized to unit positron density at infinity. The error in $Z_{\rm eff}$ is only of first order in the error in Ψ, whereas the error in the elastic scattering phase shifts is usually of second order in the error. Consequently, a calculated value of $Z_{\rm eff}$ is likely to be significantly less accurate than the phase shift and good agreement between the calculated value of $Z_{\rm eff}$ and an accurate experimental value, derived from measurements of the annihilation rate, is therefore an important test of the quality of the scattering wavefunction.

We have calculated $Z_{\rm eff}$ for positron–helium scattering, using the elaborate variational wavefunctions generated by Van Reeth and Humberston (1995) (see also Humberston and Van Reeth 1996). For s-wave scattering, the wavefunction is

$$\Psi_t = \frac{1}{\sqrt{4\pi}}\Phi_{\rm He}(\boldsymbol{r}_2, \boldsymbol{r}_3)\sqrt{k}\left\{j_0(kr_1) - \tan\eta_t n_0(kr_1)\left[1-\exp(-\delta r_1)\right]\right\} + \frac{1}{\sqrt{4\pi}}[1+P_{23}]\exp\left(-(\alpha r_1 + \beta r_2 + \beta r_3)\right)\sum_{i=1}^{N} c_i r_1^{k_i} r_2^{l_i} r_{12}^{m_i} r_3^{n_i} r_{13}^{p_i} r_{23}^{q_i} \qquad (3)$$

where P_{23} is the exchange operator for the two electrons, $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ etc and $\Phi_{\rm He}(\boldsymbol{r}_2, \boldsymbol{r}_3)$ is a very accurate approximation to the helium wavefunction, of the form

$$\Phi_{\rm He}(\boldsymbol{r}_2, \boldsymbol{r}_3) = \exp\left[-(\gamma(r_2+r_3))\right]\sum_{j=1}^{n} b_j (r_2+r_3)^{K_j}(r_2-r_3)^{M_j} r_{23}^{Nj} \qquad (4)$$

with 22 terms included in the summation. The most elaborate of these scattering wavefunctions, containing as many as 502 short-range correlation terms, give very accurate and well converged values for the phase shifts.

Positrons which thermalize in the helium gas at a temperature T before annihilation have a mean energy of $\frac{3}{2}kT$, with the value of 0.04 eV at T = 300 K. At such low energies the dominant contribution to $Z_{\rm eff}$ is from s-wave scattering and the only other contribution of any significance comes from the p-wave. Good polynomial fits to the dependence of these two partial-wave contributions to $Z_{\rm eff}$ on the positron momentum, k, over the range $0 \leqslant k < 0.4$ are given by

$$Z_{\rm eff}(l=0) = 3.9321 + 0.185\,84k - 19.563k^2 + 46.670k^3 - 38.212k^4 \qquad (5)$$

$$Z_{\rm eff}(l=1) = 3.8741k^2 - 1.6910k^3 - 0.641\,17k^4 \qquad (6)$$

which are plotted, together with the total $Z_{\rm eff}$, in figure 1. The experimental value of $Z_{\rm eff}$ is an average over the Maxwell–Boltzmann speed distribution of the positrons and we have therefore convoluted the total theoretical $Z_{\rm eff}$ with this speed distribution (Bhatia *et al* 1977) to give a value of $Z_{\rm eff} = 3.88 \pm 0.01$ at $T = 293$ K. This is in reasonable agreement with what is probably the most accurate experimental value of $Z_{\rm eff} = 3.94 \pm 0.02$ (Coleman *et al* 1975).

In the frame of reference of the centre of mass of the electron–positron pair, the two γ-rays produced in the annihilation of the spin singlet state both have the same energy, $E_0 = h\nu_0 = mc^2 = 511$ keV and they emerge in opposite directions; that is, the angle between them is π. In the laboratory frame of reference, however, the velocity of the centre of mass is $\boldsymbol{v}$ and the momentum of the electron–positron pair is therefore $\boldsymbol{p} = 2m\boldsymbol{v}$. Consequently the two γ-rays are Doppler shifted to other energies, $E_1 = h\nu_1$ and $E_2 = h\nu_2$ and the angle between their directions becomes $(\pi - \theta)$, as illustrated in a greatly exaggerated manner in figure 2. (In reality θ is typically a few milliradians.) Measurements of the energy shift and the angle θ have both been used previously in experimental investigations

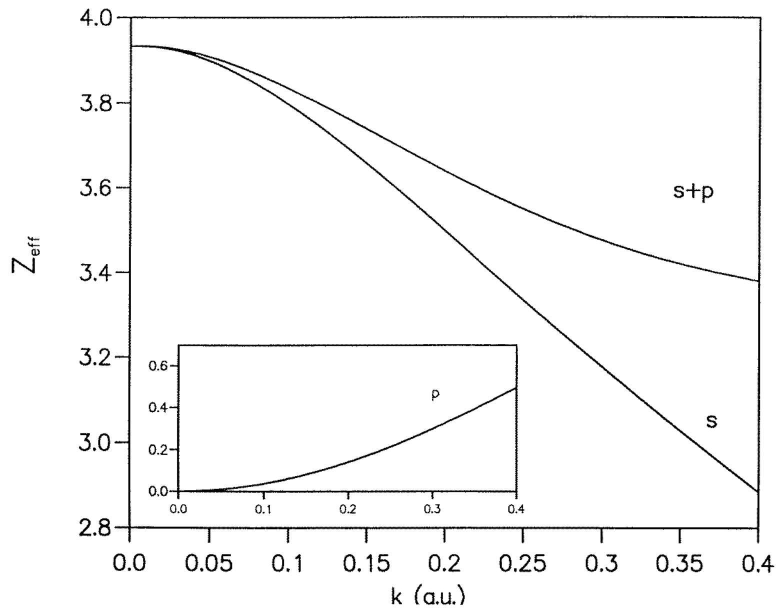

Figure 1. The theoretical dependence of Z_{eff} on the positron momentum.

of the momentum distribution of the annihilating electron–positron pair (Shizuma *et al* 1978, Coleman *et al* 1994).

In the centre-of-mass frame of reference, the momenta of the two annihilation γ-rays are both of magnitude $E_0/c = mc$ and their directions may be taken to be along the positive and negative y-axis. Also, the velocity of the centre of mass in the laboratory frame may be taken to be in the x–y plane and making an angle α with the positive x-axis, as shown in figure 2. Under the non-relativistic transformation to the laboratory frame of reference, the momenta of the two γ-rays become

$$\boldsymbol{p}_1 = mc\hat{\boldsymbol{j}} + m\boldsymbol{v} \qquad \text{and} \qquad \boldsymbol{p}_2 = -mc\hat{\boldsymbol{j}} + m\boldsymbol{v} \tag{7}$$

where $\hat{\boldsymbol{j}}$ is a unit vector along the y-axis. To first order in v/c,

$$p_1 = mc + mv\sin\alpha = mc + \tfrac{1}{2}p_y \qquad \text{and} \qquad p_2 = mc - mv\sin\alpha = mc - \tfrac{1}{2}p_y \tag{8}$$

where $p_y = 2mv\sin\alpha$ is the y-component of the momentum of the electron–positron pair. The Doppler shift in the energy of one of the γ-rays is therefore

$$\Delta E_1 = (E_1 - E_0) = c(p_1 - mc) = \tfrac{1}{2}cp_y\,. \tag{9}$$

The angle between the two γ-rays in the laboratory frame of reference is $(\pi - \theta)$ and, from figure 2,

$$\theta = \theta_1 + \theta_2 = \frac{mv\cos\alpha}{mc} + \frac{mv\cos\alpha}{mc} = \frac{p_x}{mc} \tag{10}$$

where $p_x = 2mv\cos\alpha$ is the x-component of the momentum of the electron–positron pair.

In an isotropic system such as this, all directions of the total momentum of an annihilating electron–positron pair with a given magnitude, p, are equally likely. Therefore, all components of momentum have the same distribution function, which may be obtained from either the distribution function for ΔE, equation (9), or the angular correlation function for the angle $(\pi - \theta)$ between the two γ-rays, using equation (10). From these two equations,

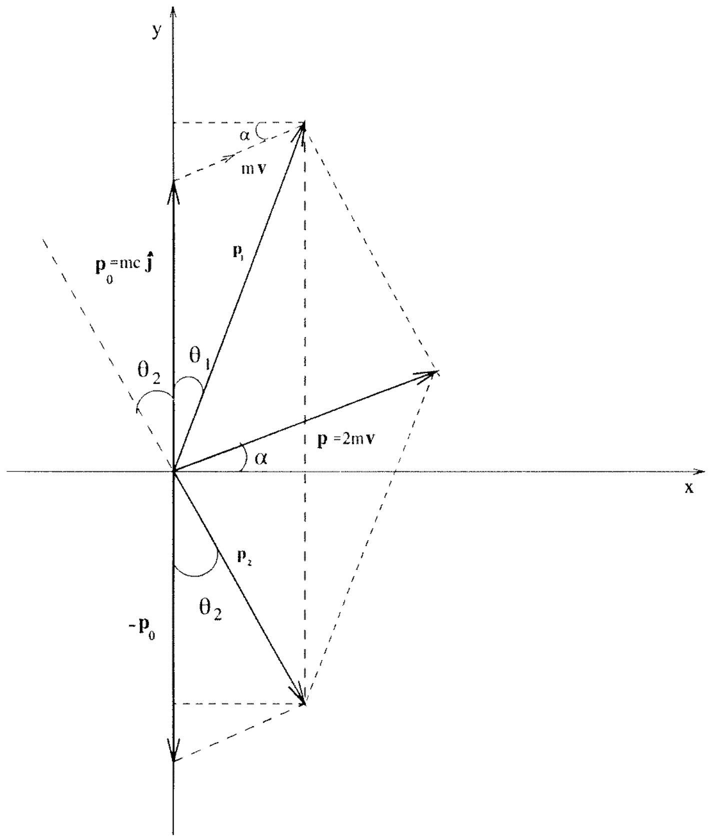

Figure 2. Illustration of the relationships between the momenta of the annihilation γ-rays in the centre-of-mass coordinate system and in the laboratory system.

the relationship between the value of one component of the centre-of-mass momentum and ΔE and θ is

$$\frac{1}{2}cp_x = \Delta E = mc^2\frac{\theta}{2}\,. \tag{11}$$

The probability of the two γ-rays emerging with the angle between them in the range $(\pi - \theta)$ to $(\pi - (\theta + \mathrm{d}\theta))$ is $F(\theta)\,\mathrm{d}\theta$, where $F(\theta)$ is the angular correlation function. This is calculated from the elastic scattering wavefunction in the following manner (Humberston 1979):

$$F(\theta) \propto \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Gamma(p_x = mc\theta,\, p_y,\, p_z)\,\mathrm{d}p_y\,\mathrm{d}p_z \tag{12}$$

where $\Gamma(\boldsymbol{p})$ is the momentum distribution function of the annihilating electron–positron pair, which for the positron–helium system has the form

$$\Gamma(\boldsymbol{p}) = \int \mathrm{d}\boldsymbol{r}_3 \left| \int \exp(-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_2)\Psi(\boldsymbol{r}_1 = \boldsymbol{r}_2, \boldsymbol{r}_2, \boldsymbol{r}_3)\,\mathrm{d}\boldsymbol{r}_2 \right|^2. \tag{13}$$

Instead of expressing the distribution function in terms of θ, it can be given as a function of the γ-ray energy $E = m_0c^2(1 + \frac{1}{2}\theta) = 511(1 + \frac{1}{2}\theta)$ keV.

Our experimental measurements of γ-ray spectra were performed in a Penning trap designed to accumulate, store and manipulate large numbers of room-temperature positrons (Surko *et al* 1989, Greaves *et al* 1994). A schematic diagram of the apparatus is shown in figure 3. High-energy positrons emitted from a 60 mCi ^{22}Na source are slowed in a solid neon moderator (Mills and Gullikson 1986, Greaves and Surko 1996) to a few eV. They are then guided through a magnetic beam line into the trap where they experience inelastic collisions with nitrogen buffer gas molecules. The inelastic collisions result in the positrons being trapped axially in a potential well imposed by an electrode structure and radially by a uniform magnetic field of 1 kG and they are cooled to room temperature within the order of a second. The positron loading rate is 1–2 $\times$ 10^6 s^{-1} and the positron lifetime is typically 30 s in the presence of the buffer gas. If the buffer gas feed is switched off after the positrons have been loaded, the positron lifetime is limited by annihilation on impurities in the vacuum system, but can be as long as 1 hour if the impurities are reduced by filling the cold trap, shown in figure 3, with liquid nitrogen.

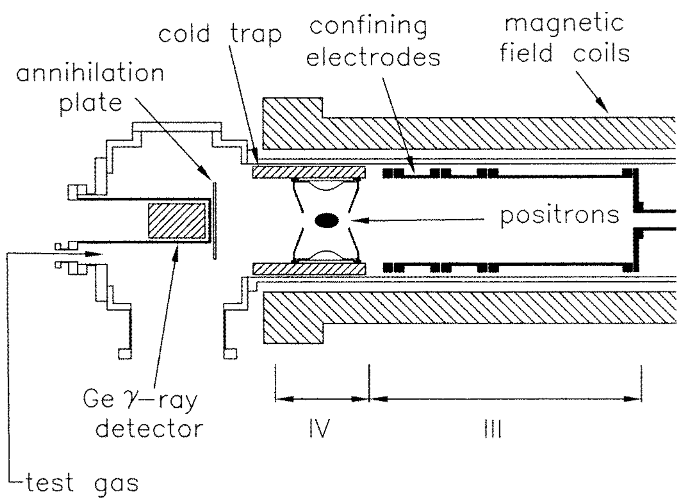

Figure 3. A schematic diagram of the positron trap showing the final two stages.

The γ-ray spectrum was obtained using a similar technique to the previous measurements by Tang *et al* (1992), but with various improvements in the experimental geometry and gas handling system. These improvements have enhanced the signal-to-noise ratio by about two orders of magnitude over our earlier measurements and the installation of a high-capacity cryogenic pump has enabled us to obtain annihilation data for helium for the first time in the trap. A detailed account of the measurements is in preparation (Iwata *et al* 1996). The experiment is operated with repetitive cycles of positron filling and annihilation as follows. Positrons are loaded into the positron trap for 30 s in the presence of the N_2 buffer gas. The buffer gas feed is then switched off, followed by an 8 s pump-out delay. The intrinsic Ge detector shown in figure 3 is then gated on before the helium gas is admitted into the system. The spectrum is accumulated for 30 s and the helium gas feed is then turned off. This cycle is repeated for 2 hours, after which time the cryogenic pumps become saturated and stop functioning. The observed spectrum, which contains a total of 9 $\times$ 10^4 γ-ray counts in the peak, also contains the detector response, which is accurately approximated with a combination of a Gaussian with FWHM of 1.16 keV and a step function convolved with the same Gaussian. (The step function in the detector response is due to Compton scattering in the Ge crystal.) The spectrum is plotted in figure 4(*a*) with the step function subtracted. A Gaussian function is fitted to the spectrum (the broken curve in figure 4(*a*)), resulting in a FWHM of 2.50 ± 0.03 keV with the detector response deconvoluted. As indicated by the residuals in figure 4(*b*), the Gaussian does not give a very good fit with χ^2/(degrees of freedom) = 4.7 instead of approximately unity if the model of the Gaussian fit were appropriate. A Gaussian form has been assumed in the analysis of the previous experimental data, but it has no proper theoretical basis. The non-Gaussian shape of the present experimental spectrum is evident from figure 4(*a*) and it demonstrates the high precision of our measurement.

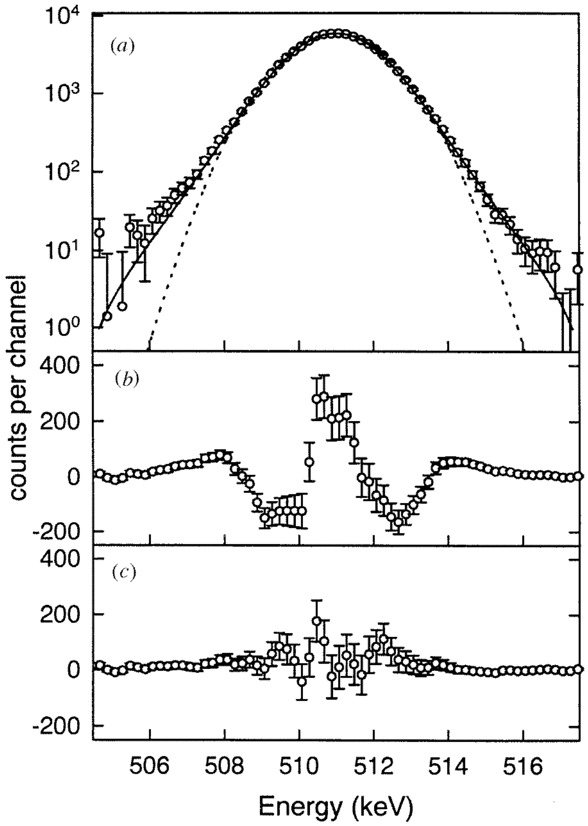

Figure 4. (*a*) Annihilation γ-ray spectrum for positrons interacting with helium atoms, as measured in the laboratory frame of reference. Full curve: theoretical prediction convolved with the response of the Ge detector; broken curve: Gaussian function fitted to the experimental data; ($\circ$), experimental measurements. (*b*) Residuals from the Gaussian fit. (*c*) Residuals from the theoretical calculation.

Before making a comparison between the theoretical and experimental distribution function, the theoretical data calculated at a positron energy of 0.04 eV were convoluted with the energy resolution function of the detector. The results, normalized to the experimental data, are shown in figure 4(*a*) as a full curve with the residuals in figure 4(*c*). We have chosen to convolute the theoretical data rather than to deconvolute the experimental data because the latter procedure was found to be numerically unstable and therefore less reliable. The agreement between the convoluted theory and experiment extends over three orders of magnitude without using fitting parameters and we find the value of χ^2/(degrees of freedom) = 1.2.

Previous measurements of the momentum distribution of the annihilating electron–positron pair mainly used the angular correlation of annihilation radiation (ACAR) technique (Stewart *et al* 1990, Coleman *et al* 1994). The angular correlation of the two γ-rays resulting from annihilation is measured using two narrow slits, but high angular resolution is achieved at the expense of count rate. In the experiment of Coleman *et al* (1994), carried out in rare dense gases, high-energy positrons are emitted directly from a source into the gas cell. This produced a significant γ-ray component from the annihilation of positronium atoms. Their FWHM in the angular correlation of the free-positron component of the annihilation radiation was obtained by fitting two Gaussians to the spectrum, yielding a value of 10.30 ± 0.05 mrad (2.63 ± 0.01 keV) for the free positron component. The experiment in liquid helium by Stewart *et al* (1990) yielded a linewidth of 9.4 ± 0.5 mrad (2.4 ± 0.1 keV). In neither of these experiments were the data sufficiently good to resolve the non-Gaussian features of the lineshape that we have observed here. Shizuma *et al* (1978) measured the γ-ray spectrum in noble gases using a Ge γ-ray detector and from the data that they presented for helium at atmospheric pressure, we estimate the FWHM of their annihilation line to be 2.0 ± 0.1 keV.

In summary, we have obtained a new theoretical estimate for the annihilation rate of positrons in helium gas and find good agreement with previously measured values. Furthermore, excellent agreement is obtained between our theoretical and experimental estimates of the γ-ray annihilation spectrum for the helium atom. This agreement provides evidence of the accuracy of both the positron–helium wavefunction used in these calculations and the experimental data.

PVR acknowledges receipt of an EPSRC Research Studentship. We thank Dr M Charlton for several helpful discussions and Mr E A Jerzewski and Dr C Kurz for technical assistance in the experiments. The experimental part of this work was supported by the National Science Foundation under grant no PHY-9221283.

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