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Capture of atomic electrons by high-velocity positrons

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Calculations, complete through second order in the collision potentials, are presented for $1s$-$1s$ capture by positrons. Some new destructive interference between second-order amplitudes is evident. This destruction interference was not important in capture by protons where one Thomas amplitude is dominant. Nevertheless, the total cross sections for capture by positrons are larger than those for capture by protons at the same velocity because of a kinematical effect.

Positron capture of electrons requires a deeper understanding than capture of electrons by protons or other heavy projectiles. Because the positron has identical mass and opposite charge to that of the electron, new and observable interference effects can occur with positrons that cannot occur with protons. These effects, presented in this paper, are conceptually simple. Furthermore, specific experiments to observe these effects are now feasible with the recent development of intense, high-energy position sources.

During the past several years there has been significant development[1–8] in the understanding of electron capture by heavy projectiles such as protons. Electron capture by such heavy particles is now understood as a two-step, or primarily second-order, process at high velocities. The intermediate states of the system are continuum intermediate states, and the capture amplitude has been expressed[2] as an integral of the ionization amplitude weighted by the momentum distribution of the final state of the captured electron. Both energy-conserving and energy-nonconserving intermediate states contribute significantly[9] to the capture cross section. At very high velocities these energy-conserving and energy-nonconserving amplitudes are interconnected[10] by a dispersion relation.

The signature of such a second-order process in the differential cross section for electron capture is the so-called Thomas peak named after L. H. Thomas who suggested in 1927 a simple two-step classical model[11] which predicts such a peak. This peak, present in the second Born approximation, dominates the total cross section at very high velocities. It has the form of a resonance in momentum transfer whose width corresponds[12] to a shift in the impact parameter of the projectile. Observation[13,14] of this Thomas peak in high-velocity electron capture has confirmed our understanding of the two-step or second-order nature of this process. The Thomas peak has also been observed[15] in capture of atoms from molecules. In electron capture by heavy projectiles from an infinitely heavy nucleus, a second peak also due to a internuclear second-order process has been predicted[16,17] and observed.[18] Another second-order peak[19] has been observed in atomic ionization by high velocity electrons. And it has recently been pointed out[20] that such second-order singularities may be systematically embedded in few-body and many-body collision cross sections.

Electron capture by positrons (or positronium formation) differs from electron capture by protons. First we note a relatively simple kinematic effect. Because the positron must transfer one-half its kinetic energy to the electron during capture, its capture cross section (which decreases rapidly with incresing energy) is larger than the capture cross section by protons of the same velocity. At high velocities in the Brinkman-Kramers approximation[21] the total cross section for positrons is about 6.6 times larger than for protons of the same velocity. More striking, however, is the disappearance of the Thomas singularity for $1s$-$1s$ capture by positrons at high velocities. The Thomas peak vanishes because of a dynamical interference first noted by Shakeshaft and Wadehra[22] and illustrated in Fig. 1. Because the mass of the positron and electron are equal, the interaction between the projectile and the target nucleus may not be ignored as it is for heavy projectiles. At the Thomas angle of 45° the internuclear contribution, corresponding to Fig. 1(b), is equal and opposite to the second-order singularity from elastic rescattering of the electron by the nucleus, corresponding to Fig. 1(a). The relative minus sign is evident from the scattering vertices, which multiply in the second Born amplitudes and are of the same sign in Fig. 1(a) and opposite sign in Fig. 1(b). It is worth noting at this point that in the $1s$-$2p$ (or any odd Δl) transitions the two amplitudes interfere constructively because of an extra minus sign in the parity of the wave functions of the final state. The destructive interference in the $1s$-$1s$ (or even Δl) cross section serves to underscore the fact that our basic understanding of heavy particle capture of electrons (as dominated by a particular second-order effect) is not sufficient for electron capture by positrons.

In this paper we address two experimentally testable[23] questions. First, how do the total cross sections for capture by positrons and protons compare? (We note that for excitation or ionization of a single electron they are expected to be the same.) That is, does the kinematic (increasing) effect of the dynamic (decreasing) effect dominate?

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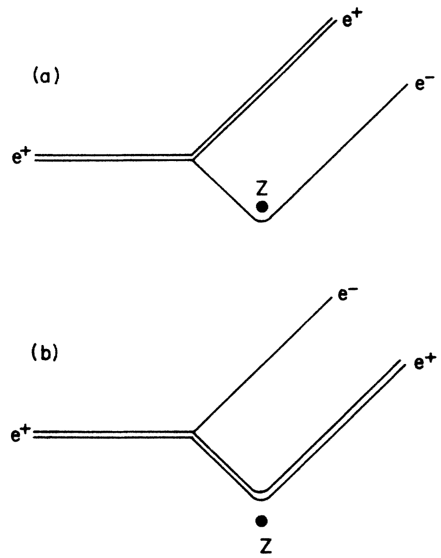

FIG. 1. Second-order scattering processes. Process (a) corresponds to the forward-angle Thomas mechanism that is dominant at very high velocity for electron capture by heavy particles. Process (b) arises as a result of the projectile-nucleus interaction, corresponding to a second-order peak at 60° for electron capture by heavy projectiles from very heavy atoms. For even Δl (odd Δl) transitions processes (a) and (b) interfere destructively (constructively) for capture by positrons.

Second, what is the shape of the differential cross section for capture by positrons, especially near the Thomas angle of 45°?

To address these questions we use the work of Shakeshaft and Wadehra[22] (SW) as a primary point of departure. Shakeshaft and Wadehra consider the two second-order processes shown in Figs. 1(a) and 1(b), but use plane waves as intermediate states. Yet, as demonstrated by Briggs, Greenland, and Kocbach,[4] such plane waves do not adequately describe the angular distribution near the Thomas peak for capture by protons. One possible set of intermediate states at high velocities is the positronium intermediate states. In this paper we extend the SW work to incorporate positronium intermediate states and include a second-order distortion term, as explained below. Corresponding calculations for proton impact collisions give[8,13,14] cross sections of the correct shape and magnitude.

In our calculation we begin by expressing the exact T matrix by

$$T_{if}=\langle\psi_f|\bar{V}_f|\Psi_i\rangle=\langle\psi_f|\bar{V}_f(1+G^+\bar{V}_i)|\psi_i\rangle$$
$$=\langle\psi_f|\left[\frac{Z}{R}-\frac{Z}{r}\right]\left[1+G^+\left[\frac{-1}{\rho}\right]\right]|\psi_i\rangle$$
$$+\langle\psi_f|\left[\frac{Z}{R}-\frac{Z}{r}\right]G^+\left[\frac{Z}{R}\right]|\psi_i\rangle=T_{a+b}+T_d\ . \quad (1)$$

We have generally followed the notation of Sil and McGuire,[8] and here Z/R, $-Z/r$, and $-1/\rho$ are the positron-electron Coulomb interactions, respectively. The first term in the bottom expression above contains the essential interfering second-order singularities, and the second term is a difference between a distorted wave and plane-wave matrix element, i.e., a second-order distortion term. We now introduce two approximations: (i) The interaction, $Z/R-Z/r$, is ignored in the Green's function, G^+, in the first term, thus giving a Coulomb Green's function, G_c^+, and (ii) the interaction $-1/\rho$ is ignored in G^+ in the second term. In the previous work of Shakeshaft and Wadehra,[22] plane-wave Green's functions were used in both parts of the T_{a+b} amplitude of Eq. (1) and T_d was neglected. We use all second-order terms, including T_d. We also include some selected higher-order terms via Coulomb Green's functions, so that our intermediate states contain Coulomb distortions. However, different Coulomb intermediate states are used for T_{a+b} and for T_d. In the first term there are positronium intermediate states. H-atom intermediate states are used in the second term. In both terms the electron propagates in the field of a positive charge. Nevertheless, the ultimate validity of this procedure will rest on comparison with appropriate experimental data or a more complete theory.

Using the approximate off-energy-shell Coulomb wave function of Macek and co-workers,[5,24] and following the technique of Sil amd McGuire,[8] the resulting amplitude for the first term in Eq. (1) is

$$T_{a+b}^{if}=-(2\pi)^2Z\int_0^\infty dp\,p^2\frac{2\sqrt{2}}{\pi}\frac{Z^{5/2}}{(p^2+Z^2)^2}\left[\frac{p^2+Z^2}{2v^2}\right]^{-i/v}$$
$$\times\frac{1}{J^2+p^2}(a_{10}I_{10}+a_{20}I_{20})\ , \quad (2)$$

where

$$\mathbf{J}=\mathbf{K}_i-\mathbf{K}_f,\ \mathbf{K}=\tfrac{1}{2}\mathbf{K}_f-\mathbf{K}_i,\ \beta=\tfrac{1}{2}\ ,$$

$$A=[(2\beta-iv)^2+J^2]/4,\ \ L=|\mathbf{J}+\mathbf{v}+2i\beta\hat{\mathbf{v}}|/4\ ,$$

$$a_{10}=2\beta\frac{2/v}{1-e^{-2\pi/v}}(i/v-1)[(\beta^2+v^2/2)^{-2+i/v}$$
$$-(\beta^2+K^2)^{-2+i/v}]\ ,$$

$$a_{20}=(-i/v)\frac{2/v}{1-e^{-2\pi/v}}[(\beta^2+v^2/2)^{-1+i/v}$$
$$-(\beta^2+K^2)^{-1+i/v}]\ ,$$

$$I_{10}=\frac{1}{2Lp(1-i/v)}[(A+Lp)^{1-i/v}-(A-2Lp)^{1-i/v}]\ ,$$

$$I_{20}=\frac{1}{2Lp(-i/v)}[(A+2Lp)^{-i/v}-(A-2Lp)^{-i/v}]\ ,$$

where $\mathbf{K}_i$ and $\mathbf{K}_f$ are the initial and final momenta, respectively. This expression may be reduced[25] to close form. Here only two leading-order terms in a (Z/v) expansion have been retained. Hence, the error is of order (Z/v) (with a large coefficient), and this expression is accurate for systems of arbitrary charges at sufficiently high velocities. The second-order distortion term T_d may be expressed[26] in terms of a one-dimensional integral.

Results for total cross sections are given in Table I. In our calculation the total cross section for electron capture by positrons is several times larger than that by protons at the same velocity (except at very high, i.e., relativistic ve-

TABLE I. Total cross sections for $1s$-$1s$ electron capture.

	Total cross sections (πa_0^2)	
v (a.u.)	p^+	e^+
6	1.47 (−6)	2.52 (−5)
8	7.51 (−8)	1.00 (−6)
10	7.07 (−9)	7.82 (−8)
14	1.79 (−10)	1.60 (−9)
20	3.30 (−12)	2.47 (−11)
30	3.29 (−14)	2.08 (−13)
50	9.51 (−17)	4.88 (−16)
100	3.47 (−20)	1.26 (−19)

locities where the Thomas peak is dominant for capture by protons).

Differential cross sections for $1s$-$1s$ capture are shown in Figs. 2 and 3. Three calculations are given in Fig. 2. In the curve labeled T_a only the amplitude for the Thomas peak, corresponding to Fig. 1(a), is included. This is the amplitude used[5,8] for capture by heavy projectiles. The large Thomas peak at about 45° dominates the total cross section for T_a at very high velocities. The T_{a+b} curve in Fig. 2 includes contributions from Figs. 1(a) and 1(b), but ignores the second-order distortion, T_d in Eq. (1). The cancellation of the Thomas peak, as predicted by Shakeshaft and Wadehra[22] is quite evident[27] near 45 °C. The dip at 23° is due to the interference between first and second Born amplitudes. The curve T_{a+b+d} represents our most complete calculation including the second-order distortion term in addition to contributions from Figs. 1(b) and 1(c). At 45° the amplitude T_{a+b} changes sign while the distortion amplitude T_d is finite and smoothly varying. The structure seen about 45° occurs because of interference due to all of the three second-order terms. In Fig. 3 we see that this interference is more pronounced at the higher energies although some effect is evident at the lower energies shown.

In our calculations $1s$-$2p$ (and other odd Δl) capture has been neglected. At energies near a few keV we estimate by scaling from $p+H$ that the $1s$-$2p$ Thomas peak is less than half of the interference structure shown. At very high velocities the $1s$-$2p$ peak should eventually dominate the total cross section.

In summary, electron capture by positrons requires a deeper understanding than capture by heavy particles. For positrons picturing $1s$-$1s$, capture simply as a two-step or second-order mechanism is insufficient because of cancellation and interference in the second-order amplitudes. Furthermore, the nature of the intermediate states (as discussed for heavy projectiles in the introduction) is not clear for positronium formation, although the amplitude in Eq. (2) may be expressed as a difference in amplitudes for ionization by electrons and positrons, weighted by the initial $1s$ momentum distribution. Development of an adequate picture of electron capture by positrons may be aided by further studies of both total and differential cross sections, experimentally and theoretically, at high velocities. We recommend (1) comparisons of total cross sections for capture by positrons and protons of the same velocity, and (2) examination of the shape of the differential cross section, especially near 45°.

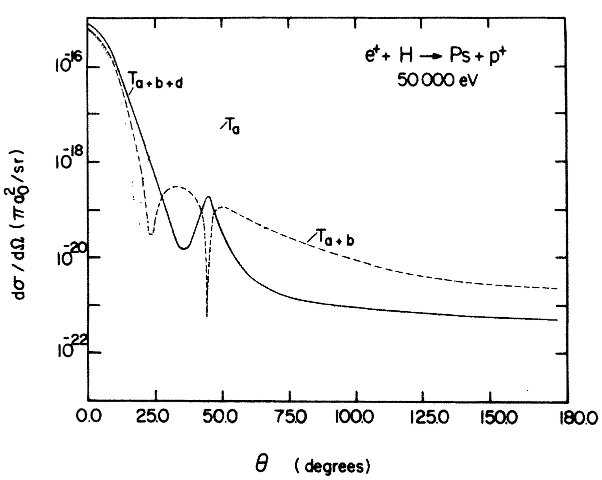

FIG. 2. Differential cross section vs scattering angle for $1s$-$1s$ capture. Curve T_a contains only the Thomas amplitude corresponding to Fig. 1(a). Curve T_{a+b} is calculated from Eq. (2) using amplitudes for both 1(a) and 1(b). The most complete calculation, T_{a+b+d} including the second-order distortion term in Eq. (1), contains three second-order amplitudes. Interference about the Thomas angle of 45° is evident.

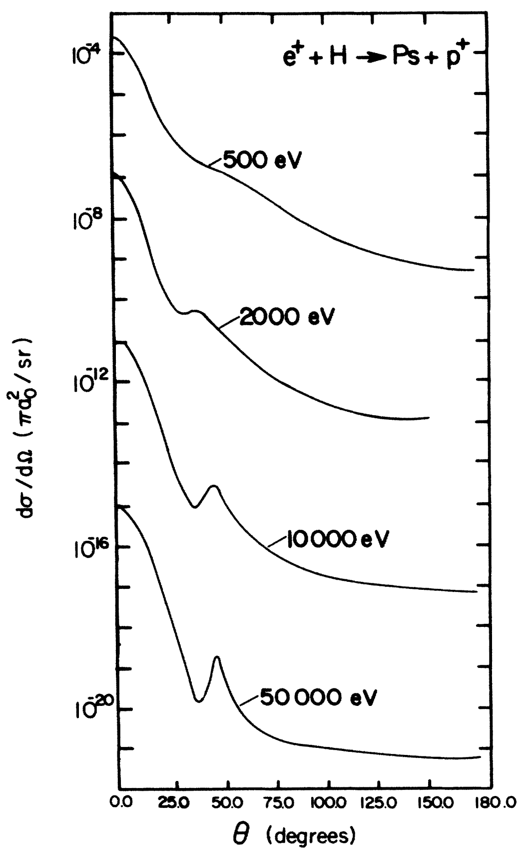

FIG. 3. Differential cross section vs scattering angle at various projectile energies for $1s$-$1s$ electron capture by positrons from atomic hydrogen.

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