Comments and Addenda

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Annihilation during positron-hydrogen collisions: Addendum and erratum

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The p-wave contribution to the positron-hydrogen annihilation rate, in terms of Z_{eff}, is corrected from a previous calculation of the authors, thereby removing the discrepancy with later calculations of Chan and McEachran. The present results should be the most accurate available. This opportunity is taken to give thermally averaged positron-hydrogen annihilation coefficients $\bar{Z}(T)$, which are of use in the analysis of solar-flare observations of the positron-electron annihilation line. For reference and experimental purposes we also present curves of the integrated elastic and momentum-transfer (i.e., diffusion) cross sections, as well as effective cross sections which account for the finite acceptance angle of the detector.

I. INTRODUCTION

Observations of the 0.51-MeV positron-electron annihilation line in solar flares[1] can be used to infer properties of the flare as well as the solar atmosphere itself,[2] provided the relevant positron cross sections are known. One process of potential importance is the annihilation in flight of positrons by atomic hydrogen. That quantity can be readily calculated from the wave function for positron-hydrogen scattering; however, for most astrophysical applications it is more useful to have the relevant quantity averaged over a Maxwellian distribution of positrons for different temperatures T.

In a previous paper[3] we calculated the effective annihilation cross section; it is the purpose of this note to present the Maxwellian averages. However, we take the opportunity to correct results of the p-wave contribution to the annihilation cross section in which our previous calculation[3] was in error. It has turned out that the correction of this error has necessitated a rather extensive recalculation.

The annihilation rate in flight is usually expressed in terms of an effective number of electrons, Z_{eff}, times the Dirac rate for free positron-electron annihilation. The quantity Z_{eff} is influenced by the interaction of the positron with the atomic system; thus it differs from the number of orbital electrons, approaching the latter only in the limit of high energy. For low-energy scattering we may conveniently calculate Z_{eff} in partial-wave components,

$$Z_{\text{eff}} = \sum_{L=0}^{\infty} Z_{\text{eff}}(L), \tag{1.1}$$

where

$$Z_{\text{eff}}(L) = \int d\vec{r}_1\, d\vec{r}_2\, |\Psi_L(\vec{r}_1, \vec{r}_2)|^2 \delta(\vec{r}_1 - \vec{r}_2) \tag{1.2}$$

and Ψ_L of the Lth partial wave function of the positron-hydrogen system. ($\vec{r}_1$ and $\vec{r}_2$ represent the positron and orbital-electron coordinates, respectively.)

II. RECALCULATION AND RESULTS

Our previous calculation of Z_{eff} was based on precision s-wave[4] and p-wave[5] e^+-H scattering calculations. These calculations were done using the Feshbach formalism[6] with generalized Hylleraas correlation functions. Briefly (the reader is referred to Refs. 5 and 6 for details), the wave function is broken into two parts,

$$\Psi_L = P\Psi_L + Q\Psi_L; \tag{2.1}$$

however, when this was done for p waves ($L=1$), it unfortunately happened that $Q\Psi_1$ was not correctly normalized relative to $P\Psi_1$. Equation (1.2) assumes the latter to approach the p component of a plane wave

TABLE I. p-wave contribution to e^+ –H annihilation.

k \ $2N(\omega)\rightarrow$	$Z_{\rm eff}(1)$ 70(5)	112(6) This calculation	168(7)	Chan and McEachran[a]	Humberston[d]	Final results $Z_{\rm eff}$(total)	ν_1 cusp, Eq. (2.4), This calculation
0						8.868[c]	
0.1	0.12109	0.130 08	•••	0.104	0.1335	7.493	−0.464
0.2	0.502 13	0.527 04	0.539 94	0.429	0.5366	6.079	−0.478
0.3	1.066 25	1.102 764	1.124 41	0.901	1.114	5.312	−0.484
0.4	1.683 11	1.734 21	1.762 92	1.40	1.719	5.100	−0.487
0.5	2.221 11	2.312 96	2.339 10	1.84	2.353	5.091	−0.484
0.6	2.724 75	2.828 00	2.849 88		2.823	5.168	−0.485
0.7	3.367 58	3.553 43	3.670 30		3.637	5.683	−0.482

[a] Reference 7.
[b] $Z_{\rm eff}(0)+Z_{\rm eff}(>1)$ from Ref. 3 plus $Z_{\rm eff}(1)$ from present calculation.
[c] $k=0$ result from S. K. Houston and R. J. Drachman (unpublished) (cf. Ref. 3).
[d] Reference 8.

$$\lim_{r_1\to\infty}\Psi_1 = P\Psi_1 = (12\pi)^{1/2}[u(r_1)/r_1]Y_{10}(\Omega_1)\varphi_0(r_2)\,, \tag{2.2}$$

where

$$\lim_{r_1\to\infty} u(r_1) = (1/k)\sin(kr_1 - \tfrac{1}{2}\pi + \eta_1)\,. \tag{2.3}$$

Although the erroneous normalization of $Q\Psi_1$ relative to $P\Psi_1$ is not involved in (and therefore does not affect) the scattering calculation itself,[5] it does require a completely new evaluation of $Z_{\rm eff}(1)$. To make matters worse, however, the tape on which Ψ_1 was stored went bad, so that we had to recalculate the whole scattering wave function Ψ_1. (The phase shifts did completely check Ref. 5, but 12 hours of IBM 360/91 time were consumed!) It should be stated that our evaluation of $Z_{\rm eff}(L=0)$ was done correctly.[3]

In Table I we give our new results versus the total number of terms $2N$, where N is the number of terms (such that $l+m+n\leq\omega$) in each symmetry needed to describe Ψ_1 (cf. Ref. 5 for details). We have found no reliable extrapolation formula, which undoubtedly is caused by the nonvariational nature of $Z_{\rm eff}$.

We also give in Table I results of Chan and McEachran, and unpublished calculations of Humberston,[8] which showed unequivocally that our original p-wave calculation of $Z_{\rm eff}(1)$ was in error.

In the last column we give the value of the cusp condition

$$\nu_1 = \frac{\langle\Psi_1|\delta(\vec{r}_1-\vec{r}_2)|\partial\Psi_1/\partial r_{12}\rangle}{\langle\Psi_1\delta(\vec{r}_1-\vec{r}_2)\Psi_1\rangle}\,. \tag{2.4}$$

For an exact wave function, $\nu_1=-\frac{1}{2}$ according to Kato's theorem.[9] We remarked in Ref. 3 that the value for the cusp that we were getting there (~ -0.19) was difficult to understand. It turns out that the same relative normalization problem affected the earlier evaluation of ν_1 also.[3] The corrected values are seen to be quite satisfactory.

Using the values of $Z_{\rm eff}(k)$ given in Table I, we can now compute the thermally averaged annihilation parameter

$$\overline{Z}(T) = \int_0^\infty dk\, f_T(k) Z_{\rm eff}(k)\,, \tag{2.5}$$

where $f_T(k)$ is the Maxwell-Boltzmann distribution function, given in atomic units by

$$f_T(k) = (4A^{3/2}/T)k^2 e^{-Ak^2}\,,$$
$$A = \hbar^2(2ma_0^2kT)^{-1} \equiv A_0/T_4\,, \tag{2.6}$$

where T_4 is the temperature in units of 10^4 K and $A_0=15.789$. Although strictly speaking the Maxwellian distribution fails above the threshold, it may be used as long as the temperature is not too high (we have therefore confined the temperature to $T_4\leq 1$).

The calculated values of $Z_{\rm eff}(k)$ were fitted with a sixth-degree polynomial of the form

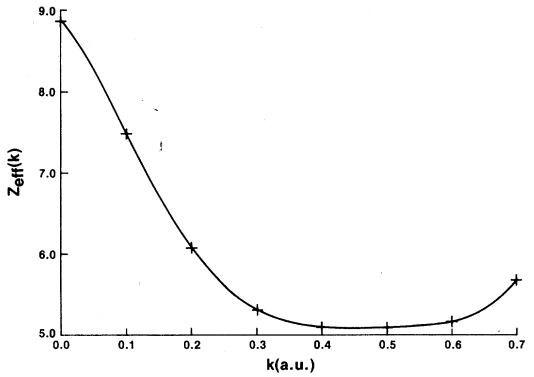

FIG. 1. Sixth-degree polynomial fit to the total $Z_{\rm eff}(k)$. The points are from Table I.

TABLE II. Coefficients of the polynomials describing the momentum and temperature dependence of the annihilation parameter: $Z_{\rm eff}(k)=\sum_{n=0}^{6} Z_n k^n$ and $\bar{Z}(T)=\sum_{n=0}^{6} \bar{Z}_n (T_4)^{n/2}$, where $\bar{Z}_n=\alpha_n Z_n A_0^{-n/2}$.

n	Z_n	$\bar{Z}_n$	α_n
0	8.868	8.868	1
1	−7.838	−2.226	$2\pi^{-1/2}$
2	−102.77	−9.763	$\frac{3}{2}$
3	527.38	18.971	$4\pi^{-1/2}$
4	−978.68	−14.722	$\frac{15}{4}$
5	773.15	5.284	$12\pi^{-1/2}$
6	−197.17	−0.658	$\frac{105}{8}$

$$Z_{\rm eff}(k)=\sum_{n=0}^{6} Z_n k^n \tag{2.7}$$

in order to perform the integral in Eq. (2.5) analytically. The fit shown in Fig. 1 is very smooth, without any unphysical oscillations; the derived coefficients are given in Table II. The integral in Eq. (2.5) then takes the form

$$\bar{Z}(T)=\sum_{n=0}^{6} Z_n \int_0^\infty dk\, f_T(k) k^n \equiv \sum_{n=0}^{6} \bar{Z}_n (T_4)^{n/2}. \tag{2.8}$$

Inserting $f_T(k)$ from (2.6) and carrying out the integrals analytically gives

$$\bar{Z}_n = \alpha_n Z_n A_0^{-n/2}, \tag{2.9}$$

where the α_N are also given in Table II.

The thermally averaged annihilation parameter $\bar{Z}(T)$ is plotted in Fig. 2. One should note that there are significant differences between $\bar{Z}(T)$ as given here and any approximation in which the mean energy $\bar{E}$ is simply assumed proportional to T in $Z_{\rm eff}(k)$. In particular, the natural choice of $\bar{E}=\frac{3}{2}k_B T$ underestimates $\bar{Z}(T)$ by as much as 8.2%,

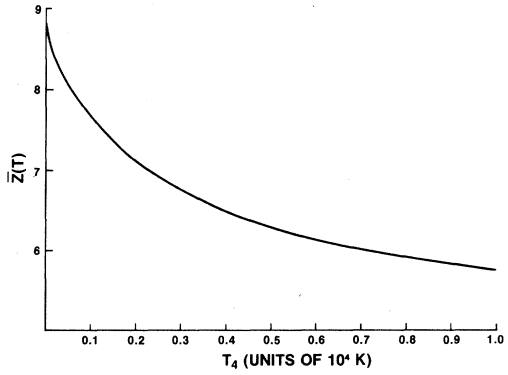

FIG. 2. Thermally averaged annihilation parameter $\bar{Z}(T)$ obtained from the polynomial fit to $Z_{\rm eff}(k)$.

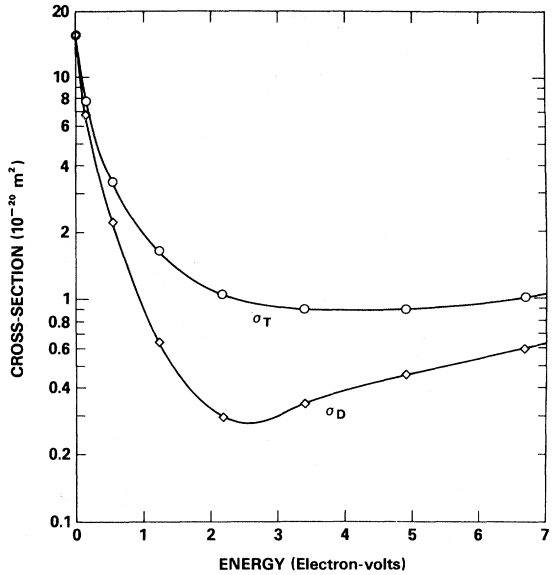

FIG. 3. Total elastic (σ_T) and diffusion (σ_D) cross sections for e^+-H scattering in units of 10^{-20} m^2 (Å^2).

while the choice of $\bar{E}=k_B T$, although better, overestimates $\bar{Z}(T)$ by 2.4% at $T=2\times10^3$ K and underestimates it by 2.7% at $T=10^4$ K.

Although, as we have indicated, accurate phase shifts for e^+-H scattering have now been calculated, actual cross-section curves based on these phase shifts have not yet been published. Using

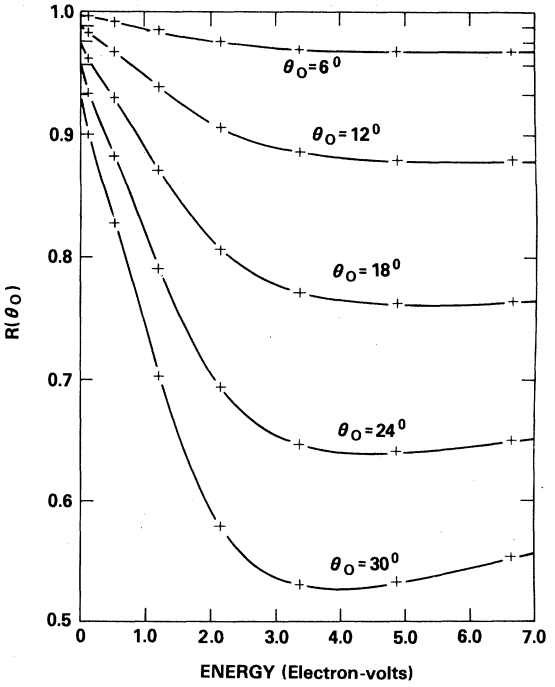

FIG. 4. Effective cross-section ratio $R(\theta_0)$ as a function of energy.

the essentially exact s-wave[4] and p-wave[5] phase shifts, the very good d-wave phase shifts given by a Kohn variational calculation,[10] and the effective range formula[11] for $3 \leq L \leq 9$, we have computed differential, total elastic, and diffusion (or momentum-transfer) cross sections up to the inelastic threshold at 6.8 eV, where

$$\sigma_T = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta, \tag{2.10}$$

$$\sigma_D = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} (1 - \cos\theta) \sin\theta \, d\theta. \tag{2.11}$$

We will not present the results for $d\sigma/d\Omega$ but will simply note that for all but the lowest energies it is strongly peaked in the forward direction, with one deep minimum occurring at an angle that depends on energy. In Fig. 3 we show the results for σ_T and σ_D; the latter becomes quite small because of the forward peaking mentioned above.

The forward scattering peak also implies that in experimental transmission experiments the inferred total cross section will be substantially underestimated if the acceptance angle of the detector is too large. Figure 4 gives the ratio of inferred to true cross sections as a function of the acceptance angle θ_0, where

$$R(\theta_0) = \frac{2\pi}{\sigma_T} \int_{\theta_0}^\pi \frac{d\sigma}{d\Omega} \sin\theta \, d\theta / \sigma_T. \tag{2.12}$$

From Fig. 4 we see that $R(\theta_0)$ is strongly energy dependent and is significantly different from unity for $\theta_0 \gtrsim 10°$.

We hope that the results presented here will be useful as the experimental positron-scattering programs turn towards the difficult atomic hydrogen target.

ACKNOWLEDGMENT

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