Annihilation during positron-hydrogen collisions

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(Received 20 September 1973)

Using the precision s- and p-wave elastic-scattering wave functions obtained previously, we have calculated the annihilation rate for positrons colliding with hydrogen atoms below the positronium-formation threshold. The s-wave results agree well with those of Humberston, while the p-wave results, which are new, contribute about 20% of the total at the higher energies.

I. INTRODUCTION

In two previous papers,[1,2] generalized Hylleraas wave functions were used in rigorous lower-bound calculations of the s-wave[1] and p-wave[2] phase shifts for positron-hydrogen elastic scattering. One of the interesting by-products of such a calculation is the annihilation cross section, which can be obtained in first-order perturbation theory, and which gives an additional test of the accuracy and reliability of the calculation.

Although annihilation calculations have been reported frequently[3] for the positron-helium system (which is under experimental examination[4]) only two such results[5,6] have been reported for atomic hydrogen, a much more difficult experimental subject. Nevertheless, it seems quite worthwhile to report the results corresponding to two very accurate wave functions.

II. FORMULATION

The partial cross section for annihilation of an incoming positron and an atomic electron with the emission of two gamma rays is[7]

$$\sigma_a = Z_{\rm eff}\alpha^3 k^{-1}(\pi a_0^2) , \tag{1}$$

where $\alpha = e^2/\hbar c$ is the fine-structure constant, $a_0 = \hbar^2/me^2$ is the Bohr radius, and k is the positron's asymptotic wave number in units of a_0^{-1}. The quantity $Z_{\rm eff}$ depends on specific properties of the positron-atom system and approaches Z, the number of atomic electrons, when the positron can be represented as a free particle. For hydrogen,

$$Z_{\rm eff} = \int\int d\vec{r}_1 d\vec{r}_2 |\Psi(\vec{r}_1\vec{r}_2)|^2 \delta(\vec{r}_1 - \vec{r}_2) , \tag{2}$$

where $\Psi(\vec{r}_1, \vec{r}_2)$ is the positron-hydrogen scattering wave function; $Z_{\rm eff}$ measures the probability that the positron and electron are at the same point.[8] In the noninteracting limit, for positron wave number k,

$$\Psi(\vec{r}_1, \vec{r}_2) = e^{i\vec{k}\cdot\vec{r}_1}\phi_0(r_2) , \tag{3}$$

where ϕ_0 is the hydrogen ground-state wave function, and $Z_{\rm eff} = 1$, independent of k. To compute $Z_{\rm eff}$ as a function of k one simply normalizes the numerically obtained function Ψ to the asymptotic form given in Eq. (3) and applies Eq. (2).

The s- and p-wave ($L = 0, 1$) scattering functions are represented as follows[1,2]:

$$\Psi_L = \{[U_L(r_1)]/r_1\} Y_{L0}(\Omega_1)\phi_0(r_2) + Q\Phi_L(\vec{r}_1\vec{r}_2) , \tag{4}$$

where

$$Q\Phi_L = \Phi_L - \phi_0(r_2)\int d\vec{r}_2' \phi_0(r_2')\Phi_L(\vec{r}_1, \vec{r}_2') . \tag{5}$$

For s waves[1] the correlation function is

$$\Phi_0 = e^{-\alpha r_{12}} f_{10} Y_{00}(\Omega_1) \tag{6a}$$

and for p waves,[2]

$$\Phi_1 = [f_{11}\cos(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1+}(\vec{\beta}) + f_{21}\sin(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1-}(\vec{\beta})](2\pi)^{1/2}, \tag{6b}$$

where

$$f_{iL} = e^{-(\delta_{iL}r_1 + \gamma_{iL}r_2)} r_i^L \sum_{l,m,n\geq 0} C_{lmn}^{iL} r_1^l r_2^m r_{12}^n . \tag{7}$$

The $\vec{\beta}$'s are symmetric Euler angles, and the $\mathfrak{D}$'s are rotational harmonics of appropriate type.[9] The normalization of Eq. (3) requires that

$$U_L(r) \sim [4\pi(2L+1)]^{1/2} k^{-1}\sin(kr - \tfrac{1}{2}(L\pi) - \eta_L) . \tag{8}$$

To evaluate the wave function for $L = 1$ at $\vec{r}_1 = \vec{r}_2$, we note that[9]

$$\cos(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1+}(\vec{\beta}) = (8\pi)^{-1/2}[Y_{10}(\Omega_1) + Y_{10}(\Omega_2)],$$
$$\sin(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1-}(\vec{\beta}) = (8\pi)^{-1/2}[Y_{10}(\Omega_1) - Y_{10}(\Omega_2)], \tag{9}$$

and hence the second term in Eq. (6b) vanishes in the limit, while the first simplifies. The final result is

$$Z_{\rm eff}(0+1) = \sum_{L=0,1}\int_0^\infty dr\{[U_L(r) - rI_L(r)] \times \phi_0(r) + rf_{1L}(r, r, 0)\}^2 , \tag{10a}$$

TABLE I. Z_{eff} as a function of positron wave number k. We quote the results of the present calculation to three decimal places, but do not imply convergence to that accuracy.

k	Z_{eff} (0)	Z_{eff} (0) (Ref. 5)	Z_{eff} (1)	Z_{eff} (>1) [Eq. (13)]	Z_{eff} (Total)
0.1	7.363	7.5	0.022	$<10^{-3}$	7.385
0.2	5.538	5.7	0.090	0.001	5.629
0.3	4.184	4.3	0.187	0.004	4.375
0.4	3.327	3.3	0.294	0.010	3.631
0.5	2.730	2.7	0.390	0.022	3.142
0.6	2.279	2.3	0.464	0.039	2.782
0.7	1.950	•••	0.528	0.063	2.541

where $I_L(r)$ is related to the integral in Eq. (5):

$$I_L = \int d\Omega \int d\vec{r}_2' \phi_0(r_2)\Phi_L(\vec{r}, \vec{r}_2') \ . \tag{10b}$$

For completeness and possible comparison with experiment, it is desirable to estimate the contribution of higher partial waves ($L>1$) to the annihilation. This can be done by using the unscattered form and omitting the last two terms in Eq. (10). That is, $U_L = [4\pi(2L+1)]^{1/2} r j_L(kr)$ and

$$Z_{\text{eff}}(L>1) \simeq 4\pi \sum_{L=2}^{\infty} (2L+1) \int_0^{\infty} dr\, r^2 \phi_0^2(r) j_L^2(kr) \ . \tag{11}$$

Using the identity

$$\sum_{L=0}^{\infty} (2L+1) j_L^2 = 1 \ , \tag{12}$$

one can write

$$Z_{\text{eff}}(L>1) \simeq 4 \int_0^{\infty} dr\, r^2 e^{-2r}(1 - j_0^2 - 3j_1^2)$$

$$= \frac{k^2}{1+k^2} + \frac{6}{k^2}\left(\frac{1}{k^2}\ln(1+k^2) - \frac{1+\frac{1}{2}k^2}{1+k^2}\right) \ . \tag{13}$$

This correction is quite small and goes like $\frac{1}{2}k^4$ for small k.

III. RESULTS

In Table I we present our best-converged values of Z_{eff} for $L=0$ and $L=1$ as a function of k up to the inelastic threshold. For $L=0$ they are compared with the results of Humberston and Wallace[5]; the agreement is good, although it improves with increasing k. No zero-energy calculations were reported in Ref. 1, so we are unable to corroborate the zero-energy value[5] $Z_{\text{eff}}=8.9$, although an independent 84-term Kohn variational calculation[10] gave $Z_{\text{eff}}=8.868$. The analytic correction [Eq. (13)] for $L>1$ is evaluated and the best total Z_{eff} is also presented.

The convergence of Z_{eff} as the trial-function expansion length increases is illustrated in Tables II and III for two different values of k. In each case, the nonlinear parameters in the trial function are selected to maximize approximately the phase shift. Since no minimum principle holds for Z_{eff}, it is rather difficult to extrapolate the results toward an exact value, and we have preferred to present our best actual values in the Tables. It is interesting to notice, however, the difference in possible convergence behavior: for $L=0$ and $k=0.1$, Z_{eff} is seen to increase monotonically with N, while for $k=0.6$ some oscillation is observed. In the former type of case, it seemed reasonable to assume the convergence to follow approximately the formula

$$(\eta_\infty - \eta_N)^{1/2} \propto [Z_{\text{eff}}(\infty) - Z_{\text{eff}}(N)], \tag{14}$$

since the phase-shift error is of second order in the wave-function error, while the error in Z_{eff} is of first order. This relation is fairly well obeyed for $k=0.1$ and 0.2, for which we obtain extrapolated values for Z_{eff} of 7.56 and 5.6, in better agreement with the results of Ref. 5. [For $k=0$, Eq. (14) is very well obeyed[10] and leads to an extrapolated value of 9.04.] Convergence for $L=1$ was always monotonic.

Schrader[11] has emphasized the importance of examining the "cusp value"

TABLE II. Convergence with increasing expansion length N of Z_{eff} (0) for two different values of k.

$N\rightarrow$	4	10	20	35	56
$k=0.1$	5.101	6.729	7.035	7.264	7.363
$k=0.6$	2.139	2.228	2.304	2.285	2.279

TABLE III. Convergence with increasing expansion length N of Z_{eff} (1) for two different values of k.

$N\rightarrow$	40	70	112	168
$k=0.2$	0.083	0.087	0.089	0.090
$k=0.6$	0.440	0.457	0.4637	0.4644

$$\nu_L = \langle \Psi_L | \delta(\vec{r}_1 - \vec{r}_2) \frac{\partial}{\partial r_{12}} | \Psi_L \rangle \Big/ \langle \Psi_L | \delta(\vec{r}_1 - \vec{r}_2) | \Psi_L \rangle , \tag{15}$$

which probes the accuracy of the trial function near the positron-electron coalescence point, and which should equal $-\frac{1}{2}$. (For $L>0$ certain angular averages must be taken[12]). We have computed ν_0 and ν_1 from the wave functions of Refs. 1 and 2 and find good convergence for $L=0$; typically our best-converged wave functions give $\nu_0 = -0.494 \pm 0.010$. We were unable to obtain reasonable results, however, for $L=1$: our best-converged wave functions give $\nu_1 \approx -0.19$. We do not understand this discrepancy, and can only remark that similar difficulties show up in $L=1$ helium bound states.[13] Because the convergence in N is reasonable, however, we believe our values for Z_{eff} are meaningful.

The numerical calculations reported here were programmed by H. Eiserike, whom we should like to thank.

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