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Addendum to "Variational Bounds in Positron-Atom Scattering"

Richard J. Drachman

Laboratory for Theoretical Studies, Goddard Space Flight Center, National Aeronautics and Space Administration, Greenbelt, Maryland 20771

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Two additional positron-atom processes are treated using previously determined [Phys. Rev. 173, 190 (1968)] variational scattering functions: (1) Positronium formation in e^+-H collisions at threshold, and (2) the angular correlation between e^+-He annihilation quanta at zero energy. In case (1), we find a large reduction below the Born approximation, in qualitative agreement with other recent theoretical work. In case (2), very close agreement is found with the experiment of Briscoe *et al.*

(1) Let us recall from the title work (referred to below as I) the form of the approximate e^+ – H scattering function:

$$\Psi_k(\vec{x},\vec{r}) = [\chi_k(\vec{x}) + F(\vec{x})G(\vec{x},\vec{r})]\phi(r)\,, \qquad (1)$$

where χ and F were obtained variationally, ϕ is the ground state of hydrogen, and G is the first-order adiabatic correlation function.[1] This function describes elastic scattering only, but just at the threshold for positronium (Ps) formation (6.8 eV) it can give some information on the S-wave formation probability.

The matrix element for Ps formation can be written as

$$M_{kk'} = \iint d^3r d^3x\, e^{i\vec{k}'\cdot\vec{R}}\, t(\xi) V \Psi_k(\vec{x},\vec{r})\,, \qquad (2)$$

where $\vec{R} = \frac{1}{2}(\vec{x}+\vec{r})$ and $\vec{\xi} = \vec{x} - \vec{r}$ are the center of mass and internal coordinates of the Ps atom, respectively, $t(\xi) = (8\pi)^{-\frac{1}{2}} e^{-\frac{1}{2}\xi}$ is the ground-state function of Ps, while $V = 2(x^{-1} - r^{-1})$ is that part of the potential not already accounted for in the final-state wave function. The matrix element is difficult to evaluate, mainly due to the appearance of the mixed coordinates $\vec{R}$ and $\vec{\xi}$ arising from the rearranged channel, while the direct channel involves $\vec{x}$ and $\vec{r}$. At threshold ($k' = 0$), however, the integrand no longer involves $\vec{R}$ and simplifies considerably. The correlation function G is expressible in elliptical coordinates, so one can write, in terms of these coordinates,

$$M = \pi 2^{-1/2} \int_0^\infty dx [U_0(x) I(x) + g_0(x) J(x)]\,, \qquad (3)$$

where

$$I, J = x^3 \int_1^\infty d\lambda\, e^{-\frac{3}{4}x\lambda} \int_{-1}^1 d\mu\, e^{-\frac{1}{4}x\mu} \times (1, G)(\lambda - \mu)(\lambda + \mu - 2)\,,$$

and U_0, g_0, and G are defined in I. The function

$$I(x) = \tfrac{64}{9}\{(64/3x)e^{-x} - [(64/3x) - 12 + 3x]e^{-\frac{1}{2}x}\}\,,$$

while $J(x)$ must be evaluated numerically, most conveniently by Gaussian quadrature. (I and J are shown in Fig. 1, and U_0 and g_0 in Fig. 2). The corresponding Born-approximation matrix element M_B is obtained by setting $U_0 = \sin kx$ and $g_0 = 0$ in Eq. (3). M was then computed using Simpson's rule and M_B analytically, with the result $(M_B/M)^2 = \sigma_B/\sigma = 28$. Thus near threshold the Born approximation seems to overestimate

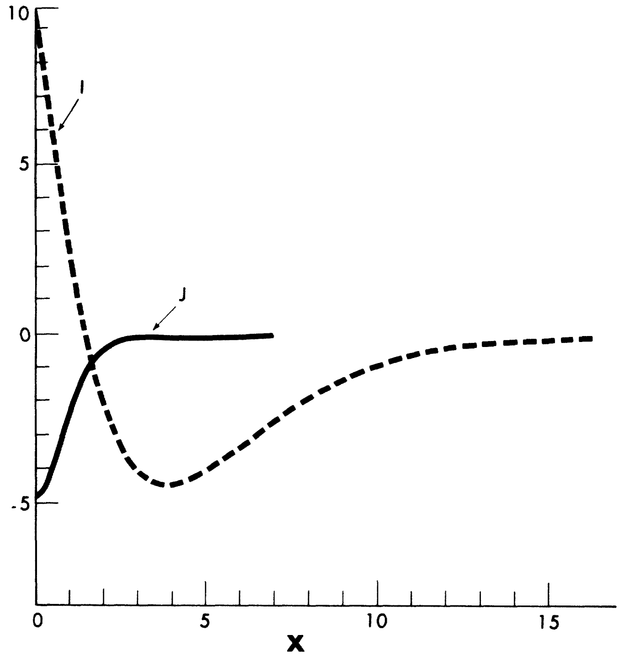

FIG. 1. Functions used in the evaluation of the positronium-formation matrix element at threshold. [See Eq. (3).]

the S-wave formation probability by a very large factor. This result is consistent with previous quite different calculations,[2] which also gave a considerable reduction. The extreme sensitivity to the details of the calculation gives the present result qualitative significance only.

(2) Recent beautiful experiments[3] have provided information on the angular correlation of the two γ rays resulting from the annihilation of low-energy positrons in liquid helium. After removing a very narrow spike around $\theta = 0$ (resulting apparently from the annihilation of singlet Ps within a cavity in the liquid), one finds that the remaining angular correlation function $P(\theta)$ has the form shown by the points in Fig. 3, which were obtained from a graph provided by Professor Stewart.[4]

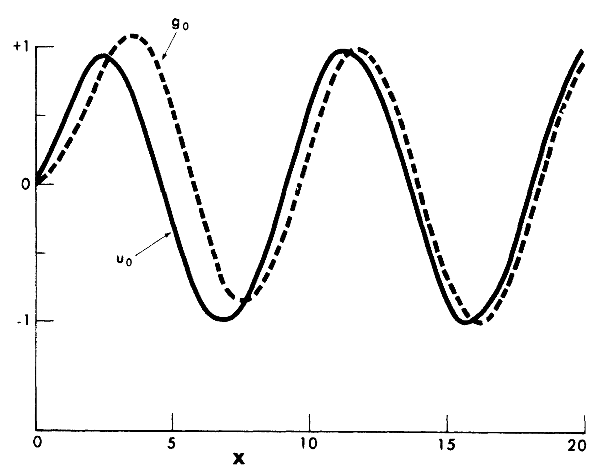

FIG. 2. S-wave scattering functions at threshold as computed variationally.

The experiment measures a single component, q_3, of the linear momentum of the annihilating $e^+ - e^-$ pair. This is always very small compared with the momentum (mc) of each of the photons, so the angle between the photon directions is $\pi - \theta$, where $\theta \cong q_3/mc$. If the wave function for the e^+-He system is $\Psi(\vec{r}_1, \vec{r}_2, \vec{x})$, then we have[5]

$$P(q_3) = \int_{-\infty}^{\infty} \int dq_1 dq_2 S(q) , \qquad (4)$$

where

$$S(q) = \int d^3r \left| \int d^3x e^{i\vec{q}\cdot\vec{x}} \Psi(\vec{r}, \vec{x}, \vec{x}) \right|^2 , \qquad (5)$$

q, x, and r are in the conventional atomic units, and $\theta = 7.297 \times 10^{-3} q_3$. Using the form

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{x}) = \{\chi(\vec{x}) + F(\vec{x}) \times [G(\vec{r}_1, \vec{x}) + G(\vec{r}_2, \vec{x})]\} \psi(r_1)\psi(r_2) , \qquad (6)$$

and keeping S waves only since we are interested only in low energies, one has

$$S(q) = \left|(4\pi/q) \int_0^\infty dx \sin qx\, A(x)\psi(x)\right|^2 + \langle |T(\vec{r}, \vec{q})|^2 \rangle . \qquad (7)$$

Here $A(x) = U_0(x) + g_0(x) G(\vec{x}, \vec{x})$,

$$T(\vec{r}, \vec{q}) = \int d^3x\, \psi(x) g_0(x) x^{-1} G(\vec{x}, \vec{r}) e^{i\vec{q}\cdot\vec{x}} ,$$

where the bracket notation means integration over r as defined in Eq. (6) of I, and the cross term vanishes since $\langle G \rangle = 0$. Converting to cylindrical coordinates one has

$$P(q_3) = 2\pi \int_0^\infty d\rho\, \rho S(q) = 2\pi \int_{q_3}^\infty dq\, q S(q) . \qquad (8)$$

In evaluating $S(q)$, the first term on the right side of Eq. (7) is straightforward, but the second is difficult and we have neglected it. To justify this neglect, we observe that the integral

$$\int d^3q S(q) = \int_{-\infty}^{\infty} dq_3 P(q_3)$$

is proportional to the total annihilation rate of zero-energy positrons in helium [Eq. (27) of I]. The second term of Eq. (7) contributes less than 1% to the annihilation rate; since it is positive definite, its effect on $P(q_3)$ must also be very

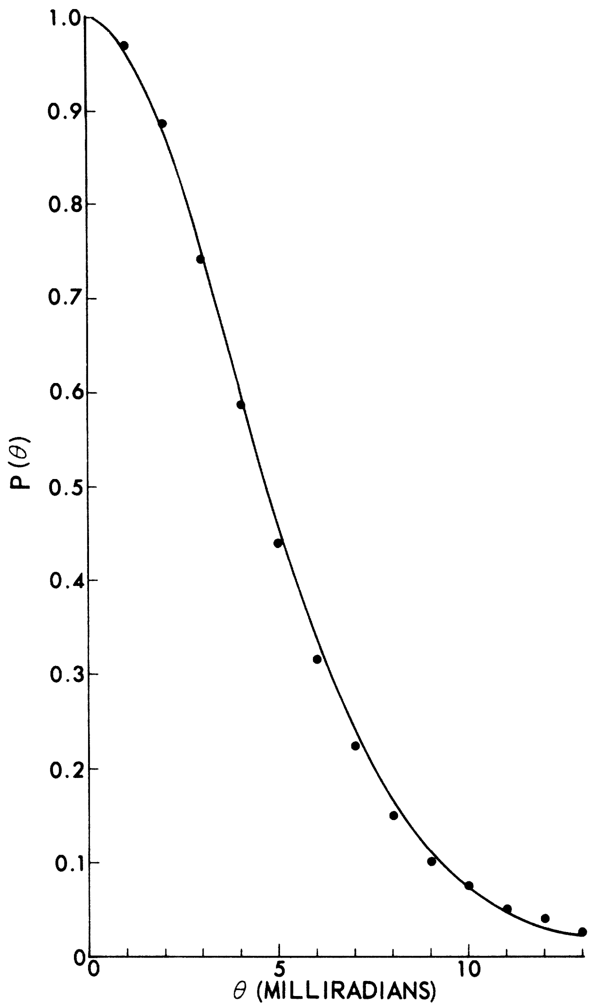

FIG. 3. Two-photon angular correlation for zero-energy positrons annihilating in helium. The curve is the present theoretical result, and the points are the experimental results of Refs. 3 and 4. [Only one side of the curve is shown since $P(\theta)$ is symmetric about $\theta = 0$.]

small.

With this neglect, we have used the numerically obtained zero-energy functions U_0 and g_0 along with $G(\vec{x}, \vec{x})$ from Eq. (A6) of I to compute the angular correlation, as shown in Fig. 3, where $P(\theta)$ is normalized to unity at $\theta = 0$. The agreement is seen to be very good.

To demonstrate that the close agreement shown in Fig. 3 is nontrivial, we have also computed $P(\theta)$ for several other plausible forms for Ψ. These included the nonvariational wave function with full monopole suppression[6] and the present variational function without correlation (i.e., with $g_0 = 0$). These were in significantly worse agreement with experiment. Still simpler wave functions, which include neither correlation nor scattering (Born approximations) were tried also. In using them one assumes that the total momentum spread of the photons comes from the ground state of the helium atom. Single exponential forms ($\Psi = e^{-\beta(r_1 + r_2)}$, with $\beta = 1.5992$ and $\beta = 27/16$) and a two-exponential form[7] ($\Psi = e^{-\alpha r_1} \times e^{-\beta r_2} + e^{-\alpha r_2} e^{-\beta r_1}$, with $\alpha = 2.1832$ and $\beta = 1.1886$) gave poor results. For clarity, the various $P(\theta)$ curves are not displayed here, but from them the full widths at half-maximum were obtained for all cases and are listed in Table I.

It is apparent that the variational method, although not in exact agreement with experiment, is significantly better than any of the others.

We conclude that the angular-correlation measurements provide a valuable test of very low-energy positron-atom scattering functions, and that the variational method of I seems rather accurate. Similar measurements at higher temperatures or with an applied electric field might provide information on the properties of finite-energy scattering functions.

TABLE I. Full width at half-maximum of the two-photon angular-correlation function $P(\theta)$ (in milliradians).

Method	Width
Experiment (Ref. 4)	9.2 ± 0.2
Variational	9.47
Nonvariational	10.07
Variational without correlation	10.82
One exponential ($\beta = 1.5992$)	11.90
Two exponentials	12.36
One exponential ($\beta = 27/16$)	12.56

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[3]C. V. Briscoe, S.-I. Choi, and A. T. Stewart, Phys. Rev. Letters 20, 493 (1968).

[4]Private communication from A. T. Stewart.

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