Elastic scattering of positrons on mercury: A negative-energy Dirac-Fock treatment

J. E. Sienkiewicz* and W. E. Baylis
Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4
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In a new extension of the Dirac-Fock method, calculations have been performed on the 80 electrons of mercury (in 22 *nlj* orbitals) plus one continuum electron of negative energy less than $-mc^2$. The asymptotic form of the numerical wave function of the negative-energy electron determines the phase shifts for the elastic scattering of positrons on Hg. The self-consistent-field calculations include the usual exchange interaction between electrons. The exchange between the bound Hg electrons and the negative-energy continuum electron represents the positron-electron annihilation-creation process. Such effects are usually computed in quantum electrodynamics to some order of approximation in a perturbation expansion. We believe ours is the first Dirac-Fock calculation of this effect, but we find its influence on the elastic positron scattering to be negligible.

I. INTRODUCTION

Low-energy positron scattering on atoms is usually calculated by treating the positron as a positively charged point particle that happens to have the same mass as the electron but is distinguishable from it. Calculations typically solve the one-particle Schrödinger[1,2] or Dirac[3] equation and include in the interaction only the direct electromagnetic terms, possibly an effective induced polarization potential and, if the Schrödinger equation is used, the spin-orbit correction.

Using the charge-conjugate relation between the positron and the electron and the *CPT* invariance of the electroweak interaction, the Stückelberg-Feynman picture of antifermions suggests that in the framework of the Dirac theory, it is more proper to consider the positron to be a negative-energy electron moving backward in time.[4] This, of course, is the way that positron interactions, such as Bhabha scattering (electron-positron scattering), are usually calculated in quantum electrodynamics.[5] Here we report what we believe to be the first Dirac-Fock (or relativistic Hartree-Fock) calculation involving both positive- and negative-energy electrons, as well as the first such calculation of the pair annihilation-creation process.

II. THEORY

The Dirac-Fock formulation of elastic positron scattering is the same as for elastic electron scattering[6] and is based on the theory and codes developed by Grant[7] and Desclaux.[8] As for (positive-energy) electron scattering, the scattering equation is the radial Dirac equation (in atomic units)

$$\left[\frac{d}{dr}+\frac{\kappa}{r}\right]P_\kappa(r)=\left[\frac{2}{\alpha}+\alpha[E-V(r)]\right]Q_\kappa(r)+X_Q(r)\ ,$$
$$\left[\frac{d}{dr}-\frac{\kappa}{r}\right]Q_\kappa(r)=-\alpha[E-V(r)]P_\kappa(r)-X_P(r)\ , \tag{1}$$

where $\alpha=c^{-1}=1/137.036$ is the fine-structure constant, but now the energy E is large and negative instead of small and positive. In terms of the asymptotic kinetic energy ε of the positron, $E=-2mc^2-\varepsilon=-2\alpha^{-2}-\varepsilon$. In terms of ε, Eq. (1) can be written

$$\left[\frac{d}{dr}+\frac{\kappa}{r}\right]P_\kappa(r)=-\alpha[\varepsilon+V(r)]Q_\kappa(r)+X_Q(r)\ ,$$
$$\left[\frac{d}{dr}-\frac{\kappa}{r}\right]Q_\kappa(r)=\left[\frac{2}{\alpha}+\alpha[\varepsilon+V(r)]\right]P_\kappa(r)-X_P(r)\ . \tag{2}$$

When comparing Eqs. (1) and (2), the scattering of positive- and negative-energy electrons is also seen to be related by the interchanges $E\leftrightarrow\varepsilon$, $P_\kappa\leftrightarrow Q_{-\kappa}$, $V\leftrightarrow -V$, and $X_Q\leftrightarrow -X_P$. This relation is simply a manifestation of the *CPT* symmetry of the Dirac theory; it provides a basis for the usual positron picture. Since the signs of the interaction terms have been reversed, Eq. (2) may be interpreted as describing an $m=1$ particle of positive unit charge $e=1$ (a positron), and whereas P (Q) is the large (small) component of the Dirac spinor for low-energy ($|E|\ll mc^2$) electrons, their roles are reversed for low-energy positrons ($|\varepsilon|\ll mc^2$). For both electrons and positrons, the quantum number $\kappa=\pm(j+\frac{1}{2})$ corresponds to the orbital angular momentum number $l=j\pm\frac{1}{2}$ associated with the larger component.

The total effective interaction potential may be written

$$V(r)=V_{\rm FC}(r)+V_{\rm pol}(r) \tag{3}$$

where the frozen-core potential $V_{\rm FC}$ is defined by

$$V_{\rm FC}(r)=-\frac{Z}{r}+\sum_{n,k}a^k(s,n)Y^k(n,n,r) \tag{4}$$

and

$$Y^k(n,n';r)=r^{-k}\int_0^r F(q)q^k dq+r^{k+1}\int_r^\infty F(q)q^{-k-1}dq \tag{5}$$

with

$$F(q)=P_n(q)P_{n'}(q)+Q_n(q)Q_{n'}(q). \tag{6}$$

The sum in (4) is over all electrons n in the target; the index s refers to the scattering electron or positron. The angular coefficients a^k have been given explicitly by Grant[7,8] The model polarization potential $V_{\rm pol}(r)$ is the lowest-order correlation correction to the interaction between the scattered particle and the frozen core (here the target atom). For a negative-energy electron moving backward in time, the polarization potential is repulsive.

In electron calculations, $X_P(r)$ [or $X_Q(r)$] is the exchange term for the component $P_\kappa(r)$ [or $Q_\kappa(r)$] of the Dirac wave function:

$$\begin{aligned} rX_P &= \alpha\sum_{n,k} b^k(s,n)Y^k(s,n;r)P_n \ , \\ rX_Q &= \alpha\sum_{n,k} b^k(s,n)Y^k(s,n;r)Q_n \ , \end{aligned} \tag{7}$$

where b^k are also standard angular coefficients.[7] In previous calculations of positron scattering from atomic targets, the positron has been treated as a distinct particle and the exchange terms X_P and X_Q have been dropped from the equations. However, when the process is considered to be the scattering of a negative-energy electron, the fermion statistics of electrons leads naturally to such "exchange" terms. In fact, within the picture of positron scattering, the same terms represent electron-positron annihilation and creation. The equivalence of the exchange and annihilation-creation diagrams can be seen by the *CPT* crossing method common in the relation of Möller (e^-e^-) to Bhabha (e^+e^-) scattering (see Fig. 1).[5] As the incident positron annihilates a bound electron, a new electron-positron pair is created.

The pair annihilation-creation process is usually calculated in quantum electrodynamics (QED) as a perturbation series of Feynman diagrams representing the transfer of virtual photons between fermions. In the Dirac-Fock calculation, the wave function of the negative-energy continuum electron is adjusted to be an eigenfunction of the Dirac Hamiltonian including the exact "electron exchange" interaction with the frozen target. Such "exchange" represents pair annihilation and creation, and the Dirac-Fock calculation of this process is equivalent to a sum over all atomic electrons of diagrams interchanging an arbitrary number of virtual quanta with the continuum positron in the Furry representation[9] (in which the interactions of the fermions with the "external" atomic field include contributions from all order of $Z\alpha$). Of course there are many QED diagrams which are omitted, for example, modifications of the process arising from vacuum polarization and self-energy. The only diagrams effectively included are tree-level ones with ladder extensions.

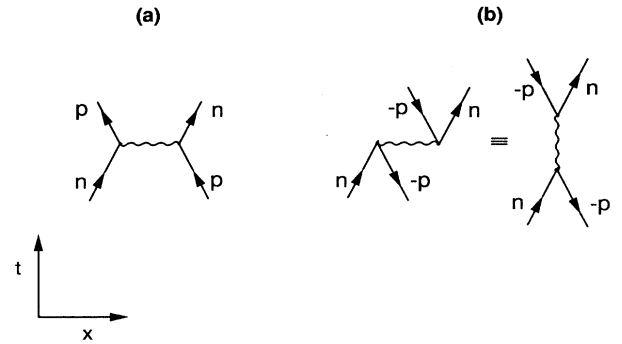

FIG. 1. The crossing relation is shown between the electron exchange (a) and the electron-positron annihilation-creation process (b). Here p is the four-momentum of the incident positron and n labels a bound electron. The photon exchanged is generally off shell (virtual). The calculation here was made not with perturbation theory but as part of a self-consistent Dirac-Fock calculation.

The pair annihilation-creation effect is much smaller than the usual exchange between positive-energy electrons because in the *CPT* crossing, as seen above, the roles of the 'small" and "large" components of the Dirac spinor are interchanged. As a result, the amplitude for the annihilation-creation process is down by a factor of the fine-structure constant at low incident positron energies compared to the size of the usual electron-electron exchange amplitude. Nevertheless, since exchange has a major effect in normal electron scattering and had not been previously considered in cases of a negative-energy electron, it seemed worthwhile to investigate effects of the corresponding annihilation-creation process on the relativistic dynamics of positron scattering. We were particularly interested in whether the process might provide an observable spin polarization of positrons scattered from heavy targets. In previous calculations, such polarization was found to be negligible because, due to Coulomb repulsion, the positron wave function is strongly suppressed near the positively charged nucleus where the spin-orbit interaction is significant.[2] It was conceivable that the annihilation-creation process might reduce the suppression of the wave function and make the spin polarization larger.

III. NUMERICAL METHOD

To test the influence of the pair annihilation-creation process on positron scattering, we have chosen the heavy target atom mercury. Both differential and total cross sections for elastic scattering, as well as the phase differences responsible for spin polarization of the positron, have been calculated. We treat the target atom as a frozen core to which correlation corrections have been added in the form of a model core-polarization potential.[10] A modified version of the Desclaux code[9,11] has been used for the computations. Analogous calculations have been successfully carried out for electron scattering on noble-gas targets.[6]

Two different models have been used in the calculations presented here (see inset in Fig. 2). One is the potential employed in previous electron-Hg scattering calculations:[12]

$$V_{\rm pol}^{(1)}(r)=\tfrac{1}{2}\alpha_d\frac{r^2}{(r^3+r_0^3)^2} \tag{8}$$

where $\alpha_d=44.9a_0^3$ is the static dipole polarizability of the target atom[13] and $r_0=3.0a_0$ represents the size of the tar-

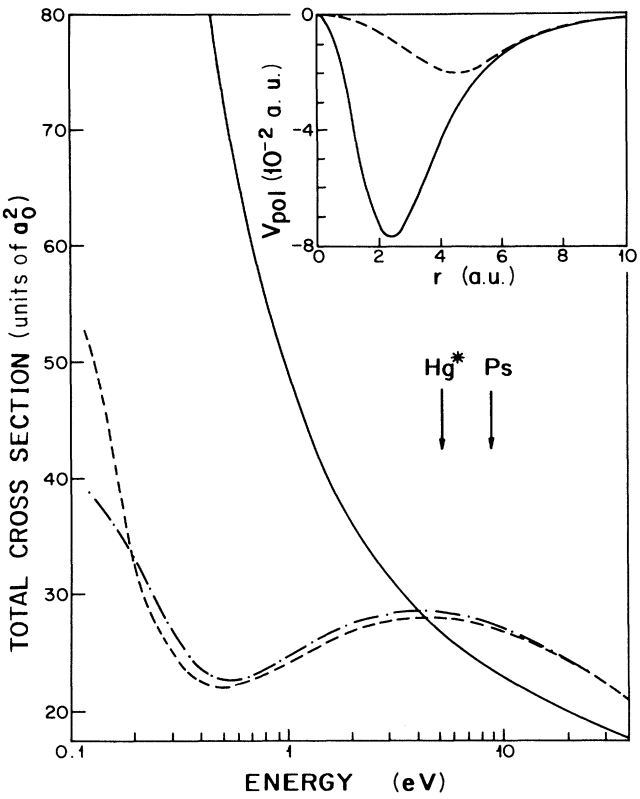

FIG. 2. Total cross section for elastic scattering of positrons on Hg: the solid line gives our results with polarization potential $V_{pol}^{(I)}(r)$; the dot-dashed line gives our results with the polarization potential $V_{pol}^{(II)}(r)$; the dashed line represents results of Sin Fai Lam (Ref. 1). Arrows show the threshold of excitation and, at higher energy, of positronium formation. The inset compares the polarization potentials: the solid line is $V_{pol}^{(I)}(r)$; the dashed line, $V_{pol}^{(II)}(r)$.

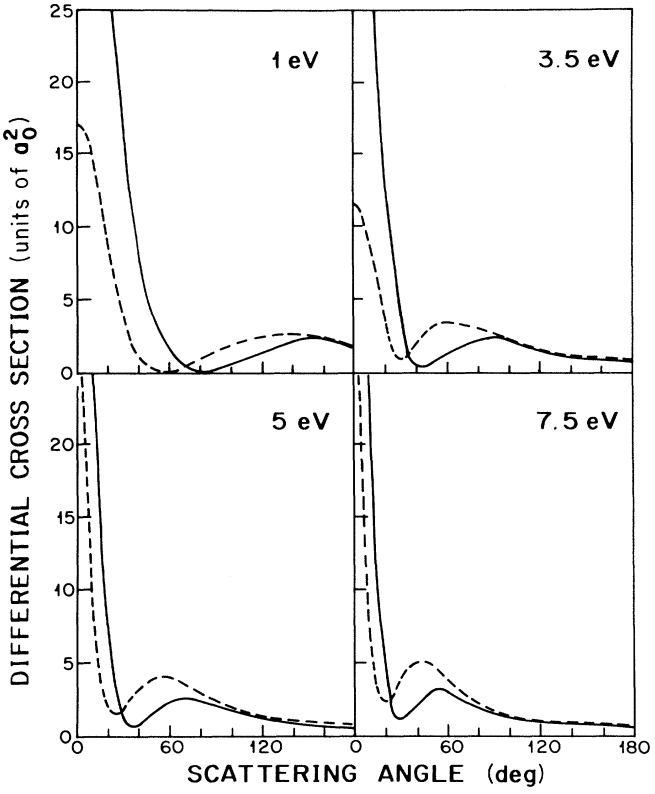

FIG. 3. Differential cross sections for elastic scattering of positrons on Hg: the solid line shows our results with $V_{pol}^{(I)}(r)$; the dashed line, our results with $V_{pol}^{(II)}(r)$.

get atom and serves as a cutoff radius. The other model is that used by Sin Fai Lam[1] in his positron-Hg calculations:

$$V_{pol}^{(II)}(r)=\frac{\alpha_d'}{2r^4}[1-\exp(-r/r_c)^6] \tag{9}$$

where $\alpha_d'=33.796a_0^3$ and $r_c=4.8a_0$.

The scattering equation (1) is solved subject to the boundary conditions $P_\kappa(0)=Q_\kappa(0)=0$. Phase shifts $\delta_l^\pm$ are obtained by comparing the numerical solutions of Eq. (1) to the asymptotic ones at large r:

$$\frac{P_\kappa(r)}{r}\sim j_l(kr)\cos\delta_l^\pm - n_l(kr)\sin\delta_l^\pm \tag{10}$$

where k is the momentum of the incident electron, and $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions. For each $l>0$ we have two scattering equations (1) corresponding to the different values of κ. We let δ_l^+ be the phase shift for $\kappa=-l-1$ (corresponding to $j=l+\frac{1}{2}$) and δ_l^- be that for $\kappa=l$ (corresponding to $j=l-\frac{1}{2}$).

In this work we calculate the relativistic phase shifts $\delta_l^\pm$ from $l=0$ to 6, and from the phase shifts we determine both the total (Fig. 2) and differential (Fig. 3) cross sections. For the differential cross sections (Fig. 3) at energies of 5 and 7.5 eV, the phase shifts for higher l up to $l=50$ were extrapolated using the nonrelativistic effective formula of Ali and Fraser.[14] At lower energies, contributions of phase shifts greater than $l=6$ were small and could be ignored.

IV. RESULTS AND DISCUSSION

When the "exchange" interaction between the negative-energy continuum electron and the bound target electrons is omitted, calculated results reproduce those found by the more common procedure[1-3] of treating the positron as a positively charged, distinguishable particle. When "exchange" (the pair annihilation-creation process) is added, the changes are minimal. The scattering phase shifts δ_l^+ are presented in Table I for energies from 0.01 to 800 eV. The polarization effects arise from the difference in phase shifts $\Delta\delta_l\equiv\delta_l^+-\delta_l^-$ for the relativistic scattering wave functions for a given orbital angular

TABLE I. Elastic phase shifts δ_l^+ in radians for positrons on Hg.

E (eV)	δ_0^+	δ_1^+	δ_2^+	δ_3^+	δ_4^+	δ_5^+	δ_6^+
0.01	0.2290	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000
0.02	0.3021	0.0028	0.0000	0.0000	0.0000	0.0000	0.0000
0.05	0.3987	0.0107	0.0002	0.0000	0.0000	0.0000	0.0000
0.10	0.4420	0.0287	0.0011	0.0000	0.0000	0.0000	0.0000
0.20	0.4416	0.1083	0.0198	0.0064	0.0032	0.0017	0.0012
0.50	0.2901	0.2079	0.0494	0.0166	0.0079	0.0049	0.0035
1.00	0.0964	0.2789	0.0935	0.0331	0.0160	0.0089	0.0060
2.00	−0.1690	0.2808	0.1585	0.0641	0.0318	0.0180	0.0121
3.50	−0.4364	0.1969	0.2060	0.1030	0.0542	0.0312	0.0195
5.00	−0.6296	0.0990	0.2146	0.1315	0.0744	0.0418	0.0277
7.50	−0.8720	−0.0507	0.1873	0.1580	0.0990	0.0603	0.0405
10.00	−1.0569	−0.1810	0.1397	0.1651	0.1180	0.0761	0.0528
12.50	−1.2069	−0.2941	0.0856	0.1592	0.1303	0.0894	0.0608
15.00	−1.3335	−0.3933	−0.0012	0.1456	0.1405	0.1000	0.0702
20.00	−1.5396	−0.5611	−0.0699	0.1050	0.1380	0.1106	0.0852
35.00	−1.9570	−0.9178	−0.3193	−0.0344	0.0788	0.1126	0.1021
50.00	−2.2343	−1.1631	−0.5030	−0.1610	0.0039	0.0736	0.0976
100.00	−2.7847	−1.6940	−0.8991	−0.4597	−0.2103	−0.0691	0.0069
150.00	−3.1094	−1.9666	−1.1490	−0.6547	−0.3670	−0.1885	−0.0831
500.00	−3.9919	−2.8169	−1.9349	−1.3142	−0.8862	−0.6060	−0.4370
800.00	−4.2555	−3.0781	−2.2029	−1.5647	−1.1064	−0.7992	−0.5579

TABLE II. Phase-shift differences $\Delta\delta_l \equiv \delta_l^+ - \delta_l^-$ for positron scattering on mercury atoms in units of 10^{-5} rad. (a) Present calculations. (b) Hasenberg (Ref. 2).

	$E=35$ eV		$E=150$ eV		$E=800$ eV	
l	(a)	(b)	(a)	(b)	(a)	(b)
1	2.96	3.05	9.99	9.92	44.20	44.23
2	2.42	2.58	10.49	10.97	55.04	52.91
3	1.36	1.34	7.86	8.97	49.89	49.88
4	0.53	0.38	5.63	6.29	38.47	42.25
5	0.07	0.02	3.86	4.10	29.31	34.05

momentum number l and for $j=l\pm\frac{1}{2}$. Table II shows these phase-shift differences for $l=1$ to 5 and for three energies of the incident positron. As may be seen, the differences increase with increasing incident energy. The results agree well with recent calculations of Hasenburg,[2] who used a nonrelativistic scattering calculation with a Dirac-Fock Hg charge density, a spin-orbit potential, and a distinct polarization potential. To the accuracy shown, our results are independent of whether or not the pair annihilation-creation process is included. Spin polarization effects generally remain at or below the 10^{-4} level and are hence very difficult to observe experimentally.

The total and differential cross sections calculated with the phase shifts are shown in Figs. 2 and 3. The results at low energies and small scattering angles are seen to be sensitive to the model polarization potential $V_{\rm pol}(r)$. When we use the same model potential $V_{\rm pol}^{(\rm II)}(r)$ as Sin Fai Lam,[1] our total cross sections agree well with his. However, our stronger model polarization potential $V_{\rm pol}^{(\rm I)}(r)$ gives a significantly larger cross section at low energies and small scattering angles. As far as we know, there are no experimental data that would confirm or rule out either model potential.

V. CONCLUSIONS

The first Dirac-Fock calculations have been made in which both positive- and negative-energy electrons are present. The negative-energy continuum electron represents a free positron, and its asymptotic wave function gives phase shifts and cross sections which are in good agreement with traditional calculations in which the positron is treated as a positively charged particle unrelated to the electrons. The usual exchange between electrons represents a virtual pair annihilation and creation in the positron picture. We believe ours to be the first Dirac-Fock calculation of this effect, which, however, is small and has little effect on the low-energy elastic scattering. Even when the annihilation-creation process is included, the spin polarization of positrons scattered from mercury lies well below present observational capabilities.[15]

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*Permanent address: Institute of Theoretical Physics and Astrophysics, University of Gdansk, 80-952 Gdansk, Poland.

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