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The relativistic polarized orbital theory of the elastic electron and positron scattering from closed-shell atoms

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Abstract. The relativistic polarized orbital theory of the elastic electron and positron scattering from closed-shell atoms is formulated in a similar way to that used in the non-relativistic case. The scattering equations involving the relativistic polarization potential for both types of projectile and also the exchange-polarization terms for the electron projectile are derived. The relativistic formula for the positron-atomic-electron annihilation coefficient Z_{eff} is presented.

1. Introduction

More than twenty years have passed since first serious attempts to study relativistic effects in low-energy electron- and positron-atom collisions. The most natural way was the generalization of non-relativistic theories and significant progress has been made in this direction. Walker (1969, 1970, 1971) attacked the problem by solving the continuous state Dirac-Fock equations. Carse and Walker (1973) formulated the electron-hydrogenic-ion scattering theory via the close-coupling formalism. Again Walker (1974, 1975) considered electron impact excitation of hydrogenic ions in the Coulomb-Born approximation using the Dirac wavefunctions. Chang (1975) presented the formulation of the R-matrix theory for systems with the Dirac Hamiltonian while Scott and Burke (1980) formulated the R-matrix method for the Breit-Pauli Hamiltonian. Johnson and co-workers (Johnson and Cheng 1979, Lee and Johnson 1980) and Chang (1983) gave the relativistic generalization of the quantum defect theory. More recently, Jaskólski and Karwowski (1986) and Jaskólski (1989) have dealt with the problem using their quasirelativistic scattering theory. On the whole, about a hundred papers have been published in which relativistic effects in low-energy $e^{\mp}$-atom collisions have been studied. But it is apparent that relativistic calculations on electron- and positron-atom collisions have achieved none of the sophistication of their non-relativistic counterparts.

Among non-relativistic $e^{\mp}$-atom or molecule scattering theories one of the most fruitful is the polarized orbital method. It was formulated originally by Temkin (1957) and applied with great success to a variety of electronic collisions. For details of the method and examples of its applications see the extensive review of Drachman and Temkin (1972). Walker (1970) used the relativistic polarized orbital method in its very simplified version to take into account the effect of the target distortion on e^- scattering from mercury. Later, Kemper *et al* (1984, 1985) applied his method to relativistic two-channel calculations of electron–noble-gas-atom scattering. However, a fully relativistic formulation of the polarized orbital method has not yet been presented and the goal of this paper is to fill this gap.

2. Formulation of the problem

We are concerned with the problem of low-energy elastic electron or positron scattering from atoms. The nucleus is assumed to be an infinitely heavy point charge $+Ze$. We neglect all second-order magnetic interactions (i.e. spin–spin, spin–other-orbit and orbit–orbit) as well as retardation effects. The complete Dirac equation for the considered system is

$$(H^0 + t + V^\mp + U^\mp - E)\cdot\Xi^\mp = 0 \tag{1}$$

where H^0 is an unperturbed target Dirac Hamiltonian, t is a kinetic energy operator of the projectile (including a rest energy operator):

$$t = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 \tag{2}$$

where $\boldsymbol{\alpha}$ and β have their usual meanings (Schiff 1968),

$$U^\mp(x) = \mp Ze^2/x \tag{3}$$

and

$$V^\mp(\boldsymbol{r},\boldsymbol{x}) = \sum_{i=1}^{N} h_i^\mp = \sum_{i=1}^{N} \frac{\pm e^2}{|\boldsymbol{r}_i - \boldsymbol{x}|} \tag{4}$$

where N is a number of target electrons and $\boldsymbol{r}_i$ denotes the position vector of the ith target electron. The upper sign in equations (1), (3) and (4) concerns the electron projectile, while the lower one applies to the positron. The projectile is described by the coordinate $\boldsymbol{x}$. It emphasizes the fact that in the polarized orbital method, which we shall develop below, the incident particle is treated quite unsymmetrically even if it is an electron.

We expand the total wavefunctions $\Xi^\mp(\boldsymbol{r},\boldsymbol{x})$ in terms of the orthonormal sets of functions $\Psi^\mp_{\mathrm{AD}i}(\boldsymbol{r},\boldsymbol{x})$ with associated energy eigenvalues $E^\mp_{\mathrm{AD}i}(\boldsymbol{x})$ generated by the adiabatic Hamiltonians $H^\mp_{\mathrm{AD}} = H^0 + V^\mp$:

$$H^\mp_{\mathrm{AD}}\Psi^\mp_{\mathrm{AD}i} = E^\mp_{\mathrm{AD}i}(\boldsymbol{x})\cdot\Psi^\mp_{\mathrm{AD}i}. \tag{5}$$

Therefore we have

$$\Xi^+(\boldsymbol{r},\boldsymbol{x}) = \sum_i \chi_i^+(\boldsymbol{x})\cdot\Psi^+_{\mathrm{AD}i}(\boldsymbol{r},\boldsymbol{x}) \tag{6a}$$

and

$$\Xi^-(\boldsymbol{r},\boldsymbol{x}) = \hat{\mathscr{A}}\sum_i \chi_i^-(\boldsymbol{x})\cdot\Psi^-_{\mathrm{AD}i}(\boldsymbol{r},\boldsymbol{x}) \tag{6b}$$

where $\hat{\mathscr{A}}$ is an antisymmetrization operator and summations run over all states including continuum states. If in equations (6a) and (6b) all terms with $i>0$ are neglected (i.e. if we suppose that only ground states $\Psi^\mp_{\mathrm{AD}i=0}$ of the adiabatic Hamiltonians $H^\mp_{\mathrm{AD}}$ contribute to the above expansions), the mathematical prescriptions for the total *adiabatic* wavefunctions are

$$\Xi^+_{\mathrm{AD}}(\boldsymbol{r},\boldsymbol{x}) = \chi^+(\boldsymbol{x})\cdot\Psi^+_{\mathrm{AD}}(\boldsymbol{r},\boldsymbol{x}) \tag{7a}$$

$$\Xi^-_{\mathrm{AD}}(\boldsymbol{r},\boldsymbol{x}) = \hat{\mathscr{A}}\chi^-(\boldsymbol{x})\cdot\Psi^-_{\mathrm{AD}}(\boldsymbol{r},\boldsymbol{x}). \tag{7b}$$

In equations (6*a*)–(7*b*) $\boldsymbol{r}$ stands for all atomic electron coordinates and $\Psi^{\mp}_{\mathrm{AD}}$ are already antisymmetric in $\boldsymbol{r}_i$, $i=1,\ldots,N$. We have omitted $i=0$ subscripts for brevity.

In order to determine $\chi^{\mp}$ we replace $\Xi^{\mp}$ in equation (1) by $\Xi^{\mp}_{\mathrm{AD}}$ and project the obtained Dirac equation onto the ground state Φ^0 of the *isolated* target. Integration over all coordinates of the target electrons leads to the following scattering equations

$$(t+U^{+}(\boldsymbol{x})+E^{+}_{\mathrm{AD}}(\boldsymbol{x})-E)\cdot\chi^{+}(\boldsymbol{x})=0 \tag{8a}$$

$$\int \mathrm{d}^{3N}\boldsymbol{r}\,\Phi^{0}(\boldsymbol{r})^{*}\hat{\mathscr{A}}\Psi^{-}_{\mathrm{AD}}(\boldsymbol{r},\boldsymbol{x})\cdot(t+U^{-}(\boldsymbol{x})+E^{-}_{\mathrm{AD}}(\boldsymbol{x})-E)\cdot\chi^{-}(\boldsymbol{x})=0. \tag{8b}$$

Therefore, the above considerations divided the scattering problem into two parts: the calculation of the distorted (adiabatic) target wavefunctions $\Psi^{\mp}_{\mathrm{AD}}$ and the calculation of the scattering functions $\chi^{\mp}$. We deal with the first problem in section 3 and with the second in section 4.

3. The polarized orbitals

In the polarized orbital method the adiabatic wavefunction is assumed to have determinantal form

$$\Psi^{\mp}_{\mathrm{AD}}=(N!)^{-1/2}\cdot\det|\psi^{\mp}_1,\psi^{\mp}_2,\ldots,\psi^{\mp}_N| \tag{9}$$

where the one-electron polarized orbital $\psi^{\mp}_a$ is

$$\psi^{\mp}_a(\boldsymbol{r}_i,\boldsymbol{x})=\varphi^0_a(\boldsymbol{r}_i)+\varphi^{1\mp}_a(\boldsymbol{r}_i,\boldsymbol{x}). \tag{10}$$

Here φ^0_a is the unperturbed orbital and $\varphi^{1\mp}_a$ is the x-dependent correction due to the interaction $V^{\mp}$. To first order in the perturbation we have

$$\Psi^{\mp}_{\mathrm{AD}}=\Phi^0+\Phi^{1\mp} \tag{11}$$

where

$$\Phi^0=(N!)^{-1/2}\cdot\det|\varphi^0_1,\varphi^0_2,\ldots,\varphi^0_N| \tag{12}$$

and

$$\Phi^{1\mp}=(N!)^{-1/2}\sum_{a=1}^{N}\det|\varphi^0_1,\varphi^0_2,\ldots,\varphi^{1\mp}_a,\ldots,\varphi^0_N|. \tag{13}$$

The coupled Dirac–Fock equations (CDF) are obtained by minimizing the adiabatic energy values $E^{\mp}_{\mathrm{AD}}(\boldsymbol{x})=\langle\Psi^{\mp}_{\mathrm{AD}}|H^{\mp}_{\mathrm{AD}}|\Psi^{\mp}_{\mathrm{AD}}\rangle$ subject to the orthonormality constraints of the $\psi^{\mp}_a$. By treating $V^{\mp}$ as a perturbation and retaining only first-order terms in the $\varphi^{1\mp}_a$ we find that φ^0_a are just the usual Dirac–Fock orbitals satisfying the following equations

$$\left[h^0_1+\sum_c^{\mathrm{occ}}\left(\langle\varphi^0_c|\frac{e^2}{r_{12}}|\varphi^0_c\rangle-|\varphi^0_c\rangle\frac{e^2}{r_{12}}\langle\varphi^0_c|\right)\right]|\varphi^0_a\rangle-\sum_c^{\mathrm{occ}}E^0_{ca}|\varphi^0_c\rangle=0 \tag{14}$$

where

$$h^0_1=c\boldsymbol{\alpha}\cdot\boldsymbol{p}_1+\beta mc^2-Ze^2/r_1 \tag{15}$$

while the $\varphi_a^{1\mp}$ satisfy the CDF equations

$$\left[h_1^0+\sum_c^{\rm occ}\left(\langle\varphi_c^0|\frac{e^2}{r_{12}}|\varphi_c^0\rangle-|\varphi_c^0\rangle\frac{e^2}{r_{12}}\langle\varphi_c^0|\right)\right]|\varphi_a^{1\mp}\rangle-\sum_c^{\rm occ}E_{ca}^0|\varphi_c^{1\mp}\rangle$$
$$=-\left[h_1^{\mp}+\sum_c^{\rm occ}\hat\delta_c^{\mp}\left(\langle\varphi_c^0|\frac{e^2}{r_{12}}|\varphi_c^0\rangle-|\varphi_c^0\rangle\frac{e^2}{r_{12}}\langle\varphi_c^0|\right)\right]|\varphi_a^0\rangle+\sum_c^{\rm occ}E_{ca}^{1\mp}|\varphi_c^0\rangle \tag{16}$$

where $\hat\delta_c^{\mp}$ is the replacement operator:

$$\hat\delta_c^{\mp}\langle\varphi_c^0|\frac{1}{r_{12}}|\varphi_c^0\rangle=\langle\varphi_c^{1\mp}|\frac{1}{r_{12}}|\varphi_c^0\rangle+\langle\varphi_c^0|\frac{1}{r_{12}}|\varphi_c^{1\mp}\rangle \tag{17a}$$

$$\hat\delta_c^{\mp}|\varphi_c^0\rangle\frac{1}{r_{12}}\langle\varphi_c^0|=|\varphi_c^{1\mp}\rangle\frac{1}{r_{12}}\langle\varphi_c^0|+|\varphi_c^0\rangle\frac{1}{r_{12}}\langle\varphi_c^{1\mp}| \tag{17b}$$

and $h_1^{\mp}$ is defined by equation (4) with $i=1$. An explicit expression for the Lagrange multiplier corrections $E_{ca}^{1\mp}(x)$ can be easily obtained from equation (16):

$$E_{ca}^{1\mp}(x)=\langle\varphi_c^0|h_1^{\mp}|\varphi_a^0\rangle+\sum_d^{\rm occ}\hat\delta_d^{\mp}\left(\langle\varphi_c^0\varphi_d^0|\frac{e^2}{r_{12}}|\varphi_a^0\varphi_d^0\rangle-\langle\varphi_c^0\varphi_d^0|\frac{e^2}{r_{12}}|\varphi_d^0\varphi_a^0\rangle\right). \tag{18}$$

It follows immediately from equations (16)-(18) that

$$\varphi_c^{1-}=-\varphi_c^{1+}\qquad\text{and}\qquad E_{ca}^{1-}=-E_{ca}^{1+}. \tag{19}$$

It means that it is sufficient to solve equation (16) only for φ_a^{1+} and then use equation (19). Therefore below we shall consider equations (16)-(18) with the lower sign (+) and we shall omit this sign for brevity.

Now we restrict ourselves to the closed-shell systems and reduce the CDF equations (16) to radial form following Grant's method for the Dirac-Fock equations (Grant 1970). We write the unperturbed orbital in the form

$$\varphi_a^0(\boldsymbol r)=\frac{1}{r}\cdot\begin{pmatrix}P_A(r)\cdot\Omega_a(\hat{\boldsymbol r})\\ \mathrm{i}Q_A(r)\cdot\tilde\Omega_a(\hat{\boldsymbol r})\end{pmatrix} \tag{20}$$

where $P_A(r)$ and $Q_A(r)$ are solutions of the radial Dirac-Fock equations and

$$\Omega_a(\hat{\boldsymbol r})\equiv\Omega_{\varkappa_A,m_a}(\hat{\boldsymbol r})\qquad\tilde\Omega_a(\hat{\boldsymbol r})\equiv\Omega_{-\varkappa_A,m_a}(\hat{\boldsymbol r}) \tag{21}$$

are standard angular momentum eigenfunctions with

$$\varkappa_A=(2j_A+1)\cdot(l_A-j_A). \tag{22}$$

It is convenient to expand the correction φ_a^1 as

$$\varphi_a^1(\boldsymbol r,x)=\sum_{k=0}^{\infty}\sum_{q=-k}^{+k}\sum_b d^{kq}(a,b)\cdot C_q^{k*}(\hat{\boldsymbol x})\cdot\frac{1}{r}\cdot\begin{pmatrix}P_{A\to B}^{(k)}(r,x)\cdot\Omega_b(\hat{\boldsymbol r})\\ \mathrm{i}Q_{A\to B}^{(k)}(r,x)\cdot\tilde\Omega_b(\hat{\boldsymbol r})\end{pmatrix} \tag{23}$$

where

$$d^{kq}(a,b)=(-1)^{m_b+1/2}\cdot\Lambda_k(A,B)\cdot\begin{pmatrix}j_B&k&j_A\\-m_b&q&m_a\end{pmatrix} \tag{24}$$

is an angular coefficient introduced by Grant (1970) with

$$\Lambda_k(A,B)=\Lambda_k(B,A)=[j_A\quad j_B]^{1/2}\cdot\begin{pmatrix}j_B&k&j_A\\\frac12&0&-\frac12\end{pmatrix}\cdot\pi(l_A,l_B,k) \tag{25}$$

with

$$\pi(l_A, l_B, k) = \begin{cases} 1 & \text{for } l_A + l_B + k \text{ even} \\ 0 & \text{for } l_A + l_B + k \text{ odd} \end{cases} \tag{26}$$

$[xy \ldots z] \equiv (2x+1)(2y+1)\ldots(2z+1)$, $C_q^k(\hat{x})$ is a spherical harmonic (Brink and Satchler 1968) and $P_{A\to B}^{(k)}(r, x)$ and $Q_{A\to B}^{(k)}(r, x)$ are radial functions which should be determined. The sum over b runs over all pairs $(\varkappa_B, m_b)$ for which $d^{kq}(a, b)$ does not vanish. We introduce the two-component radial orbitals

$$F_A(r) = \begin{pmatrix} P_A(r) \\ Q_A(r) \end{pmatrix} \tag{27}$$

and

$$F_{A\to B}^{(k)}(r, x) = \begin{pmatrix} P_{A\to B}^{(k)}(r, x) \\ Q_{A\to B}^{(k)}(r, x) \end{pmatrix}. \tag{28}$$

With the aid of equations(18), (21) and summation formulae (A2)–(A5) for $d^{kq}(a, b)$ coefficients given in the appendix, the CDF equations (16) for closed-shell systems can be rewritten as a set of coupled radial integro-differential equations

$$\begin{aligned} &\begin{pmatrix} mc^2 - E_A - \dfrac{Z(r)\cdot e^2}{r} & -c\hbar\cdot\left(\dfrac{\mathrm{d}}{\mathrm{d}r} - \dfrac{\varkappa_B}{r}\right) \\ c\hbar\cdot\left(\dfrac{\mathrm{d}}{\mathrm{d}r} + \dfrac{\varkappa_B}{r}\right) & -mc^2 - E_A - \dfrac{Z(r)\cdot e^2}{r} \end{pmatrix} \cdot F_{A\to B}^{(k)}(r, x) \\ &\quad = \sum_{\nu=0}^{\infty} \sum_{C}^{\mathrm{occ}} \frac{\Lambda_\nu^2(B, C)}{[j_B]} \cdot \frac{e^2}{r} \cdot R_\nu(F_C, F_{A\to B}^{(k)}|r, x) \cdot F_C(r) \\ &\quad - \sum_{C}^{\mathrm{occ}} \sum_{\varkappa_D} \Bigg[2\cdot \frac{\Lambda_k^2(C, D)}{[k]} \cdot \frac{e^2}{r} \cdot R_k(F_C, F_{C\to D}^{(k)}|r, x) \cdot F_A(r) \\ &\quad - \sum_{\nu=0}^{\infty} \Bigg(\Gamma_{DCBA}^{k\nu} \cdot \frac{e^2}{r} \cdot R_\nu(F_A, F_{C\to D}^{(k)}|r, x) \cdot F_C(r) \\ &\quad + \Gamma_{CDBA}^{k\nu} \cdot \frac{e^2}{r} \cdot Y_\nu(F_A, F_C|r) \cdot F_{C\to D}^{(k)}(r, x) \Bigg) \Bigg] \\ &\quad + e^2 \cdot \gamma_k(r, x) \cdot F_A(r) + e^2 \cdot \sum_{C}^{\mathrm{occ}} \lambda_{CA}^{(k)}(x) \cdot F_C(r) \cdot \delta_{\varkappa_B \varkappa_C} \end{aligned} \tag{29}$$

where $E_A \equiv E_{AA}^0$,

$$Z(r) = Z - \sum_{C}^{\mathrm{occ}} [j_C] \cdot Y_0(F_C, F_C|r) \tag{30}$$

$$\gamma_k(r, s) = r_<^k / r_>^{k+1} \tag{31}$$

with $r_< = \min(r, s)$ and $r_> = \max(r, s)$,

$$Y_\nu(F_A, F_B|r) = r \cdot \int_0^\infty \mathrm{d}s\, \gamma_\nu(s, r) \cdot (P_A(s)\cdot P_B(s) + Q_A(s)\cdot Q_B(s)) \tag{32}$$

$$\begin{aligned} &R_\nu(F_A, F_{B\to C}^{(k)}|r, x) \\ &\quad = r \cdot \int_0^\infty \mathrm{d}s\, \gamma_\nu(s, r) \cdot (P_A(s)\cdot P_{B\to C}^{(k)}(s, x) + Q_A(s)\cdot Q_{B\to C}^{(k)}(s, x)) \end{aligned} \tag{33}$$

and

$$\lambda_{AB}^{(k)}(x) = -\frac{1}{x} \cdot Y_k(F_A, F_B|x) + \sum_{C}^{\mathrm{occ}} \sum_{\kappa_D} \left(2 \cdot \frac{\Lambda_k^2(C, D)}{[k]} \cdot W_k(F_A, F_B; F_{C\to D}^{(k)}, F_C|x) \right.$$
$$- \sum_{\nu=0}^{\infty} [\Gamma_{CDBA}^{k\nu} \cdot W_\nu(F_A, F_C; F_{C\to D}^{(k)}, F_B|x)$$
$$\left. + \Gamma_{CDAB}^{k\nu} \cdot W_\nu(F_B, F_C; F_{C\to D}^{(k)}, F_A|x)]\right) \tag{34}$$

with $W_\nu(F_A, F_B; F_{C\to D}^{(k)}, F_E|x)$ defined as

$$W_\nu(F_A, F_B; F_{C\to D}^{(k)}, F_E|x) = \int_0^\infty \mathrm{d}s \frac{1}{s} \cdot Y_\nu(F_A, F_B|s) \cdot (P_{C\to D}^{(k)}(s, x) \cdot P_E(s) + Q_{C\to D}^{(k)}(s, x) \cdot Q_E(s)). \tag{35}$$

A definition of the $\Gamma_{ABCD}^{k\nu}$ coefficients is given in the appendix. Note that $\lambda_{AB}^{(k)}(x) = \lambda_{BA}^{(k)}(x)$. Summations over C in equations (29), (30) and (34) run over all occupied subshells. We have also utilized the fact that for closed-shell systems the off-diagonal Lagrange multipliers E_{AB}^0 vanish (Johnson and Cheng 1985).

The non-relativistic counterpart of equation (29) was derived by McEachran *et al* (1977) and applied to calculations of the $e^{\mp}$ elastic scattering on noble gas atoms.

4. The scattering equations

With the aid of equations (11)–(13) the scattering equations (8*a*) and (8*b*) can be rewritten in the form

$$(t + V_S^+ + V_P^+ - \mathscr{E})|\chi^+\rangle = 0 \qquad \text{for } e^+ \text{ projectile} \tag{36}$$

$$\left(1 - \sum_a^{\mathrm{occ}} |\psi_a^-\rangle\langle\varphi_a^0|\right)(t + V_S^- + V_P^- - \mathscr{E})|\chi^-\rangle = 0 \qquad \text{for } e^- \text{ projectile} \tag{37}$$

where $V_S^{\mp}$ is a static potential

$$V_S^{\mp}(\boldsymbol{x}) = U^{\mp}(\boldsymbol{x}) \pm e^2 \cdot \sum_c^{\mathrm{occ}} \langle\varphi_c^0| \frac{1}{|\boldsymbol{r} - \boldsymbol{x}|} |\varphi_c^0\rangle \tag{38}$$

$V_P^{\mp}$ is a polarization potential

$$V_P^{\mp}(\boldsymbol{x}) = \pm e^2 \cdot \sum_c^{\mathrm{occ}} \langle\varphi_c^0| \frac{1}{|\boldsymbol{r} - \boldsymbol{x}|} |\varphi_c^{1\mp}\rangle \tag{39}$$

and $\mathscr{E}$ is an initial projectile energy (including the rest energy mc^2). Note that $V_S^-(\boldsymbol{x}) = -V_S^+(\boldsymbol{x})$ and because of equation (19) $V_P^-(\boldsymbol{x}) = V_P^+(\boldsymbol{x})$. In equation (37) the notation $\Sigma_a^{\mathrm{occ}} |\psi_a^-\rangle\langle\varphi_a^0|$ should be understood symbolically because ψ_a^- depends parametrically on an integration variable.

For closed-shell systems $V_S^{\mp}(\boldsymbol{x})$ and $V_P^{\mp}(\boldsymbol{x})$ are spherically symmetric and the scattering equations (36) and (37) can be reduced to radial form. Let us expand the scattering functions $\chi^{\mp}(\boldsymbol{x})$ as

$$\chi^{\mp}(\boldsymbol{x}) = \sum_d a_D^{\mp} \cdot (\Omega_d^*(\hat{\boldsymbol{K}}) \cdot A(\hat{\boldsymbol{K}})) \cdot \frac{1}{x} \cdot \begin{pmatrix} f_D^{\mp}(x) \cdot \Omega_d(\hat{\boldsymbol{x}}) \\ \mathrm{i} g_D^{\mp}(x) \cdot \tilde{\Omega}_d(\hat{\boldsymbol{x}}) \end{pmatrix} \tag{40}$$

where $\hat{\boldsymbol{K}}$ is a direction of the incident beam, the two-component normalized spinor $A(\hat{\boldsymbol{K}})$ specifies the spin direction of the projectile in its rest frame, while $a_D^{\mp}$ are some phase factors. If we introduce the two-component radial orbitals

$$S_D^{\mp}(x)=\begin{pmatrix} f_D^{\mp}(x) \\ g_D^{\mp}(x) \end{pmatrix} \tag{41}$$

then equations (36) and (37) take the form

$$\begin{pmatrix} mc^2-\mathscr{E}+V_S^+(x)+V_P^+(x) & -c\hbar\cdot(\mathrm{d}/\mathrm{d}x-\varkappa_D/x) \\ c\hbar\cdot(\mathrm{d}/\mathrm{d}x+\varkappa_D/x) & -mc^2-\mathscr{E}+V_S^+(x)+V_P^+(x) \end{pmatrix}\cdot S_D^+(x)=0 \tag{42}$$

and

$$\begin{aligned} &\begin{pmatrix} mc^2-\mathscr{E}+V_S^-(x)+V_P^-(x) & -c\hbar\cdot(\mathrm{d}/\mathrm{d}x-\varkappa_D/x) \\ c\hbar\cdot(\mathrm{d}/\mathrm{d}x+\varkappa_D/x) & -mc^2-\mathscr{E}+V_S^-(x)+V_P^-(x) \end{pmatrix}\cdot S_D^-(x) \\ &\quad=\sum_A^{\mathrm{occ}}(E_A-\mathscr{E})\cdot\Delta(F_A,S_D^-)\cdot F_A(x)\cdot\delta_{\varkappa_A\varkappa_D} \\ &\quad+e^2\cdot\sum_{k=0}^{\infty}\sum_{A,B}^{\mathrm{occ}}\frac{\Lambda_k^2(A,B)}{[j_A]}\cdot M_k(F_A,F_B;F_B,S_D^-)\cdot F_A(x)\cdot\delta_{\varkappa_A\varkappa_D} \\ &\quad-\sum_{k=0}^{\infty}\sum_{A}^{\mathrm{occ}}(E_A-\mathscr{E})\cdot\frac{\Lambda_k^2(A,D)}{[j_D]}\cdot G_{A\to D}^{(k)}(x) \\ &\quad-e^2\cdot\sum_{k=0}^{\infty}\sum_{\nu=0}^{\infty}\sum_{A,B}^{\mathrm{occ}}\sum_{\varkappa_C}\Gamma_{ABCD}^{k\nu}\cdot\frac{\Lambda_k^2(C,D)}{[j_D]}\cdot L_{BA\to D}^{(k\nu)}(x) \\ &\quad-e^2\cdot\sum_{k=0}^{\infty}\sum_{A,B}^{\mathrm{occ}}\sum_{\varkappa_C}\frac{\Lambda_k^2(B,C)}{[k]}\cdot N_k(F_B,F_{B\to C}^{(k)};F_A,S_D^-)\cdot F_A(x)\cdot\delta_{\varkappa_A\varkappa_D} \end{aligned} \tag{43}$$

where

$$V_S^{\mp}(x)=\mp\frac{Ze^2}{x}\pm e^2\cdot\sum_A^{\mathrm{occ}}[j_A]\cdot\frac{1}{x}\cdot Y_0(F_A,F_A|x)=\mp\frac{Z(x)\cdot e^2}{x} \tag{44}$$

$$V_P^{\mp}(x)=-e^2\cdot\sum_{k=0}^{\infty}\sum_{A}^{\mathrm{occ}}\sum_{\varkappa_B}\frac{\Lambda_k^2(A,B)}{[k]}\cdot\frac{1}{x}\cdot R_k(F_A,F_{A\to B}^{(k)}|x,x) \tag{45}$$

$$\Delta(F_A,S_B^-)=\int_0^{\infty}\mathrm{d}s\,(P_A(s)\cdot f_B^-(s)+Q_A(s)\cdot g_B^-(s)) \tag{46}$$

$$M_k(F_A,F_B;F_C,S_D^-)=\int_0^{\infty}\mathrm{d}s\frac{1}{s}\cdot Y_k(F_A,F_B|s)\cdot(P_C(s)\cdot f_D^-(s)+Q_C(s)\cdot g_D^-(s)) \tag{47}$$

$$\begin{aligned} G_{A\to B}^{(k)}(x)&=\begin{pmatrix} u_{A\to B}^{(k)}(x) \\ w_{A\to B}^{(k)}(x) \end{pmatrix} \\ &=\int_0^{\infty}\mathrm{d}s\,(P_A(s)\cdot f_B^-(s)+Q_A(s)\cdot g_B^-(s))\cdot\begin{pmatrix} P_{A\to B}^{(k)}(x,s) \\ Q_{A\to B}^{(k)}(x,s) \end{pmatrix} \end{aligned} \tag{48}$$

$$\begin{aligned} L_{AB\to C}^{(k\nu)}(x)&=\begin{pmatrix} y_{AB\to C}^{(k\nu)}(x) \\ z_{AB\to C}^{(k\nu)}(x) \end{pmatrix} \\ &=\int_0^{\infty}\mathrm{d}s\frac{1}{s}\cdot Y_k(F_A,F_B|s)\cdot(P_A(s)\cdot f_C^-(s)+Q_A(s)\cdot g_C^-(s))\cdot\begin{pmatrix} P_{B\to C}^{(\nu)}(x,s) \\ Q_{B\to C}^{(\nu)}(x,s) \end{pmatrix} \end{aligned} \tag{49}$$

and

$$N_\nu(F_A, F^{(k)}_{B\to C}; F_D, S^-_E)$$
$$= \int_0^\infty \mathrm{d}s \frac{1}{s} \cdot R_\nu(F_A, F^{(k)}_{B\to C}|s, s) \cdot (P_D(s) \cdot f^-_E(s) + Q_D(s) \cdot g^-_E(s)). \qquad (50)$$

The first two terms on the right-hand side of equation (43) are the static-exchange terms, while the last three ones are the exchange-polarization terms. In equation (43) we have neglected the term

$$\sum_a^{\mathrm{occ}} \langle \varphi^0_a | V^-_{\mathrm{P}} | \varphi^{1-}_a \chi^- \rangle \qquad (51)$$

which is of third order in the perturbation V^-.

Note that equation (45) gives the possibility of calculating the polarizabilities for closed-shell targets. Indeed, for $k > 0$ we have

$$\alpha_k = \lim_{x\to\infty} 2 \cdot \sum_A^{\mathrm{occ}} \sum_{\varkappa_B} \frac{\Lambda^2_k(A, B)}{[k]} \cdot x^{2k+1} \cdot R_k(F_A, F^{(k)}_{A\to B}|x, x). \qquad (52)$$

Equations (42) and (43) must be solved subject to the asymptotic conditions

$$f^\mp_D(0) = g^\mp_D(0) = 0 \qquad (53)$$

and for large x

$$f^\mp_D(x) \to \frac{4\pi}{K} \cdot \left(\frac{\mathscr{E} + mc^2}{2\mathscr{E}}\right)^{1/2} \cdot (\hat{j}_{l_D}(Kx) \cdot \cos \delta^{(\mp)}_{\varkappa_D} - \hat{n}_{l_D}(Kx) \cdot \sin \delta^{(\mp)}_{\varkappa_D}) \qquad (54)$$

where $\delta^{(\mp)}_\varkappa$ is the scattering phaseshift,

$$K^2 = (\mathscr{E} - mc^2) \cdot (\mathscr{E} + mc^2)/(c\hbar)^2 \qquad (55)$$

while $\hat{j}_l(Kx)$ and $\hat{n}_l(Kx)$ are the Riccati–Bessel functions. The upper and lower signs in equation (54) concern the electron and positron scattering respectively.

5. Annihilation coefficient Z_{eff}

During e^+–atom scattering one of the possible processes is the annihilation of a positron–atomic-electron pair. The cross section for this process is (Fraser 1968)

$$\sigma_A = Z_{\mathrm{eff}}(v) \cdot \frac{\pi \cdot r_0^2 \cdot c}{v} + \mathrm{O}(v^2/c^2) \qquad (56)$$

where r_0 is the classical electron radius, v is the speed of the positron and Z_{eff} is an effective number of electrons per atom for the annihilation process:

$$Z_{\mathrm{eff}} = \sum_{i=1}^N \langle \Xi^+_{\mathrm{AD}} | \delta(\boldsymbol{r}_i - \boldsymbol{x}) | \Xi^+_{\mathrm{AD}} \rangle = \sum_a^{\mathrm{occ}} \langle \psi^+_a \chi^+ | \delta(\boldsymbol{r} - \boldsymbol{x}) | \psi^+_a \chi^+ \rangle. \qquad (57)$$

In order to be consistent with the derivation of the polarized orbitals we should retain in equation (57) only terms up to first order in φ_a^{1+}. For closed-shell systems, with the aid of equations (20), (23) and (40) equation (57) can be written as

$$Z_{\text{eff}}=\frac{1}{32\pi^2}\cdot\sum_{\varkappa_D}[j_D]\cdot\int_0^\infty \mathrm{d}x\frac{1}{x^2}\cdot(f_D^2(x)+g_D^2(x))\cdot\sum_A^{\text{occ}}\left[[j_A]\cdot(P_A^2(x)+Q_A^2(x))\right.$$
$$\left.+2\cdot\sum_{k=0}^{\infty}\sum_{\varkappa_B}\Lambda_k^2(A,B)\cdot(P_A(x)\cdot P_{A\to B}^{(k)}(x,x)+Q_A(x)\cdot Q_{A\to B}^{(k)}(x,x))\right] \tag{58}$$

where we have omitted (+) superscripts at f_D^+ and g_D^+ for brevity. According to equations (40) and (54) f_D and g_D are normalized to correspond to a density of one positron per unit volume asymptotically.

6. Conclusions

We have formulated the relativistic polarized orbital theory of elastic electron and positron scattering from closed-shell atoms. Derived equations involve the relativistic polarization potential for both types of the projectile and also the exchange-polarization terms for the electron projectile. The relativistic formula for the positron-atomic-electron annihilation coefficient Z_{eff} has been presented. An appropriate computer program is now being written.

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Appendix

Useful formulae for $d^{kq}(a,b)$ coefficients:

$$d^{kq}(a,b)=(-1)^q\cdot d^{k,-q}(b,a) \tag{A1}$$

$$\sum_{m_b} d^{kq}(b,b)=[j_B]\cdot\delta_{k0}\cdot\delta_{q0} \tag{A2}$$

$$\sum_{m_a m_b} d^{kq}(a,b)\cdot d^{\nu\mu}(a,b)=\frac{\Lambda_k^2(A,B)}{[k]}\cdot\delta_{k\nu}\cdot\delta_{q\mu} \tag{A3}$$

$$\sum_{m_b q} d^{kq}(a,b)\cdot d^{kq}(c,b)=\frac{\Lambda_k^2(A,B)}{[j_A]}\cdot\delta_{\varkappa_A\varkappa_C}\cdot\delta_{m_a m_c} \tag{A4}$$

$$\sum_{m_a m_b \mu} d^{kq}(a,b)\cdot d^{\nu\mu}(b,c)\cdot d^{\nu\mu}(a,d)=\Gamma_{ABCD}^{k\nu}\cdot d^{kq}(d,c) \tag{A5}$$

where

$$\Gamma_{ABCD}^{k\nu}=(-1)^{k+\nu+1}\cdot\Lambda_k(A,B)\cdot\Lambda_\nu(B,C)\cdot\Lambda_\nu(A,D)\cdot\Lambda_k^{-1}(C,D)\cdot\begin{Bmatrix} j_A & k & j_B\\ j_C & \nu & j_D\end{Bmatrix}. \tag{A6}$$

Note that $\Gamma_{ABCD}^{k\nu}=\Gamma_{BADC}^{k\nu}$.

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