Recurrence relations for relativistic two centre matrix elements.

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Abstract. Recursion formulae are derived for the calculation of two centre matrix elements of a radial function in relativistic quantum mechanics. The recursions are obtained between not necessarily diagonal radial eigensates using arbitrary radial potentials and any radial functions. The only restriction is that the potentials have to share a common minimum. Among other things, the relations so obtained can help in evaluating relativistic corrections to transition probabilities between atomic Rydberg states.

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1. Introduction

The bridge between quantum calculations and experimental results is made at the level of matrix elements of the appropriate operators (Wong and Yeh 1983a,b, De Lange and Raab 1991, Dobrovolska and Tutik 1999, Quiney et al. 1997, Elboudali and Joulakian 2001, Ilarraza-Lomelí et al. 2002). In atomic and molecular physics this usually means matrix elements of powers of a radial coordinate between states of the system at hand (Blanchard 1974, Brack 1983, Bessis et al. 1985, Nana Engo et al. 1997, Owono Owono et al. 2002, West 2001). Matrix elements of more general radial functions are also very useful (Avram and Drăganescu 1997, Charro and Martin 2002, Nagy and Végh 1992). In nonrelativistic quantum mechanics, the importance of hypervirial results, and other related techniques, follows from this fact, since the task of calculating matrix elements is simplified using such techniques (Morales 1987, Fernández and Castro 1987, 1996, De Lange and Raab 1991, Núñez-Yépez et al. 1995). These techniques are also important for atomic physics in the relativistic realm (Martínez-y-Romero et al. 2001). This is especially important at present given the precision attained in atomic physics experiments using synchrotron radiation and other state-of-the-art sources of photons (Schippers et al. 2002, 2003, Müller et al. 2002, Aguilar et al. 2003).

In this work we exhibit that hypervirial-like formulas and other operator techniques suffice to obtain recurrence relations between relativistic matrix elements of an arbitrary radial function between states corresponding to two different arbitrary potentials. Such relation generalizes other recurrence relations between relativistic hydrogenic matrix elements of powers of \( r \) and of \( \beta r \) [\( \beta \) is a Dirac matrix, see equation (2)] we have recently calculated (Ilarraza-Lomelí et al. 2002, Martínez-y-Romero et al. 2000, 2001, 2002). In subsections 2.1, 2.2 and 2.3 of the paper we obtain the four recursion relations between the matrix elements of an arbitrary radial function, \( f(r) \), with the corresponding matrix elements of its first and second derivatives, taken between eigenstates of different potential functions, \( V_1(r) \) and \( V_2(r) \), with the corresponding matrix elements of its first and second derivatives. These generalized recurrence relations follow from a hypervirial-like result together with operator algebra computations. The recursions so obtained may be useful for studying radiative transitions in Rydberg atoms, in analysing atomic photorecombination and photoionization processes, for calculating relativistic corrections to ionic oscillator strengths, or in analysing impact ionization or vibrational transitions in molecules — albeit in the last two cases in a crude manner — (Schippers et al. 2002, Owono Owono et al. 2002, Semenov and Cherepkov 2003, Weck et al. 2001, Bauche-Arnoult et al. 1989). Section 3 contains the conclusions and other final remarks.

2. Relations for two centre integrals in relativistic quantum mechanics

General hypervirial results, the virial theorem, and other algebraic and operator techniques have been always very useful for calculating matrix elements in quantum
mechanics. Nonetheless they have been little used in relativistic situations, see, however, (Brack 1983, Lucha and Schöberl 1990). We want to show in this paper that they have similar importance for obtaining recursion relations between matrix elements of radial functions between eigenstates of different radial potentials in relativistic quantum mechanics. Thus, let us consider two radial Dirac Hamiltonians with two possibly different radial potentials (each behaving as the temporal component of a 4-vector) \( V_1(r) \) and \( V_2(r) \). We further assume that these potentials have the same equilibrium position which, furthermore, is assumed coincident with the origin of coordinates. That is, the recurrence relations correspond to the so-called unshifted case. The potentials could be regarded as describing the electronic configurations in processes involving electronic rearrangements in atomic transitions. For example, any transition to an autoionizing state studied in the central field approximation where the electron motion is solution of the Dirac equation with an effective central potential created by a \( k \) or a \( k - x \) electron ion core; or any other atomic process involving highly excited electrons which needs to be studied using multichannel spectroscopy or quantum defect theory (Owono Owono et al 2002, Mannervik et al 1998, Xiao-Min et al 1994, Aymar et al 1996).

The Hamiltonians can be written as (Martínez-y-Romero 2000)

\[
H_1 = c_\alpha r \left[ p_r - i \beta \epsilon_1 (j_1 + 1/2)/r \right] + M_1 \beta c^2 + V_1(r), \\
H_2 = c_\alpha r \left[ p_r - i \beta \epsilon_2 (j_2 + 1/2)/r \right] + M_2 \beta c^2 + V_2(r),
\]

in writing equation (1) we assume \( M_1 \neq M_2 \) since it is convenient for the calculations we perform for deriving the recurrence relations. The eigenstates of these radial Hamiltonians correspond to a definite value of the total angular momentum (orbital plus spin) \( J = L + S \) and of the quantum number \( \epsilon = (-1)^{j+l-1/2} \), where, respectively, \( j \) is the total, \( l \) the orbital, and \( s \) the spin angular momentum quantum numbers, the operators

\[
\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \alpha_r = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix},
\]

are Dirac matrices in the two-dimensional representation appropriate for the radial problem we are discussing, and the subscript simply distinguishes between the systems pertaining to the different potentials. Each Dirac equation can be written as

\[
H_k \psi_k(r) = E_k \psi_k(r)
\]

where the energy eigenvalues \( E_{n_jk} \equiv E_k \) and the corresponding eigenfunctions \( \psi_{n_jk} \equiv \psi_k(r) \) are assumed known. In this work we use atomic units \( (\hbar = m_e = e = 1) \) so the masses in (1) are given in units of the electron mass. The radial eigenstates \( \psi_k(r) \) are the purely radial spinors (Drake 1996, Greiner 1991)}
\[ \psi_k(r) \equiv \psi_{n_kj_k\epsilon_k}(r) = \frac{1}{r} \left( F_{n_kj_k\epsilon_k}(r) + i G_{n_kj_k}(r) \right); \quad (4) \]

\( F \) and \( G \) are, respectively, the big and the small components of the energy eigenstate. In the following we employ, as we did in equation (3), the shorthand \( k \) for describing the whole set of quantum numbers \( n_kj_k\epsilon_k \). We also use the ket notation for the relativistic eigenstates \( |n_kj_k\epsilon_k\rangle \equiv |k\rangle \).

2.1. The first recurrence relation for the case of two centres

Taking the difference between the radial Hamiltonians \( H_1 \) and \( H_2 \) in (1), we obtain

\[ H_1 = H_2 + i \alpha r \beta \frac{\Delta^-}{2r} - c^2 \beta M - (V_2(r) - V_1(r)). \quad (5) \]

where \( M^\pm \equiv M_2 \pm M_1 \), and \( \Delta^\pm \equiv \epsilon_2(2j_2 + 1) \pm \epsilon_1(2j_1 + 1) \). On employing (1) again, we can directly evaluate the commutator

\[ [H_1, f(r)] = -i \alpha r \frac{df(r)}{dr} \quad (6) \]

where \( f(r) \) is an arbitrary radial function and \( [H, f(r)] \) stands for the commutator between \( H \) and \( f(r) \). We can calculate this commutator again, but now using equation (5), to get the alternative form

\[ [H_1, f(r)] = H_2 f(r) - f(r) H_1 + \left( i \alpha r \beta \frac{\Delta^-}{2r} - c^2 \beta M - V^- \right) f(r). \quad (7) \]

It is now simple to obtain, from equations (6) and (7), the relation

\[ (E_2 - E_1) \langle 2 | f | 1 \rangle = \langle 2 | (c^2 \beta M^- + V^-) f | 1 \rangle - i c \langle 2 | \alpha r \left( f' + \beta \frac{\Delta^-}{2r} f \right) | 1 \rangle; \quad (8) \]

where we have additionally taken matrix elements between the eigenstates (4), we use the notation \( \langle 1 \rangle \equiv \langle n_1j_1\epsilon_1 | \) and \( |n_2j_2\epsilon_2\rangle \equiv |2\rangle \), and we have defined

\[ V^\pm \equiv V_2(r) \pm V_1(r). \quad (9) \]

Equation (8) may lead to recursions between relativistic matrix elements of radial functions between hydrogenic states (Martínez-y-Romero et al 2003, Ilarraza-Lomelí et al 2002, Martínez-y-Romero et al 2002, Martínez-y-Romero et al 2001) and generalizes a nonrelativistic one useful for similar purposes (Núñez-Yépez et al 1995). Equation (8) is an exact relation for the calculation of any \( f(r) \) two-centre matrix elements in
relativistic quantum mechanics. Taking the potentials as equal, i.e. $V_1(r) = V_2(r)$, we recover a relation which has proved useful for obtaining recurrence relations between atomic matrix elements in relativistic quantum mechanics (Ilarraza-Lomelí et al 2002, equation (6); Martínez-y-Romero et al 2001, equation (24)).

Albeit exact, equation (8) is not entirely convenient due to the presence of the operator $\alpha_r \beta$. To get rid of this factor, we found it convenient to deal directly with operator relations and not with the matrix elements themselves. The matrix elements will be evaluated at the end of the operator calculations.

Let us first establish that

$$H_2 f - f H_1 = \left( c^2 \beta M^- + V^- \right) f - i c \alpha_r \left( f' + \beta f \frac{\Delta^-}{2 r} \right), \quad (10)$$

notice that equation (8) above can be obtained from (10) just by taking matrix elements. The following result is also easily established

$$H_2 f + f H_1 = \left( c^2 \beta M^+ + V^+ \right) f - i c \alpha_r \left( 2 f \frac{d}{d r} + f' + \frac{2 f}{r} + \beta f \frac{\Delta^+}{2 r} \right), \quad (11)$$

Then, it can be seen that

$$-i c \left( H_2 \alpha_r f + \alpha_r f H_1 \right) = i c \alpha_r \left( c^2 \beta M^- - V^+ \right) f - c^2 \left( 2 f \frac{d}{d r} + f' + \frac{2 f}{r} - \beta f \frac{\Delta^-}{2 r} \right), \quad (12)$$

and that

$$H_2 f V^- - f V^- H_1 = \left( c^2 \beta M^- + V^- \right) V^- f - i c \alpha_r \left( V^- f' + \frac{d V^-}{d r} f + \beta f V^- \frac{\Delta^-}{2 r} \right). \quad (13)$$

The next relation is also readily apparent

$$-i c \left[ H_2 \alpha_r \beta \frac{f}{r} + \alpha_r \beta \frac{f}{r} H_1 \right] = -i c \alpha_r \beta V^+ \frac{f}{r} - c^2 \left[ \beta \left( \frac{f'}{r} - \frac{f}{r^2} \right) - \frac{\Delta^+}{2 r} \frac{f}{r} \right]. \quad (14)$$

To further proceed, let us define $\psi(r) \equiv H_2 f(r) + f(r) H_1$, and evaluate

$$H_2 \psi - \psi H_1 = c^2 \beta \frac{\Delta^+}{2 r} f' + c^2 \left( \frac{\Delta^-}{2 r} \right)^2 f + (c^2 \beta M^- + V^-)^2 f$$

$$-c^2 f'' - c^2 \beta \frac{\Delta^-}{2 r} \left( 2 f \frac{d}{d r} + f' + \frac{f}{r} \right)$$

$$-i c \alpha_r \left[ \left( f' + \beta f \frac{\Delta^-}{2 r} \right) (V^- - c^2 \beta M^+) + c^2 \beta M^- \left( 2 f \frac{d}{d r} + f' + \frac{2 f}{r} \right) \right]$$

$$+ V^- f' + \frac{d V^-}{d r} f + c^2 M^- \frac{\Delta^+}{2 r} f + V^- \frac{\Delta^-}{2 r} \beta f \right]. \quad (15)$$
Given these last expressions [equations (10)–(15)], it is relatively simple to obtain, from (10),

\[-i \alpha r \left( f' + \beta f \frac{\Delta^-}{2r} \right) = \left( H_2 f - f H_1 \right) - (c^2 \beta M^- + V^-) f, \quad (16)\]

and from (11),

\[-i \alpha_r \beta \left( 2f \frac{d}{dr} + f' + \frac{2f}{r} \right) = \left( H_2 \beta f + \beta f H_1 \right) - (c^2 \beta M^+ + V^+) \beta f + i \alpha_r \frac{\Delta^+}{2r} f. \quad (17)\]

From equation (12) we obtain

\[-c^2 \beta \frac{\Delta^-}{2r} \left( 2f \frac{d}{dr} + f' + \frac{2f}{r} \right) = -ic \left( H_2 \alpha_r \frac{\Delta^-}{2r} f + \alpha_r \frac{\Delta^-}{2r} f H_1 \right) - i \alpha_r \frac{\Delta^-}{2r} \left( c^2 \beta M^- - V^+ \right) f - c^2 f \left( \frac{\Delta^-}{2r} \right)^2. \quad (18)\]

From equation (13) we obtain

\[-ic \alpha_r \left( V^- f' + \frac{dV^-}{dr} f \right) = \left( H_2 f V^- - f V^- H_1 \right) - (c^2 \beta M^- + V^-) V^- f + ic \alpha_r V^- \frac{\Delta^-}{2r} \beta f. \quad (19)\]

Substituting equations (16), (17), (18), and (19), into equation (15), we get

\[H_2 \psi - \psi H_1 = -c^2 \left( f'' - \beta f' \frac{\Delta^+}{2r} \right) + c^2 \frac{\Delta^-}{2r^2} \beta f + (M^-)^2 \left( c^2 f \right) \]

\[-c^2 M^+ \left( H_2 \beta f - \beta f H_1 \right) + c^2 M^+ V^- \beta f + c^2 M^- \left( H_2 \beta f + \beta f H_1 \right) \]

\[-c^2 M^- V^+ \beta f + V^- \left[ 2 \left( H_2 f - f H_1 \right) - V^- \right] \]

\[-ic \left( H_2 \alpha_r \frac{\Delta^-}{2r} f + \alpha_r \frac{\Delta^-}{2r} f H_1 \right) - ic \alpha_r \frac{\Delta^-}{2r} \left( c^2 \beta M^- - V^+ \right) \beta f. \quad (20)\]

The terms which include the operator \( ic \alpha_r \) can be also obtained from (14), thus we get the expression

\[-ic \left( H_2 \alpha_r \frac{\Delta^-}{2r} f + \alpha_r \frac{\Delta^-}{2r} f H_1 \right) - ic \alpha_r \frac{\Delta^-}{2r} \left( c^2 \beta M^- - V^+ \right) \beta f = -c^2 \frac{\Delta^-}{2r} \left[ \beta \left( f' - \frac{f}{r} \right) - \frac{\Delta^+}{2r} f \right]. \quad (21)\]
Substituting now equation (21) into (20), it easily yields

\[
H_2\psi - \psi H_1 = -c^2 \left( f'' - \beta f' \frac{\Delta^+}{2r} \right) + 2c^2 \frac{\Delta^-}{2r} \beta f + (M^-)^2 e^4 f \\
- c^2 M^+ (H_2 \beta f - \beta f H_1) + c^2 M^+ V^- \beta f + c^2 M^- (H_2 \beta f + \beta f H_1) \\
- c^2 M^- V^+ \beta f + V^- \left[ 2 (H_2 f - f H_1) - V^- \right] - c^2 \frac{\Delta^-}{2r} \left( \beta f' - \frac{\Delta^+}{2r} f \right).
\]

(22)

Evaluating the matrix elements between the Dirac eigenstates \( \langle 2 | \) and \( | 1 \rangle \) and rearranging, we finally obtain the relation

\[
a_0 \langle 2 | f | 1 \rangle + a_2 \langle 2 | \frac{f}{r^2} | 1 \rangle - 2E^- \langle 2 | V^- f | 1 \rangle + \langle 2 | (V^-)^2 f | 1 \rangle + c^2 \langle 2 | f'' | 1 \rangle \\
= b_0 \langle 2 | \beta f | 1 \rangle + b_1 \langle 2 | \frac{\beta f}{r^2} | 1 \rangle - c^2 M^- \langle 2 | V^+ \beta f | 1 \rangle + c^2 M^+ \langle 2 | V^- \beta f | 1 \rangle + b_4 \langle 2 | \frac{\beta f'}{r} | 1 \rangle,
\]

(23)

where

\[
a_0 = (E^-)^2 - (c^2 M^-)^2 \\
a_2 = - c^2 \frac{\Delta^- \Delta^+}{4} \\
b_0 = c^2 (M^- E^+ - M^+ E^-) \\
b_1 = c^2 \Delta^- \\
b_4 = \frac{c^2}{2} (\Delta^+ - \Delta^-)
\]

(24)

This is the first relation between matrix elements of an arbitrary radial function \( f(r) \) between eigenstates of two different potentials as a function of the eigenenergies in relativistic quantum mechanics.

2.2. The second two-centre recurrence relation

Given that the radial eigenstates have two components in relativistic quantum mechanics, it should be clear that we need more relations. To obtain such second equation, let us evaluate the following operator identity — i.e. again we calculate with the basic operators before any matrix element is taken.

\[
H_2 f V^- + f V^- H_1 = (c^2 \beta M^+ + V^+) V^- f \\
- ic\alpha_r \left( 2V^- \frac{d}{dr} f V^- f' + \frac{dV^-}{dr} f + 2V^- \frac{f}{r} + \beta V^- \frac{\Delta^+}{2r} \right).
\]

(25)

Using again the definition \( \psi(r) \equiv H_2 f(r) - f(r) H_1 \), we obtain
\[ H_2\psi + \psi H_1 = c^2 f \frac{\Delta^-}{4r^2} - ic\alpha_r \left( f' + \beta f \frac{\Delta^-}{2r} \right) (V^+ - c^2 \beta M^-) \]

\[ + (c^2 \beta M^+ + V^+) (c^2 \beta M^- + V^-) f - c^2 \left( 2f' \frac{d}{dr} + f'' + \frac{2f'}{r} - \beta f \frac{\Delta^-}{2r^2} \right) \]

\[-ic\alpha_r \left( 2V^- f \frac{d}{dr} + V^- f' + \frac{dV^-}{dr} f + 2V^- \frac{f}{r} + \beta V^- f \frac{\Delta^+}{2r} + c^2 \beta M^- f' + c^2 M^- \frac{\Delta^-}{2r} f \right). \]

The calculations required for getting to the recurrence relation are similar to that used in the last section. So, from equation (10) we obtain

\[-ic\alpha_r c^2 \beta M^- \left( f' + \beta f \frac{\Delta^-}{2r} \right) = c^2 M^- (H_2 f - f H_1) - c^2 M^- (c^2 \beta M^- + V^-) \beta f, \] (27)

from (12) we get

\[-c^2 \left( 2f' \frac{d}{dr} + f'' + \frac{2f'}{r} \right) = -ic (H_2 \alpha_r f' + \alpha_r f' H_1) \]

\[-ic\alpha_r (c^2 \beta M^- - V^+) f' - c^2 \beta f' \frac{\Delta^-}{2r}, \] (28)

and from equation (25), we obtain

\[-ic\alpha_r \left( 2V^- f \frac{d}{dr} + V^- f' + \frac{dV^-}{dr} f + 2V^- \frac{f}{r} + \beta V^- f \frac{\Delta^+}{2r} \right) = (H_2 f V^- + f V^- H_1) \]

\[+ic\alpha_r V^- \beta f \frac{\Delta^+}{2r} - (c^2 \beta M^+ - V^+) V^- f. \] (29)

Using equations (16), (27), (28) and (29), in equation (26), it yields

\[ H_2\psi + \psi H_1 = -c^2 \beta \frac{\Delta^-}{2r} \left( f' - \frac{f}{r} \right) + c^2 \frac{\Delta^+}{2r^2} f - V^- V^+ f \]

\[+M^- M^+ c^4 f + V^+ (H_2 f - f H_1) + V^- (H_2 f + f H_1) \]

\[-ic (H_2 \alpha_r f' + \alpha_r f' H_1) - ic\alpha_r (c^2 \beta M^- - V^+) f'. \] (30)

Again, the last two terms of (30) can be obtained from (14), and combining these with

\[ -ic (H_2 \alpha_r f' + \alpha_r f' H_1) - ic\alpha_r (c^2 \beta M^- - V^+) f' = \]

\[-c^2 \left( f'' - \frac{f'}{r} \right) + c^2 \frac{\Delta^+}{2r} \beta f'. \] (31)
we get

\[ H_2 \psi + \psi H_1 = -c^2 \beta \frac{\Delta^+}{2r} \left( f' - \frac{f}{r} \right) + c^2 \frac{\Delta^+ \Delta^-}{2r} f - V^- V^+ f \]
\[ \quad + M^- M^+ c^4 f + V^+ (H_2 f - f H_1) + V^- (H_2 f + f H_1) \]  
\[ -c^2 \left( f'' - \frac{f'}{r} \right) + c^2 \frac{\Delta^+}{2r} \beta f', \]  

(32)

Taking matrix elements, we obtain the recurrence relation

\[ c_0 \langle 2 | f | 1 \rangle + a_2 \langle 2 | \frac{f}{r^2} | 1 \rangle - E^+ \langle 2 | V^- f | 1 \rangle - E^- \langle 2 | V^+ f | 1 \rangle + \langle 2 | V^+ V^- f | 1 \rangle \]
\[ -c^2 \langle 2 | \frac{f'}{r} | 1 \rangle + c^2 \langle 2 | f'' | 1 \rangle = b_2 \langle 2 | \beta f | 1 \rangle + b_4 \langle 2 | \beta f' | 1 \rangle, \]  

where the only newly defined coefficient is

\[ e_0 = E^+ E^- - c^4 M^+ M^- . \]  

(33)

2.3. The third and fourth two-centre recurrence relations

To get the third recurrence relation, we have to substitute, in a similar way to what we have done for getting the previous two relations, equations (10), (12), (14) and (25) into (26) and, after some juggling with the resulting terms, and taking matrix elements, we finally obtain the third recurrence relation

\[ e_0 \langle 2 | f | 1 \rangle = g_0 \langle 2 | \beta f | 1 \rangle - \langle 2 | (V^+ - V^-) \beta f | 1 \rangle, \]  

where

\[ e_0 = c^2 (M^+ - M^-) \]
\[ g_0 = E^+ - E^- . \]  

(34)

(35)

This is a very simple equation that, besides, allows writing the matrix elements of \( f \) in terms of those of \( \beta f \). To take advantage of this fact, substitute equation (35) into (23) to obtain a new relation

\[ A_0 \langle 2 | \beta f | 1 \rangle + A_1 \langle 2 | \beta f | 1 \rangle + A_2 \langle 2 | V^- \beta f | 1 \rangle + A_3 \langle 2 | (V^-)^2 \beta f | 1 \rangle \]
\[ + \langle 2 | (V^-)^3 \beta f | 1 \rangle + A_5 \langle 2 | V^+ \beta f | 1 \rangle + 2E^- \langle 2 | V^- V^+ \beta f | 1 \rangle \]
\[ - \langle 2 | (V^-)^2 V^+ \beta f | 1 \rangle + a_2 \langle 2 | (V^+ - V^-) \beta f' | 1 \rangle = \]
\[ A_9 \langle 2 | \beta f' | 1 \rangle + c^2 g_0 \langle 2 | \beta f'' | 1 \rangle - c^2 \langle 2 | (V^+ - V^-) \beta f'' | 1 \rangle. \]  

(37)
where the newly defined coefficients are

\[
A_0 = (E^-)^2 (E^+ - E^-) + c^2 E^- [(M^-)^2 + (M^+)^2] - c^4 M^+ M^- (E^+ + E^-)
\]

\[
A_1 = - \frac{c^2}{4} (E^+ - E^-) \Delta^+ \Delta^- - c^4 \Delta^- (M^+ - M^-)
\]

\[
A_2 = -2E^- (E^+ - E^-) + (E^-)^2 - (c^2 M^-)^2 - c^4 M^+ (M^+ - M^-)
\]

\[
A_3 = E^+ - 3E^- 
\]

\[
A_5 = c^4 M^+ M^- - (E^-)^2
\]

\[
A_9 = \frac{c^4}{2} (M^+ - M^-) (\Delta^+ - \Delta^-).
\]

Equation (37) is the fourth recurrence relation for the calculation of relativistic \( f(r) \) two centre matrix elements in terms of the energy eigenvalues of the intervening potentials. Notice that, at difference of the previous relations [equations (23), (33) and (35)], equation (37) just relates among themselves matrix elements of \( \beta f \) and its derivatives times a certain function of \( r \).

3. Conclusions

We have obtained recurrence relations for the calculation of two-centre matrix elements of a radial function between states of two different radial potentials. The obtained recursions are given in the most general case of an arbitrary function taken between any non necessarily diagonal radial eigenstates of two radial potentials. These recursion relations have, as particular cases, recursions between one-centre integrals or, in other particular cases, between overlap and one centre integrals in Dirac relativistic quantum mechanics. We expect the obtained recursions, together with the previous one-centre relations we have obtained (Ilarraza-Lomelí et al 2002, Martínez-y-Romero et al 2001, 2002), to be useful in atomic or molecular physics calculations as they may simplify calculation in the range of applicability of Dirac’s relativistic quantum mechanics (Bang and Hansteen 2002, Moss 1972). For most uses of the relations we first have to set \( M_1 = M_2 \), i.e. \( M^- = 0 \) and \( M^+ = 2 \) —if the particles are electrons; since the use of unequal masses is just a recourse of our calculational method.

From a practical angle, there is little that can be done for the analytical evaluation of two centre integrals of atomic physics interest beyond the Coulomb and the few similarly exactly solvable potentials. However, there are numerical methods that, after being adapted to relativistic conditions, can provide the crucial “seed” results needed for the systematic use of the recurrence relations obtained here (Chen et al 1993). Our results can be also useful in the so-called perturbation theory of relativistic corrections, in relativistic quantum defect calculations, and for the relativistic extension of the calculations of exchange integrals using Slater orbitals or
Coulomb-Dirac wave functions (Owono Owono et al. 2002, Bang and Hasteen 2002, Charro et al. 2001, Kuang and Lin 1996, Rutkowski 1996). It is also possible that our relations could be applied to a generalization of an approximate two-centre technique used for studying electron-impact ionization of simple molecules (Weck et al. 2001).

On the other hand, our results can be also of interest in nuclear studies. Since the 3D Woods-Saxon potential, used in the Dirac equation for describing the interaction of a nucleon with a heavy nucleus, has been explicitly solved recently and its eigenfuctions expressed in terms of hypergeometric functions (Jian-You et al. 2002), so it has the features needed for the direct use of our recurrence relations.

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References

Aguilar A, West J B, Phaneuf R A, Brooks R L, Folkmann F, Kjeldsen H, Bozek J D, Schlachter A S, and Cisneros C 2003 Phys. Rev. A 67 012701
Avram N M and Drăganescu Gh E 1997 Int. J. Quantum Chem. 65 655
Aymar M, Greene C H, Luc-Koenig E 1996 Rev. Mod. Phys. 68 1015
Bang J M and Hansteen J M 2002 J. Phys. B: At. Mol. Opt. Phys. 35 3979
Bauche-Arnould C, Bauche J, Luc-Koenig E, Wyart J-F, More R M, Chenais-Popovics C, Gauthier J-C, Geindre J-P, and Tragín N 1989 Phys. Rev. A 39 1053
Bessis N, Bessis G, and Roux D 1985 Phys. Rev. A 32 2044
Blanchard P 1974 J. Phys. B: At. Mol. Opt. Phys. 7 1993
Brack M 1983 Phys. Rev. D 27 1950
Charro E, López-Ferrero S, Martín I 2001 J. Phys. B: At. Mol. Opt. Phys. 34 4243
Charro E and Martín I 2002 J. Phys. B: At. Mol. Opt. Phys. 35 3227
Chen Z, Bessis D and Msezane A Z 1993 Phys. Rev. A 47 4756
De Lange O L and Raab R E 1991 Operator Methods in Quantum Mechanics (Oxford: Clarendon)
Dobrovolska I V and Tutik R S 1999 Phys. Lett. A 260 10
Drake G W F (Ed) 1996 Atomic, Molecular and Optical Physics Handbook (Woodbury: American Institute of Physics) Ch 22
Elboudali F and Jouklian B 2001 J. Phys. B: At. Mol. Opt. Phys. 34 4877
Fernández F M and Castro E A 1987 Hypervirial Theorems (Berlin: Springer)
Fernández F M and Castro E A 1996 Algebraic Methods in Quantum Chemistry and Physics (Boca Raton: CRC)
Greiner W 1991 Theoretical Physics 3: Relativistic quantum mechanics (Berlin: Springer)
Ilarrazo-Lomeí A C, Valdés-Martínez M N, Salas-Brito A L, Martínez-y-Romero R P, and Núñez-Yépez H N 2002 Int. J. Quantum Chem. 90 195
Jian-You G, Xian Cheng F, and Fu-Xin X 2002 Phys. Rev. A 66 062105
Kuang J and Lin C D 1996 J. Phys. B: At. Mol. Opt. Phys. 29 L889
Lucha W and Schöberl F F 1990 Phys. Rev. Lett. 23 2733
Mannervik S, DeWitt D, Engström L, Lindberg J, Lindroth E, Schuch R, and Zong W 1998 Phys. Rev. Lett. 81 313
Martínez-y-Romero R P 2000 Am. J. Phys. 68 1050
Martínez-y-Romero R P, Núñez-Yépez H N, and Salas-Brito H N 2000 J. Phys. B: At. Mol. Opt. Phys. 33 L367
Martínez-y-Romero R P, Núñez-Yépez H N, and Salas-Brito A L 2001 J. Phys. B: At. Mol. Opt. Phys. 34 1261
Martínez-y-Romero R P, Núñez-Yépez H N, and Salas-Brito A L 2002 J. Phys. B: At. Mol. Opt. Phys. 35 L71
Martínez-y-Romero R P, Núñez-Yépez H N, and Salas-Brito A L 2003 J. Phys. B: At. Mol. Opt. Phys. 2003 submitted
Morales J 1987 Phys. Rev. A 36 4101
Moss R E 1972 Advanced Molecular Quantum Mechanics (London: Chapman and Hall)
Müller A, Phaneuf R A, Aguilar A, Gharaibeh M F, Schlachter A S, Alvarez I, Cisneros C, Hinojosa G, and McLaughlin B M 2002 J. Phys. B: At. Mol. Opt. Phys. 35 L137
Nana Engo S G, Kwato Njock M G, Owono Owono L C, Lagmago Kamta G and Motapon O 1997 Phys. Rev. A 56 2624
Núñez-Yépez H N, López-Bonilla J and Salas-Brito A L 1995 J. Phys. B: At. Mol. Opt. Phys. 28 L525
Nagy L and Végh L 1992 Phys. Rev. A 46 284
Owono Owono L C, Kwato Njock M G and Oumaro B 2002 Phys. Rev. A 66 052503
Quiney H M, Skaane H and Grant I P 1997 J. Phys. B: At. Mol. Opt. Phys. 30 L829
Rutkowski A 1996 Phys. Rev. A 53 145
Schippers S, Müller A, Ricz S, Bannister M E, Dunn G H, Bosek J, Slachter A S, Hinojosa G, Cisneros C, Aguilar A, Covington A M, Gharaibeh M F, and Phaneuf R F 2002 Phys. Rev. Lett. 89 193002
Schippers S, Müller A, Ricz S, Bannister M E, Dunn G H, Slachter A S, Hinojosa G, Cisneros C, Aguilar A, Covington A M, Gharaibeh M F, and Phaneuf R F 2003 Phys. Rev. A 67 032702
Semenov S K and Cherepkov N A 2003 J. Phys. B: At. Mol. Opt. Phys. 36 1409
Weck P, Fojón O A, Hanssen J, Joulkian B, and Rivarola R D 2001 Phys. Rev. A 63 042709
West J B 2001 J. Phys. B: At. Mol. Opt. Phys. 34 R45
Wong M K F and Yeh H-Y 1983a Phys. Rev. A 27 2300
Wong M K F and Yeh H-Y 1983b Phys. Rev. A 27 2305
Xiao-Min Ton, Lei Liu, Jia-Ming Li 1994 Phys. Rev. A 49 4641