Low-energy elastic scattering of positrons on argon

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Elastic scattering of positrons from argon has been calculated for incident-positron energies of up to 300 eV. The target atom is represented by a frozen core in a continuum relativistic Hartree-Fock calculation with dipole- and quadrupole-polarization corrections. The cutoff parameter r_0 is fitted to reproduce measured values of the scattering length. Scattering lengths near -4 a.u. give good agreement of the calculations with recent measurements of total, differential, and momentum-transfer cross sections below 3 eV. Relativistic and positron-polarization effects are found to be much smaller than for electrons. The relativistic effects are dominated by the relativistic contraction of the target atom.

I. INTRODUCTION

From a theoretical point of view, the elastic scattering of positrons on noble-gas atoms is one of the simplest scattering problems and is therefore suitable for testing different calculational methods. The absence of any exchange potential in the one-electron Hamiltonian for the positron and, in comparison to electron scattering, the change in sign of the electrostatic interaction but not of the polarization terms permit a sensitive test of different polarization potentials. Also, relativistic effects in positron scattering can be calculated and compared with the unexpectedly significant ones found for electron scattering.^{1,2}

Experiments on positron-atom scattering have been reviewed recently by Charlton,³ Raith,⁴ Stein and Kauppi-la,⁵ and Kauppila and Stein.⁶ The theoretical work on this subject has been reviewed by McEachran,⁷ Drachman,⁸ and Schrader and Svetic.⁹ Total cross sections of e^+ -Ar scattering have been measured by several groups.¹⁰⁻¹⁶ At low energies, there is a significant discrepancy between different experimental results, reaching 30% at 2-3 eV. Kauppila et al.¹³ have found a shallow Ramsauer-Townsend minimum in the vicinity of 2 eV. This minimum had been predicted earlier by Massey et al.¹⁷ in their semiempirical approach. Coleman and McNutt,¹⁸ using a time-of-flight technique, reported the first differential elastic scattering cross sections for 2- to 9-eV positrons on argon for angles 20° to 60°. The first crossed-beam experiment with positrons was recently performed by Hyder *et al.*¹⁹ who measured relative elastic differential cross sections for 100-, 200-, and 300-eV positrons scattered at 30° to 135° from argon atoms. The same group²⁰ recently extended their measurements to lower energies (6-40 eV).

Calculations of the e^{+} -Ar elastic cross sections have been published by Montgomery and LaBahn,²¹ McEachran *et al.*,²² and McEachran and Stauffer²³ using polarized-orbital approximations. Other approaches with a model-potential or pseudopotential method have been reported by Schrader,²⁴ Datta *et al.*,²⁵ and Nakanishi and Schrader.²⁶ Nahar and Wadera,²⁷ using a localexchange approximation, have recently presented nonrelativistic calculations for positrons in the energy range 3-300 eV. Theirs is a semiempirical calculation in that they employ an energy-dependent polarization potential which is adjusted to each energy to reproduce the *electron*-scattering cross sections.

The well-established features of polarization potentials are their asymptotic forms. In this paper we study the influence of the short-range behavior of the dipoleand quadrupole-polarization potentials on the elasticscattering phase shifts as well as on total, momentumtransfer, and differential cross sections. The short-range behavior of the polarization potential is determined by a cutoff parameter in the polarization function. The values of this parameter are chosen to reproduce different scattering lengths derived from the experimental data. $^{28-30}$ Although we use relativistic Dirac-Fock wave functions for the description of the argon atom and the two-component Dirac wave function for the incident positron, we do not expect large relativistic effects for this system. Nevertheless, we examine these effects and compare with ones found for electron scattering in our previous papers.^{1,31}

II. THEORY

A. Scattering equation

Consider the elastic scattering of a positron by a target atom in its ground state. The scattered positron is represented by a four-component Dirac spinor: $^{32-34}$

$$U_{\kappa m}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{\kappa}(r)\Omega_{\kappa m}(\hat{\mathbf{r}}) \\ iQ_{\kappa}(r)\Omega_{-\kappa m}(\hat{\mathbf{r}}) \end{pmatrix}, \qquad (1)$$

where

$$\Omega_{\kappa m}(\hat{\mathbf{r}}) = \sum_{\sigma=\pm 1/2} \langle jm | l, \frac{1}{2}; m - \sigma, \sigma \rangle Y_l^{m-\sigma}(\hat{\mathbf{r}}) \chi_{\frac{1}{2}}^{\sigma}$$
(2)

is the angular momentum eigenfunction. Here $\langle jm|l, \frac{1}{2}; m-\sigma, \sigma \rangle$ is a Clebsch-Gordan coefficient, $Y_l^{m-\sigma}(\hat{\mathbf{r}})$ is a spherical harmonic, χ_{\perp}^{σ} is the spin eigen-

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function, P and Q are the large and small components of the Dirac wave function, respectively, and

$$\kappa = \pm (j + \frac{1}{2}) \text{ for } l = j \pm \frac{1}{2},$$
 (3)

where j is the total angular momentum and l is the orbital quantum number.

The effective one-electron Hamiltonian of the scattered positron is

$$H = c \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m c^2 + V_{FC}(r) + V_p(r)$$
(4)

where the matrices α and β have their usual meaning^{32,33} and $V_{FC}(r)$ is the relativistic frozen-core potential between the scattered positron and the electrons of the target. The model polarization potential $V_p(r)$ represents the polarization of the target atom by the electric field of the scattered positron. Formally, V_p is the scatteredpositron-frozen-core (here the target atom) correlation term which is the main correction to the frozen-core calculations.³⁵ We have taken a model potential in the form

$$V_{p}(r) = -\frac{1}{2} \frac{\alpha_{d} r^{2}}{(r^{3} + r_{0}^{3})^{2}} - \frac{1}{2} \frac{(\alpha_{q} - 6\beta)r^{4}}{(r^{5} + r_{0}^{5})^{2}}$$
(5)

where α_d is the static dipole polarizability, α_q is the static quadrupole polarizability, and β is the coefficient of the first-order dynamical correction to α_d . For argon we have used the values (in atomic units) $\alpha_d = 10.77$ and $\alpha_q = 50.12$ from Johnson and Kolb³⁶ and the value $\beta = 8.33$ from Dalgarno *et al.*³⁷ Uncertainties in the second-order corrections to the dipole polarizability make it pointless to include either higher-order dipole corrections or higher-order multipole polarizabilities beyond the static contribution. The value r_0 may be viewed as an effective size of the target atom; it serves as a cutoff parameter which prevents divergence at r=0.

The scattering equation we solve is the radial Dirac-Fock equation (compare $Desclaux^{38}$)

$$\left[\frac{d}{dr} + \frac{\kappa}{r}\right] P_{\kappa}(r) = \left[2c + \frac{1}{c} \left[E - V_{\rm FC}(r) - V_p(r)\right]\right] Q_{\kappa}(r) ,$$
(6a)

$$\left[\frac{d}{dr} - \frac{\kappa}{r}\right] Q_{\kappa}(r) = -\frac{1}{c} \left[E - V_{\rm FC}(r) - V_{p}(r)\right] P_{\kappa}(r) \qquad (6b)$$

where the speed of light c=137.036 a.u. and E is the energy of the incident electron. The frozen-core potential for the positron is defined by

$$V_{\rm FC}(r) = \frac{Z}{r} - \sum_{j,k} a^{k}(s,j) Y^{k}(j,j;r)$$
(7)

where the index s refers to the scattered positron, Z is the nuclear charge, and the sums are over all electrons of the target atom. The radial function Y^k is

$$Y^{k}(j,j;r) = \frac{1}{r^{k}} \int_{0}^{r} F(q)q^{k}dq + r^{k+1} \int_{r}^{\infty} F(q)q^{-k-1}dq$$

 $F(q) = P_j^2(q) + Q_j^2(q) .$ (9)

The terms a^k and b^k are standard angular coefficients.^{32,33}

Equation (6) is solved subject to the boundary conditions

$$P_{\kappa}(0) = Q_{\kappa}(0) = 0 \tag{10}$$

with the asymptotic forms at large r

$$\frac{P_{\kappa}(r)}{r} \approx j_{l}(kr) \cos\delta_{l}^{\pm} - n_{l}(kr) \sin\delta_{l}^{\pm} , \qquad (11)$$

$$\frac{Q_{\kappa}(r)}{r} \approx \left[\frac{E}{E+2c^2}\right]^{1/2} [j_{\bar{l}}(kr)\cos\delta_{\bar{l}}^{\pm} - n_{\bar{l}}(kr)\sin\delta_{\bar{l}}^{\pm}] \quad (12)$$

where $k = (2E + \alpha^2 E^2)^{1/2}$ is the momentum of the incident positron, $\tilde{l} = l \pm 1$ for $j = l \pm \frac{1}{2}$, and δ_l^{\pm} are the phase shifts. For each *l* value greater than zero there are two equations corresponding to the two values of κ [see Eq. (3)]. In conformity with Walker³⁹ we let δ_l^+ be the phase shift for $\kappa = -l - 1$ and let δ_l^- be that for $\kappa = l$. Here, $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively.

B. Elastic-scattering cross sections

We obtain the relativistic phase shifts δ_l^{\pm} for l=0 to l=12 by comparing the numerical solution of our scattering equations (6) to the asymptotic analytic solutions for the large component of the scattering wave function (11). Nonrelativistic phase shifts for l=13 to 50 are estimated by means of the effective formula given by Ali and Fraser.⁴⁰ From the phase shifts we determine the two scattering amplitudes^{41,42}

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{ (l+1) [\exp(2i\delta_l^+) - 1] + l [\exp(2i\delta_l^-) - 1] \} P_l(\cos\theta)$$
(13)

and

$$g(\theta) = \frac{1}{2ik} \sum_{l=1}^{\infty} \left[\exp(2i\delta_l^-) - \exp(2i\delta_l^+) \right] P_l^1(\cos\theta)$$
(14)

where P_l and P_l^1 are the Legendre polynomials and the Legendre associated functions, respectively, and θ is the scattering angle. The scattering amplitude $f(\theta)$ is the direct amplitude corresponding to the nonrelativistic amplitude, whereas $g(\theta)$ is the spin-flip amplitude.

The differential cross section for an unpolarized positron beam is

$$\frac{d\sigma}{d\Omega} = |f|^2 + |g|^2 \equiv I(\theta) .$$
(15)

In addition, we have calculated the total cross section σ_t and the momentum-transfer cross section σ_m given by

$$\sigma_{l} = \frac{4\pi}{k^{2}} \sum_{l} \left[(l+1)\sin^{2}\delta_{l}^{+} + l\sin^{2}\delta_{l}^{-} \right] , \qquad (16)$$

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where

$$\sigma_{m} = \frac{4\pi}{k^{2}} \sum_{l} \left[\frac{(l+1)(l+2)}{2l+3} \sin^{2}(\delta_{l}^{+} - \delta_{l+1}^{+}) + \frac{l(l+1)}{2l+1} \sin^{2}(\delta_{l}^{-} - \delta_{l+1}^{-}) + \frac{l+1}{(2l+1)(2l+3)} \sin^{2}(\delta_{l}^{+} - \delta_{l+1}^{-}) \right]. \quad (17)$$

C. The nonrelativistic limit

By eliminating the small component Q_{κ} from the Dirac equation (6) one obtains a second-order differential equation for the large component P_{κ} which reduces to the Schrödinger equation in the limit $c \to \infty$. In the same limit, the small component itself vanishes [see Eq. (6b)]. We calculate our nonrelativistic limits with the same code for the coupled first-order equations (6) as in our relativistic calculations, but with c made very large (about 10^{10}).

III. RESULTS AND DISCUSSION

A. Polarization effects

The cutoff parameter r_0 in our model polarization potential, Eq. (5), can be regarded as an effective target radius. It is chosen to reproduce the experimental scattering length for the e^+ -Ar system. Three different scattering lengths have been reported. The highest value, $-2.8a_0$, was obtained from the analysis of total crosssection data by Tsai *et al.*⁴³ The value $-3.5a_0$ was determined from the temperature and electric-field dependence of the equilibrium positron-electron annihilation rate by Hara and Fraser.⁴⁴ The scattering length $a = -4.4a_0$ reported by Lee and Jones⁴⁵ was derived from the effective-range parametrization of the momentum-transfer cross section. We find three different values of r_0 corresponding to the three scattering lengths (see Table I).

It is interesting that the r_0 values given in Table I for positron scattering are generally smaller than those appropriate for electron scattering.^{1,31} This difference, noted earlier by Nakanishi and Schrader, is expected because the exchange contribution to the two-electron part of the polarization interaction³⁵ (*not* included here) reduces the electron-argon polarization strength relative to that of the positron-argon interaction. The fact that Nahar and

TABLE I. Cutoff parameters r_0 fit to different experimental scattering lengths a.

a (units of a_0)	r_0 (units of a_0)	
-2.8ª	1.393	
-3.5 ^b	1.212	
4.4 ^c	1.070	

^aReference 43.

^bReference 44.

^cReference 45.



FIG. 1. Total elastic scattering cross section. Theory: —, presents results; — —, Datta et al. (Ref. 25); -.-.-, Schrader (Ref. 24); ----, Nakanishi and Schrader (Ref. 26); – –, McEachran et al. (Ref. 22). Experiment: \times , Kauppila et al. (Ref. 13); \bigcirc , Coleman et al. (Ref. 14); \bullet , Sinapius et al. (Ref. 15); ∇ , Charlton et al. (Ref. 16).



FIG. 2. Momentum-transfer cross section. Theory: —, present results; --, McEachran *et al.* (Ref. 22); --, Montgomery and LaBahn (Ref. 21); ---, Nakanishi and Schrader (Ref. 26). Experiment: the shaded area indicates the results of Lee and Jones (Ref. 28).



FIG. 3. Differential cross section for incident momentum k=0.4 and 0.5 a.u. Theory: —, present results; – –, McEachran *et al.* (Ref. 22). Experiment: –-–, Nakanishi and Schrader (Ref. 26); –·–·–, Schrader (Ref. 24); –··–, Datta *et al.* (Ref. 25). Experiment: Φ , Coleman and McNutt (Ref. 18).

Wadera²⁷ obtain good results with the same short-range polarization potential for electrons and positrons may be a fortuitous consequence of their local-exchange approximation.

The total cross sections corresponding to scattering lengths $-3.5a_0$ and $-4.4a_0$ are shown in Fig. 1. The curve corresponding to the scattering length $-2.8a_0$ of

Tsai *et al.*⁴³ is not shown because the values are unrealistically small and for energies greater than 2 eV lie below the bottom of the figure $(\sigma_t < 2\pi a_0^2)$. Thus from our approach it appears that the scattering length is lower than $-2.8a_0$. On the other hand, the curves for scattering lengths $-3.5a_0$ and $-4.4a_0$ lie on either side of the experimental values of Kauppila *et al.*¹³ at energies < 3 eV.



FIG. 4. As for Fig. 3 but with k=0.7 and 0.8 a.u.

The main difference in these results is that the curve corresponding to $-4.4a_0$ drops down at higher energies whereas that corresponding to $-3.5a_0$ exhibits a very shallow Ramsauer-Townsend minimum. Another theoretical calculation which displays this minimum is that of Datta *et al.*,²⁵ who also used a scattering length of $-3.5a_0$. The unpredicted rise in the cross section above k=0.8 a.u. is associated with positronium formation, the threshold for which lies just below 9 eV.

In Fig. 2 we compare our calculated momentumtransfer cross sections with other theoretical results and with the limited data of Lee and Jones,²⁸ derived from their measured annihilation rates. Figure 3 shows our differential cross sections for both $-3.5a_0$ and $-4.4a_0$ scattering lengths at k=0.4 and 0.5 a.u. together with other theoretical results and the experimental data of Coleman and McNutt.¹⁸ At k=0.4 a.u., both theoretical curves are within the range of the experimental data, but a scattering length of about $-4.0a_0$ would give the best fit. At k=0.5 a.u., the curve with $a = -3.5a_0$ fits better at low angles ($< 30^\circ$), whereas the curve with $a = -4.4a_0$ is in better agreement at higher angles (40° to 65°). It may be seen that none of the theoretical curves shows good agreement with experiment at all scattering angles. At k=0.7 a.u. (see Fig. 4), the curve corresponding to $a = -4.4a_0$ is in very good agreement with experiment, but at k=0.8 a.u. (Fig. 4), none of the theoretical curves can reproduce the experimental data of Coleman and McNutt¹⁸ for scattering angles of 30 to 40°.

Figure 5 shows the relative elastic differential cross section at 20 eV. The measurements of Smith *et al.*²⁰ have been normalized at $\theta = 75^{\circ}$ to the calculations of Nahar and Wadera²⁷ and of McEachran and Stauffer.²³ We have normalized our results for $a = -3.5a_0$ to the others at 75° by moving our curve up by $0.19a_0^2$. Only the ad-



FIG. 5. Differential cross section at 20 eV. Theory: —, present result; — —, McEachran and Stauffer (Ref. 23); —, —, Nahar and Wadera (Ref. 27). Experiment: Φ , Smith *et al.* (Ref. 20).



FIG. 6. Differential cross section at 45°. Theory: —, present results; --, McEachran and Stauffer (Ref. 23); $-\cdot - \cdot - \cdot$, Nahar and Wadera (Ref. 27). Experiment: Φ , Smith *et al.* (Ref. 20).

justed model-potential calculations of Nahar and Wadera²⁷ agree with experiment at small angles. The relative differential cross sections from 6 to 40 eV are shown in Fig. 6 for $\theta = 45^{\circ}$. Our theoretical results and the experimental data of Smith *et al.*²⁰ are normalized to the results of McEachran and Stauffer²³ at 40 eV. Again, the best agreement with the measurements is achieved by the semiempirical curve of Nahar and Wadera.²⁷ Because Nahar and Wadera have adjusted the short-range part of their polarization potential to fit electron-scattering cross sections at each energy, their curves may include effects of inelastic excitation channels on the elastic-scattering process (the first excitation threshold lies at 11.55 eV).

B. Relativistic effects

The spin polarization we calculate for positrons scattered on argon is three orders of magnitude smaller than for electrons.³¹ The small size of this relativistic effect is reflected in the miniscule difference between "spin-up" δ_l^+ and "spin-down" δ_l^- phase shifts (see Table II). Hasenburg⁴⁶ has explained the smallness by showing that the positrons hardly penetrate the region where spinorbit effects are significant.

TABLE II. The polarization phase-shift difference $\delta_l^+ - \delta_l^-$ for elastic scattering of positrons on argon.

1	30 eV	100 eV	300 eV
1	2.87	8.02	20.86
2	1.28	6.14	17.51
3	0.10	3.42	12.78

F (aV)	1=0	e^{-} -Ar ^a	1=2	1=0	e^+ -Ar	1=2
	1-0	1-1	1-2	1-0	1-1	1-2
1.0	6.59[-3]	-5.43[-4]	-8[-8]	1.29[-3]	8.91[-5]	-1.84[-6]
5.0	8.69[-3]	-1.98[-3]	-9.94[-4]	1.63[-3]	5.70[-4]	4.78[-5]
10.0	9.44[-3]	-2.54[-3]	-7.70[-3]	1.85[-3]	9.55[-4]	1.93[-4]
20.0	1.02[-2]	-2.75[-3]	-9.47[-3]	2.13[-3]	1.40[-3]	5.29[-4]
40.0	1.09[-2]	-2.56[-3]	-6.58[-2]	2.39[-3]	1.82[-3]	1.62[-3]

TABLE III. Relativistic contributions to phase shifts. A comparison of electron (e^{-}) and positron (e^{+}) scattering from argon. The numbers in square brackets represent powers of 10.

^aReference 1.

Other relativistic effects of low-energy positron scattering on heavy atoms, like Xe, Hg, Rn, and Ra, have been studied theoretically by Sin Fai Lam⁴⁷ and Jaskolski.⁴⁸ Both direct and indirect relativistic effects play important roles for electron scattering from heavy atoms, but only indirect relativistic effects are important for positron scattering. These effects are caused by the change in the electron distribution of the target due to direct relativistic effects on the innermost orbitals and to the selfconsistency of the other electrons with these orbitals. The direct relativistic effect on the positron is much smaller than on an electron because the amplitude of the positron wave function close to the nucleus, where direct effects are most important, is greatly suppressed by the repulsive character of the Coulomb interaction between the positron and the nucleus. In Table III we compare the difference between the relativistic and nonrelativistic phase shifts for electron and positron scattering from argon. In the energy range examined (1-40 eV), the relativistic effects in positron scattering are at least three times smaller than those for electron scattering.

In additional calculations we have isolated the relativistic effects on the scattering wave function from those on the target atom by solving the scattering equations (6) in the nonrelativistic limit $(c \rightarrow \infty)$ with a relativistic target and in the proper relativistic limit with a nonrelativistic target (see Sec. II C). The direct effect on the scattering wave function causes a very small *reduction* in the scattering phase shift (for example, a reduction of 10^{-5} rad at 20 eV) due to the change in the expansion of the wave function at the origin (r=0).⁴⁹ Relativistic effects on the target cause an overall contraction of the argon orbitals and hence a more effective screening of the nuclear charge. These *increase* the phase shifts, and the increase, although quite small, is much larger than the decrease caused by the direct effect on the wave function (for example, at 20 eV, it is about 100 times larger). The net effect for positrons, unlike *s*-wave scattering of electrons, is thus dominated by the indirect effect on the target for all partial waves (see Table III).

IV. CONCLUSIONS

The scattering of low-energy positrons by argon has been investigated in a fully relativistic approach with an added model polarization potential. Our results for the total elastic, momentum-transfer, and differential cross sections are in good agreement with existing experimental and theoretical data. The adjustment of the size parameter r_0 of the model potential to the scattering lengths determined from experiments indicates that while the lengths $-3.5a_0$ of Hara and Fraser⁴⁴ and $-4.4a_0$ of Lee and Jones⁴⁵ give reasonable results within our theoretical approach, the value $-2.8a_0$ of Tsai *et al.*⁴³ appears distinctly too high. The *s*- and *p*-wave shifts are sensitive to the short-range behavior of the polarization function.

Relativistic effects play a much smaller role in positron scattering than in electron scattering, evidently as a result of the repulsive Coulombic interaction between the positron and the nucleus. In particular, the spin-polarization effects of positron scattering are extremely small. The most pronounced relativistic effect is the small phaseshift increase associated with the relativistic contraction of the target orbitals.

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