$e^+ + H$ direct annihilation above the positronium formation threshold

C-.Y. Hu, D. Caballero, A. Forrester and Z. Papp[1]

[1] *Department of Physics and Astronomy, California State University, Long Beach, California 90840*

(Dated: October 12, 2004)

A long-standing problem with the solution of the Schrödinger equation has been its inability to account for the electron-positron annihilation in positron hydrogen scattering above the positronium formation threshold. This letter shows that this problem has been resolved by the use of the modified Faddeev equations. A number of e^-e^+ annihilation cross sections in the energy gap between $Ps(1s)$ and $H(n=2)$ thresholds are reported for both the positron plus hydrogen incoming channel as well as the proton plus positronium incoming channel. However the indirect annihilation cross sections after formation of the positronium themselves are well known, they will not be included in this report.

PACS numbers: 36.10.Dr, 34.90.+q

arXiv:physics/0410071 v1 12 Oct 2004

When the possibility of e^+e^- annihilation in flight is neglected the $e^+ + H$ collision in the energy region between $Ps(1s)$ and $H(n=2)$ thresholds can have only two open channels. They are: the elastic channel and the rearrangement channel, where the e^+ capture the electron from H and form a positronium in $Ps(1s)$. Under this assumption annihilation can occur only after the formation of the positronium. The lifetime of the $Ps(1s)$ is known to depend on the total spin S. The singlet para-Ps, $^1S_0$, decays into 2γ rays with a lifetime $\tau \approx 0.13ns$. The triplet ortho-Ps, $^3S_1$, decay into 3γ rays with $\tau \approx 140ns$ [1]. These well known annihilation will not be included in this report. We calculate the e^+e^- direct annihilation using the standard relation [2]

$$\sigma_{an} = \pi r_0^2 (c/v) Z_{\text{eff}}, \tag{1}$$

$r_0 = e^2/m_e c^2$, Z_{eff} is the annihilation coefficient defined by

$$Z_{\text{eff}} = \langle \Psi | \delta(\vec{r}) \Psi \rangle, \tag{2}$$

$\vec{r}$ is the distance between e^+e^- in the three-body wave function Ψ. The calculation of e^+e^- in flight thus compensate for the shortcoming of the quantum three-body calculation where the annihilation channel is closed.

The modified Faddeev equation [3, 4] explicitly separates the three-body wave function into the direct channel and the rearrangement channel

$$\Psi = \Psi_1(\vec{x}_1, \vec{y}_1) + \Psi_2(\vec{x}_2, \vec{y}_2). \tag{3}$$

Here $\vec{x}_\alpha, \vec{y}_\alpha$, $\alpha = 1, 2$ are the corresponding mass-scaled Jacobi vectors [4] defined by

$$\begin{aligned} \vec{x}_\alpha &= \tau_\alpha(\vec{r}_\beta - \vec{r}_\gamma) \\ \vec{y}_\alpha &= \mu_\alpha \left(\vec{r}_\alpha - \frac{m_\beta \vec{r}_\beta + m\gamma \vec{r}_\gamma}{m_\beta + m_\gamma} \right), \end{aligned} \tag{4}$$

where $(\alpha\beta\gamma)$ are cyclic permutations of (123), m_α and $\vec{r}_\alpha$ are the particle mass and position vectors,

$$\tau_\alpha = \sqrt{\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}}, \quad \mu_\alpha = \sqrt{2m_\alpha \left(1 - \frac{m_\alpha}{M}\right)}, \tag{5}$$

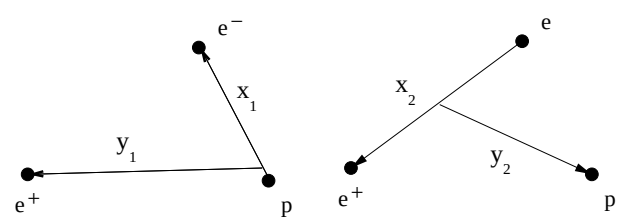

FIG. 1: Jacobi vectors in the $e^+ - H$ system.

and $M = m_\alpha + m_\beta + m_\gamma$.

The Jacobi vectors corresponding to different channels are related by the orthogonal transformation

$$\begin{pmatrix} \vec{x}_\alpha \\ \vec{y}_\alpha \end{pmatrix} = \begin{pmatrix} C_{\beta\alpha} & S_{\beta\alpha} \\ -S_{\beta\alpha} & C_{\beta\alpha} \end{pmatrix} \begin{pmatrix} \vec{x}_\beta \\ \vec{y}_\beta \end{pmatrix} \tag{6}$$

with

$$C_{\beta\alpha} = -\left[\frac{m_\beta m_\alpha}{(M - m_\beta)(M - m_\alpha)} \right]^{1/2}$$

and

$$S_{\beta\alpha} = (-)^{\beta-\alpha} \text{sgn}(\alpha - \beta)(1 - C_{\beta\alpha}^2)^{1/2}.$$

In this calculation we used the Jacobi vectors given in Fig. 1.

Using bipolar expansion we have

$$\psi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \sum_{\vec{l}+\vec{\lambda}=\vec{L}} \frac{\psi^L_{\alpha l\lambda}(x_\alpha, y_\alpha)}{x_\alpha y_\alpha} Y^{LM}_{l\lambda}(\hat{x}_\alpha, \hat{y}_\alpha) \tag{7}$$

where $\alpha = 1, 2$ and the bipolar basis is

$$Y^{LM}_{l\lambda}(\hat{x}_\alpha, \hat{y}_\alpha) = \sum_{m_l + m_\lambda = M} \langle l m_l \lambda m_\lambda | LM \rangle Y^{m_l}_l(\hat{x}_\alpha) Y^{m_\lambda}_\lambda(\hat{y}_\alpha).$$

Here L is the total angular momentum of the three-body system and l, λ are the relative angular momenta corresponding to the Jacobi vectors $\vec{x}_\alpha$ and $\vec{y}_\alpha$, respectively. The modified Faddeev equations for angular momentum L are given by

$$\left[H_{l\lambda}^{(\alpha)} + V_\alpha - E\right] \psi_{\alpha l\lambda}^L(x_\alpha, y_\alpha) + \sum_{\vec{l}'+\vec{\lambda}'} W_{l\lambda,l'\lambda'}^{\alpha L} \psi_{\alpha l'\lambda'}^L(x_\alpha, y_\alpha) = -V_\alpha^{(s)} \sum_{\vec{l}'+\vec{\lambda}'} (h_{l\lambda,l'\lambda'}^{\alpha\beta L} \psi_{\beta l'\lambda'}^L)(x_\alpha, y_\alpha), \tag{8}$$

where

$$H_{l\lambda}^{(\alpha)} = -\partial_{x_\alpha}^2 - \partial_{y_\alpha}^2 + \frac{l(l+1)}{x_\alpha^2} + \frac{\lambda(\lambda+1)}{y_\alpha^2},$$

V_α is the Coulomb potential,

$$W_{l\lambda,l'\lambda'}^{\alpha L} = \langle Y_{l\lambda}^{LM}(\hat{x}_\alpha, \hat{y}_\alpha) | \bar{V}_\alpha | Y_{l'\lambda'}^{LM}(\hat{x}_\alpha, \hat{y}_\alpha) \rangle,$$

$$\bar{V}_\alpha = V_3(x_3) + V_\beta^{(l)}(x_\beta, y_\beta)$$

$$V_\alpha^{(s)} = V_\alpha \zeta_\alpha(x_\alpha, y_\alpha)$$

$$V_\alpha^{(l)} = V_\alpha(1 - \zeta_\alpha(x_\alpha, y_\alpha)),$$

$$\zeta(x, y)) = 2\left\{1 + \exp\left[\frac{(x/x_0)^\nu}{1 + y/y_0}\right]\right\}^{-1},$$

x_0, y_0, $\nu > 2$ are the Merkuriev cut-off parameters, and

$$(h_{l\lambda,l'\lambda'}^{\alpha\beta L} \psi_{\beta l'\lambda'}^L)(x_\alpha, y_\alpha) = \int_{-1}^{1} dz_\alpha \; (h_{l\lambda,l'\lambda'}^{\alpha\beta L}(x_\alpha, y_\alpha, z_\alpha) \psi_{\beta l'\lambda'}^L(x_\beta, y_\beta)$$

where

$$\begin{aligned} h_{l\lambda,l'\lambda'}^{\alpha\beta L}(x_\alpha, y_\alpha, z_\alpha) \;=\; & \frac{(-)^{L+\lambda'}}{2} \sum_{k=0}^{(l+\lambda+l'+\lambda')/2} (-)^k (2k+1) P_k(z_\alpha) \sum_{l_1+l_2=l'} \sum_{\lambda_1+\lambda_2=\lambda'} (2l'+1)(2\lambda'+1) \\ & \times \sqrt{(2l+1)(2\lambda+1)} \left(\frac{2l'!2\lambda'!}{2l_1!2l_2!2\lambda_1!2\lambda_2!}\right)^{1/2} (-)^{\lambda_1} (c_{\beta\alpha})^{l_2+\lambda_1} (s_{\beta\alpha})^{l_1+\lambda_2} \frac{x_\alpha^{l_2+\lambda_2+1} y_\alpha^{l_1+\lambda_1+1}}{x_\beta^{l'+1} y_\beta^{\lambda'+1}} \\ & \times \sum_{l''\lambda''} (2l''+1)(2\lambda''+1) \begin{pmatrix} k & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & \lambda'' & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l'' & \lambda_2 & l_2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda'' & \lambda_1 & l_1 \\ 0 & 0 & 0 \end{pmatrix} \\ & \times \begin{pmatrix} l & \lambda & L \\ \lambda'' & l'' & k \end{pmatrix} \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda' \\ l_1 & l_2 & l' \\ \lambda'' & l'' & L \end{pmatrix}. \end{aligned}$$

The components $\psi_{\alpha l\lambda}(x_\alpha, y_\alpha)$ in (8) are further expanded in terms of quintic Hermite polynomial splines for each of the variables x_α, y_α. The wave functions are solved and normalized according to the asymptotic wave function [4, 5]

$$\psi^{(\sigma)} \sim f_\sigma + \sum_{\sigma'=1}^{\text{open channels}} \tilde{K}_{\sigma'\sigma} f^{\sigma'}. \tag{9}$$

In the Ore gap, the f's are the product of the standard spherical Bessel functions and the radial part of the bound-state hydrogenic wave functions. $\tilde{K}_{\sigma'\sigma}$ differs from the standard K-matrix elements $K_{\sigma'\sigma}$ by only a kinematic factor.

According to Fig. 1 and Eq. (2) annihilation takes place when $\vec{x}_2 = 0$. However, it is clear that the integrals in (2) diverge whenever $\psi_2(\vec{x}_2, \vec{y}_2)$ is involved. Thus, all previous calculations of Z_{eff} using (2) were limited to energies below the positronium formation threshold. Only recently, Ref. [6] used an imaginary absorption potential to replace the dynamics of e^-e^+ annihilation. In solving the Schrödinger equation they found the annihilation cross section below the $Ps(1s)$ threshold joins smoothly to the positronium formation cross section just above the threshold. But this imaginary potential is too week to represent the annihilation dynamics above and away from the $Ps(1s)$ threshold. According to this model, above the $Ps(1s)$ threshold only indirect annihilation after formation is possible. Ref. [7] renormalized the singularity in (2) near the $Ps(1s)$ threshold using the physical 2γ-lifetime of $Ps(1s)$. They also showed the smooth transition of the annihilation cross section across $Ps(1s)$ threshold. Theirs is essentially a threshold law, valid only near the threshold. Nevertheless, we will show that the integral

$$Z_{\text{inf}} = \langle \psi_1 | \delta(\vec{r}_2 | \psi_1 \rangle \tag{10}$$

is well defined and exists even above the $Ps(1s)$ threshold. In principle, the divergent part of (2) must be renormalized to the physical indirect annihilation cross section after the positronium is formed. This part is related to the positronium formation cross sections that we have already reported in [4, 8]. This report is devoted to the calculation of (10). To avoid confusion, we define (10) to be the annihilation coefficient of e^-e^+ annihilation in flight. Thus (10) truly represents the missing open channel, the neglected dynamics in the quantum mechanical solution (8) of the $e^+ + H$ system or other e^++ atom systems.

At $\vec{x}_2 = 0$, Eq. (6) gives

$$\vec{y}_1 = -C_{21}/S_{21}\vec{x}_1, \qquad \vec{y}_2 = -1/S_{21}\vec{x}_1,$$

and

$$Y^{LM}_{l\lambda}(\hat{x}_1, \hat{y}_1)|_{\vec{x}_2=0} = \sqrt{\frac{(2l+1)(2\lambda+1)}{4\pi}} \begin{pmatrix} l & \lambda & L \\ 0 & 0 & 0 \end{pmatrix} Y^M_L(\hat{y}_2),$$

where $Y^M_L(\hat{y}_2)$ is the spherical harmonic. Then,

$$\begin{aligned} Z_{\text{inf}} &= \int |\Psi_1(\vec{x}_1, -C_{21}/S_{21}\vec{x}_1)|^2 y_2^2 dy_2 d\Omega_{y_2} \qquad (11) \\ &= 4\pi\cos^2\delta \sum_{L=0}^{\infty}(2L+1)\sum_{l\lambda}\int dx_1 \frac{1}{|S_{21}|}\left[\frac{1}{|C_{21}|x_1}\sqrt{\frac{(2l+1)(2\lambda+1)}{4\pi}}\begin{pmatrix} l & \lambda & L \\ 0 & 0 & 0 \end{pmatrix}\Psi_{1\,l\lambda}^{\,L}(x_1, -C_{21}/S_{21}x_1)\right]^2, \end{aligned}$$

where δ is the phase shift of the scattering problem as a result of the normalization according to the asymptotic wave function (9).

When the incoming channel is $e^+ + H$, ψ_2 is solely responsible for all positronium formation cross section. When $p+Ps$ is the incoming channel, ψ_1 is responsible for all the hydrogen formation cross section . In either case, annihilation in flight calculated using (10) exists. Thus $Z_{1\text{inf}}$ and $Z_{2\text{inf}}$ are calculated for these two cases respectively. In Table I we present the $L = 0$ contribution to (11) for a number of k values in the Ore gap. Table II gives the corresponding annihilation cross sections. The point $k = 0.71a_0^{-1}$ is just above the positronium formation threshold, where the point $k = 0.8612a_0^{-1}$ is near a Feshbach resonance. Even though the S-state annihilation is relatively smooth in the Ore gap, the sudden increase near a Feshbach resonance is quite noticeable.

All calculations were carried out with a cut-off radii $y_1^{\max} = 125a_0$, $y_2^{\max} = 228a_0$, except near the Feshbach resonance where $y_1^{\max} = 150a_0$, $y_2^{\max} = 250a_0$ was used. Z_{inf} is very sensitive to the cut-off radii $y_1^{\max}$ and $y_2^{\max}$ especially when the energies are close to either the lower or upper thresholds. Converged results are obtained only for sufficiently large $y_1^{\max}$ and $y_2^{\max}$ values. This is demonstrated in Table III for the case $k = 0.71$, the $Ps(1s)$ formation threshold is located at $k = 0.70653$. In contrast, the scattering cross sections were well converged at a cut-off radii of less then $100a_0$ [4, 8], which were cross-checked by another method that solves the Faddeev-Merkuriev integral equations by using the Coulomb-Sturmian separable expansion approach [9] and by numerous previous calculations using the Schrödinger equation.

Calculations with considerable large cut-off radii require substantial computer resources, even for relatively low energies such as that used in the present calculations where all energies are inside the Ore gap between $H(n = 2)$ and $Ps(n = 1)$ thresholds. The three-body wave functions were obtained by using a quintic spline collocation procedure on the Jacobi coordinates [4, 5]. The dimension of the converged calculations have reached 175000. Calculations at much higher energies and near Feshbach resonances are quite demanding in terms of computer resources. Yet such calculations are important, for example in the creating of the antihydrogen and the studying of its spectroscopy. In the formation of antihydrogen using the process $\bar{p} + Ps \to \bar{H} + e^-$, e^-e^+ annihilation in the outgoing channel can be an important consideration when excited states are involved, where numerous Feshbach resonance exist.

Beyond the likely practical applications in antihydrogen research, this calculation represents the first breakthrough of a long-standing problem in positron-atom quantum scattering, i.e. its inability to account for the e^-e^+ annihilation above the positronium formation threshold. Using Schrödinger equation, the calculations in [6] are valid only in the immediate vicinity of the positronium formation threshold at $k = 0.70653a_0^{-1}$. The modified Faddeev equations enable the explicit separation of the $e^+ + H$ and the $p + Ps$ channels. The annihilation cross sections in the $e^+ + H$ channel are well defined by (10). The singularity involving the $p + Ps$ channels are renormalized to the indirect annihilation which can be calculated using the known physical annihilation cross sections of the positronium themselves and the respective positronium formation cross sections obtained in the solution of (8). Thus

TABLE I: S-state annihilation parameters in the Ore gap. The wave number k's are given in a_0^{-1} units, where a_0 is the Bohr radius.

k	0.71	0.75	0.80	0.85	0.8608	0.8612
Z_1	0.630	0.592	0.531	0.478	0.446	0.403
Z_2	1.699	1.417	0.749	1.055	1.367	7.632

TABLE II: S-state annihilation cross sections in the Ore gap. The σ's are given in $10^{-6}\pi a_0^2$ units.

k	0.71	0.75	0.80	0.85	0.8608	0.8612
σ_1	0.3446	0.3067	0.2578	0.2183	0.2010	0.1819
σ_2	0.9293	0.7337	0.3636	0.4820	0.6167	3.442

a quantum mechanical theory which includes the annihilation channel is obtained.

This work has been supported by the NSF Grant No.Phy-0243740 and by PSC and SDSC supercomputing centers under grant No. MCA96N011P.

TABLE III: S-state annihilation parameters at $k = 0.71$ with 6 pairs of cut-off radii.

$y_1^{\max}$	50	50	55	50	100	125
$y_2^{\max}$	120	150	174	180	228	228
Z_1	0.541	0.574	0.535	0.537	0.633	0.630
Z_2	0.406	101.8	2.128	0.471	1.766	1.699

[1] A. Rich, Rev. Mod. Phys. **53**, 127 (1981).
[2] P. A. Fraser, Adv. At. Mol. Phys. **4**, 63 (1968).
[3] S. P. Merkuriev, Ann. Phys. (NY), **130**, 395 (1980); L. D. Faddeev and S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems*, (Kluver, Dordrech), (1993).
[4] C-.Y. Hu, J. Phys. B: At. Mol. Opt. Phys. **32**, 3077 (1999).
[5] A. A. Kvitsinsky, C-.Y. Hu, J. Phys. B: At. Mol. Opt. Phys. **29**, 2059 (1996).
[6] A. Igarashi, M. Kimura and I. Shimamura, Phys. Rev. Lett., **89**, 123201 (2002)
[7] G. F. Gribakin and J. Ludlaw, Phys. Rev. Lett., **88**, 163202 (2002);
[8] A. A. Kvitsinsky, A. Wu, C-.Y. Hu, J. Phys. B: At. Mol. Opt. Phys. **28**, 275 (1995).
[9] Z. Papp, C-.Y. Hu, Z. T. Hlousek, B. Kónya and S. L. Yakovlev, Phys. Rev. A, **63**, 062721 (2001).