Relativistic recursion relations for transition matrix elements

R. P. Martínez-y-Romero\textsuperscript{1,*}, H. N. Núñez-Yépez\textsuperscript{2†},
A. L. Salas-Brito\textsuperscript{3‡}

1 Facultad de Ciencias, Universidad Nacional Autónoma de México,
Apartado Postal 50-542, Coyoacán 04510 D. F., México.

2 Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534 Iztapalapa 09340 D. F., México.

3 Laboratorio de Sistemas Dinámicos, Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, Apartado Postal 21-267, Coyoacán 04000 D. F., México.

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Abstract

We review some recent results on recursion relations which help evaluating arbitrary non-diagonal, radial hydrogenic matrix elements of $r^\lambda$ and of $\beta r^\lambda$ ($\beta$ a Dirac matrix) derived in the context of Dirac relativistic quantum mechanics. Similar recursion relations were derived some years ago by Blanchard in the non relativistic limit. Our approach is based on a generalization of the second hypervirial method previously employed in the non-relativistic Schrödinger case. An extension of the relations to the case of two potentials in the so-called unshifted case, but using an arbitrary radial function instead of a power one, is also given. Several important results are obtained as special cases of our recurrence relations, such as a generalization to the relativistic case of the Pasternack-Sternheimer rule. Our results are useful in any atomic or molecular calculation which take into account relativistic corrections.

1 Introduction

In atomic or molecular physics it is customary the use of sum rules to handle the matrix elements that appear in many computations\textsuperscript{[1] - [6]}. One of the conspicuous examples is the Blanchard relation \textsuperscript{[8]} which is a useful recurrence formula for non diagonal, non-relativistic arbitrary matrix elements, of the form $\langle n_1 l_1 | r^\lambda | n_2 l_2 \rangle$. Here $|nl\rangle$ stand for non-relativistic

\textsuperscript{*}e-mail: rodolfo@dirac.fcien.unam.mx, corresponding author
\textsuperscript{†}e-mail: nyhn@xanum.uam.mx
\textsuperscript{‡}e-mail: asb@correo.azc.uam.mx
hydrogenic radial energy eigenstates, and $\lambda$ is an arbitrary, even non-integer power of $r$.\footnote{Though perhaps of relatively little physical interest, it is nevertheless worth noting that the exponent, $\lambda$, can be complex, see \cite{8} for details}

According to this relation, once we know any three successive matrix elements of powers of the radial coordinate, $r$, any other of these elements can be deduced in terms of the three previous ones. The Blanchard recurrence relation was derived more thirty years ago using a calculation-intensive method. In the intervening years a simplified method has been proposed for deriving the Blanchard rule and, also, new potentially useful relations \cite{6} - \cite{12}. Different approaches have been studied for obtaining sum rules between hydrogenic matrix elements of these sorts. Some of them are based on the non relativistic hypervirial theorem \cite{5}, \cite{9}, \cite{10}, \cite{11}.

Most of the sum rules yet discovered are of a non relativistic nature despite the physical and chemical interest for obtainig relativistic results \cite{9}, \cite{10}, \cite{25}, \cite{26}. Nevertheless, there has been some effort in constructing new sum rules in the relativistic and quasi-relativistic approach \cite{12} - \cite{14}, \cite{24}, \cite{25}. In this review we want to present some of the results obtained by us in the relativistic case, using an approach inspired on the non relativistic hypervirial method proposed by some of us some years ago \cite{6}, \cite{7}.

In atomic and molecular physics the non-relativistic approach usually means non relativistic matrix elements of powers of a radial coordinate between states of the system at hand \cite{8} - \cite{20}. But in the relativistic approach we must to take into account, in the general case, the presence of the Dirac’s $\beta$ matrix in an explicit way in our calculations. This point seems natural since the $\beta$ matrix has an eigenvalue +1 for the positive energy eigenstates of the Hamiltonian and −1 for the negative ones, giving some differences in the treatment of both matrix elements. This point gives in general, two series of sum rules, one for matrix elements without the $\beta$ matrix and other one for matrix elements with the $\beta$ explicitly appearing. To this end we employ a relativistic calculation inspired directly on the hypervirial method \cite{0} to deduce new recurrence relations for the, in general, non-diagonal radial matrix elements of successive powers of $r^\lambda$ and of $\beta r^\lambda$—where $\beta$ is a $4 \times 4$ Dirac matrix \cite{18}— for relativistic hydrogenic states in the energy basis. The assumptions we use here are that the nucleus is point-like and fixed in space, and that a description using the Dirac equation is, of course, valid. We first study the recurrence relations in the general case, in which the matrix elements are taken between states with different principal quantum numbers $n_1 \neq n_2$, different total angular momentum quantum numbers $j_1 \neq j_2$, $m_{j_1} \neq m_{j_2}$, and different parity. For the sake of convenience, we employ the quantum number $\epsilon \equiv (-1)^{l+j-rac{1}{2}}$ instead of parity for labelling the hydrogenic eigenstates, where $\epsilon_1 \neq \epsilon_2$ is defined by

$$\epsilon = \begin{cases} 1 & \text{if } l = j + \frac{1}{2}, \\ -1 & \text{if } l = j - \frac{1}{2}; \end{cases}$$

(1)

As we mentioned above, we find that in general the recurrence relations depend on matrix elements of both powers of $r$ and of $\beta r$, in practical terms this means that we need two recurrence relations as the relativistic version of the single-equation Blanchard relation. Given its special interest, we in particular study the case where the total angular momentum and parity become equal, $j_1 = j_2$ and $\epsilon_1 = \epsilon_2$, in the two states—not mattering the relative
values of the principal quantum number \( n \). We also address the completely diagonal case where \( n_1 = n_2, j_1 = j_2, \) and \( \epsilon_1 = \epsilon_2 \). Both of the particular cases mentioned above require special treatment for avoiding possible divisions by zero in the general expressions; such results are immediately used to obtain a relativistic version of the Pasternack-Sternheimer relation \([30]\) and to obtain an expression for the relativistic virial theorem \([12], [31]\).

The results reported in this paper are important because the link between quantum calculations and experimental results is made at the level of matrix elements of the appropriate operators. In atomic and molecular physics this usually means matrix elements of powers of a radial coordinate between states of the system at hand \([20] - [23], [25] - [28], [32]\). But matrix elements of more general radial functions are also very useful \([33] - [36]\). Any contribution making less cumbersome the evaluation of a series of these elements is potentially very useful. In nonrelativistic quantum mechanics the importance of hypervirial results and other related techniques follows from this fact, since the task of calculating matrix elements can be indeed simplified \([9], [6]\). These techniques are also important for atomic physics in the relativistic realm \([12] - [15]\). This can be significative at present given the precision attained in atomic physics experiments using synchrotron radiation which is typically less than the expected values of relativistic corrections in some processes \([37] - [41]\).

In section 2 of this paper, we review the non-relativistic second hypervirial scheme and we use it to derive the Blanchard relation. In section 3, we deduce a radial Hamiltonian, completely equivalent to the Dirac equation for central potentials and we employ our result to implement a corresponding hypervirial result in relativistic quantum mechanics, and we proceed to use it to deduce by a long, but direct calculation, the relativistic recurrence formulae. In section 4 we study in particular the diagonal case \((j_2 = j_1, \epsilon_2 = \epsilon_1)\), which needs special treatment to avoid division by zero, to derive the relativistic Pasternack-Sternheimer rule and use it \( (\text{when } n_1 = n_2) \) to obtain a version of the relativistic virial theorem. In section 5 we use Dirac equation to obtain analytic expressions for the bound-bound, diagonal and non-diagonal matrix elements for arbitrary powers of \( r \). As it becomes evident, such results are rather cumbersome for relatively large values of the power; for small values, on the other hand, they are better regarded as starting values for the recurrence relations derived in section 3 and 4 of this article. In section 6 we explore the extension of our method to the calculation of generalized recurrence relations for the case of two different potentials. We call the results general recurrence relations as they relate matrix elements of a radial function with those of its derivatives. Also because in the case the function is chosen as a power of the radial coordinate and the potential is of the Coulomb type we obtain the sum rules of the preceding sections.

2 The non-relativistic hypervirial method

In this section we develop an alternative approach based on a generalization of the virial method to obtain the original Blanchard relation. We remind that both Blanchard relation and its predecessor the Kramers selection rule, were originally obtained employing directly the Schrödinger equation together with appropriate boundary conditions in a rather long way \([8], [11]\). The method proposed originally by us is a much simpler one \([6]\). It is based on a generalized hypervirial result and certain Hamiltonian identities that has been developed to
such a choice we can readily show

\[ H_k |n_k l_k\rangle = E_{n_k l_k} |n_k l_k\rangle, \]

(2)

where \( |n_k l_k\rangle = \psi_{n_k l_k}(r) \) and \( E_{n_k l_k} \) are respectively, an energy eigenfunction and its energy eigenvalue corresponding to principal and angular momentum quantum numbers, \( n_k \) and \( l_k \); \( k \) is a label that we will employ to identify the left bra and right ket in more complex expressions. \( H_k \), the non-relativistic radial Hamiltonian, is given by

\[ H_k = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{l_k (l_k + 1)}{2r^2} + V(r). \]

(3)

### 2.1 A nonrelativistic hypervirial relation

Although we want to calculate the radial matrix elements for terms of the form \( r^\lambda \), it is best for our purposes to consider first matrix elements of an arbitrary radial function \( f(r) \); with such a choice we can readily show

\[ (E_i - E_k) \langle n_i l_i | f(r) | n_k l_k\rangle = \langle n_i l_i | (\frac{-1}{2} f'' - f' \frac{d}{dr} - \frac{1}{r} f' + \frac{\Delta_{ik}}{2} \frac{f}{r^2}) | n_k l_k\rangle, \]

(4)

where we use \( \Delta_{ik} \equiv l_i (l_i + 1) - l_k (l_k + 1) \), \( E_k \equiv E_{n_k l_k} \), and the primes stand for radial derivatives. Please recall that the matrix element of an arbitrary radial function \( f(r) \) is

\[ \langle n_i l_i | f(r) | n_k l_k\rangle = \int_0^\infty r^2 \psi_{n_k l_k}^* (r) f(r) \psi_{n_k l_k} (r) dr. \]

(5)

To establish the result we are after, we apply the previous result to the radial function \( \xi(r) \equiv H_i f(r) - f(r) H_k \), to find

\[ 2(E_i - E_k)^2 \langle n_i l_i | f(r) | n_k l_k\rangle = \]

\[ \langle n_i l_i | (H_i (H_k f(r) - f(r) H_k) - (H_i f(r) - f(r) H_k) H_k + H_i (H_k f(r) - f(r) H_k) - (H_i f(r) - f(r) H_k) H_k) | n_k l_k\rangle. \]

(6)

This is a recurrence relation valid for arbitrary radial potential energy functions, \( V(r) \), introduced in [6].

### 2.2 The Blanchard sum rule

The second hypervirial takes a particularly simple form when \( f(r) \) is a power of the position, let us say \( f(r) = r^{\lambda+2} \); using this expression for \( f(r) \) and restricting ourselves to the Coulomb potential, \( V(r) = -Z/r \), we obtain, after a shorter calculation than in [8], the Blanchard relation.
\[
\lambda (E_i - E_k)^2 \langle n_i l_i | r^{\lambda+2} | n_k l_k \rangle = c_0 \langle n_i l_i | r^\lambda | n_k l_k \rangle + c_1 \langle n_i l_i | r^{\lambda-1} | n_k l_k \rangle + c_2 \langle n_i l_i | r^{\lambda-2} | n_k l_k \rangle;
\]

where the hydrogenic energy eigenvalues are \( E_a = -Z^2/2n_a^2 \), independent of \( l \), and

\[
c_0 = Z^2(\lambda + 1) \left[ (l_i - l_k)(l_i + l_k + 1) \left( \frac{1}{n_i^2} - \frac{1}{n_k^2} \right) + \lambda(\lambda + 2) \left( \frac{1}{n_k^2} + \frac{1}{n_i^2} \right) \right] \]

\[
c_1 = -2Z\lambda(\lambda + 2)(2\lambda + 1)
\]

\[
c_2 = \frac{1}{2}(\lambda + 2) \left[ \lambda^2 - (l_k - l_i)^2 \right] \left[ (l_k + l_i + 1)^2 - \lambda^2 \right].
\]

### 2.3 The Pasternack-Sternheimer selection rule and the non-relativistic virial theorem

From this result we can also obtain, as special cases of the relation, the Pasternack - Sternheimer rule [30]

\[
\langle n_i l_i | \frac{Z}{r^2} | n_k l_k \rangle = 0
\]

which says that the matrix element of the potential \( 1/r^2 \) vanishes between radial states of central potentials when 1) their angular momenta coincide and 2) their energy eigenvalues depend only on the principal quantum number. In the completely diagonal case \((n_i = n_k, \; l_i = l_k)\), we can further obtain the non-relativistic quantum virial theorem [3]

\[
\langle V \rangle = -Z\langle \frac{1}{r} \rangle = 2\langle E \rangle.
\]

As we exhibit in section 3, we can obtain analogous results using our recurrence relations in relativistic quantum mechanics.

### 3 The relativistic case

The method sketched in the previous section can be extended to the relativistic Dirac case. To that end, we need to start with the equivalent of the non-relativistic radial Hamiltonian of the Schrödinger equation for a central potential \( V(r) \) (Eq. 3) in the relativistic case. To obtain such expression we begin with the Dirac Hamiltonian \( H_D \) for a central potential

\[
H_D = c\alpha \cdot p + \beta c^2 + V(r), \quad H_D \Psi(r) = E \Psi(r);
\]

where we are using again atomic units, \( \alpha \) and \( \beta \) are the \( 4 \times 4 \) Dirac matrices in the Dirac representation

\[
\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]
Here the 1’s and 0’s stand, respectively, for $2 \times 2$ unit and zero matrices and the $\sigma$ is the standard vector composed by the three Pauli matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$. Since the Hamiltonian $H_D$ is invariant under rotations, we look for simultaneous eigenfunctions of $H_D$, $|J|^2$ and $J_z$, where $J = L + S$ and

$$S \equiv \frac{1}{2} \Sigma = \frac{1}{2} \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}.$$  

Hence the solutions of the Dirac equation can be written in the alternative but entirely equivalent forms [12]

$$\Psi(r, \theta, \phi) = \frac{1}{r} \begin{pmatrix} F_{nj}(r)\mathcal{Y}_{jm}(\theta, \phi) \\ iG_{nj}(r)\mathcal{Y}_{jm}(\theta, \phi) \end{pmatrix} = \frac{1}{r} \begin{pmatrix} F_{nk}(r)\chi_{km}(\theta, \phi) \\ iG_{nk}(r)\chi_{-km}(\theta, \phi) \end{pmatrix},$$  

where $\chi_{km}$ and $\chi_{-km}$, or $\mathcal{Y}_{jm}$ and $\mathcal{Y}_{jm}'$, are spinor spherical harmonics of opposite parity, and $\kappa = -\epsilon(j + 1/2)$ is the eigenvalue of the operator $\Lambda \equiv \beta(1 + \Sigma \cdot L)$ which commutes with $H_D$ (where $\Sigma \equiv \sigma \otimes I = \text{diag}(\sigma, \sigma)$). Parity is a good quantum number in the problem because central potentials are invariant under reflections; parity varies as $(-1)^l$ and, according to the triangle’s rule of addition of momenta, the orbital angular momentum is given by $l = j \pm 1/2$. But, instead of working directly with parity or with $\kappa$, we prefer the quantum numbers $j$ and $\epsilon$, introduced above, which can be shown also to satisfy $l = j + \epsilon/2$ in all cases. We also define $l' = j - \epsilon/2$; accordingly, the spherical spinor $\mathcal{Y}_{jm}$ depends on $l$ whereas the spherical spinor $\mathcal{Y}_{jm}'$, which has the opposite parity, depends on $l'$. Writing the solutions in the form (16) completely solves the angular part of the problem.

### 3.1 The relativistic radial Hamiltonian

To construct the radial Hamiltonian, we use the relation

$$(\alpha \cdot r)(\alpha \cdot p) = (\Sigma \cdot r)(\Sigma \cdot p) = r \cdot p + i\Sigma \cdot L;$$  

we then use $J^2 = [L + (1/2)\Sigma]^2 = L^2 + \Sigma \cdot L + 3/4$. For the term $L \cdot \Sigma$ we also need an expression for $L^2$ acting on the eigenfunctions (16). Directly from this equation we see that when $L^2$ is applied to any central potential state, the big component of the state function behaves with the orbital quantum number $l = j + \epsilon/2$, whereas the small one does so with the orbital quantum number $l' = j - \epsilon/2$; we have then,

$$l(l + 1) = j(j + 1) + \epsilon(j + \frac{1}{2}) + \frac{1}{4},$$  

for the big component, and

$$l'(l' + 1) = j(j + 1) - \epsilon(j + \frac{1}{2}) + \frac{1}{4},$$  

for the small one. The action of $L^2$ upon a solution of the form (16) is therefore always of the form

$$L^2 = j(j + 1) + \beta \epsilon(j + \frac{1}{2}) + \frac{1}{4},$$  

(20)
where $\beta$ is the Dirac matrix (14). From this result we obtain the term $L \cdot \Sigma$ and, substituting it into $(\alpha \cdot p)$, we finally obtain

$$c(\alpha \cdot p) = \alpha_r \left[ p_r - i \beta c^2 \frac{\epsilon}{r} \left( j + \frac{1}{2} \right) \right],$$

(21)

where

$$\alpha_r \equiv \frac{1}{r} \alpha \cdot r, \quad p_r = -i \frac{r}{r} \left( 1 + r \frac{d}{dr} \right).$$

(22)

We are now ready to write the relativistic radial Hamiltonian, and the corresponding radial Dirac equation, as $H_k \psi_k(r) = E_k \psi_k(r)$, with $H_k$ given by

$$H_k = c \alpha_r \left[ p_r - i \beta \frac{\epsilon_k}{r} \left( j_k + \frac{1}{2} \right) \right] + \beta c^2 + V(r),$$

(23)

where we introduced the purely radial eigenfunctions

$$\psi_k(r) \equiv \frac{1}{r} \left( F_{n_k j_k \epsilon_k} (r) \right)$$

(24)

in a $2 \times 2$ representation where, $\beta = \text{diag}(+1, -1)$, $\alpha_r = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$, and the radial Dirac equation becomes then $\text{[12][18]}

$$\begin{bmatrix} c^2 + (V_k(r) - E_k) & \epsilon_k c \left( j_k + 1/2 \right) /r - d/dr \\ \epsilon_k c \left( j_k + 1/2 \right) /r + d/dr & -c^2 + (V_k(r) - E_k) \end{bmatrix} \begin{bmatrix} F_{n_k j_k \epsilon_k} (r) \\ G_{n_k j_k \epsilon_k} (r) \end{bmatrix} = 0.$$ 

(25)

We want to remark that though this explicit representation can be used for our problem $\text{[14][17]}$, it is not really necessary, since all our results are representation independent.

### 3.2 The relativistic hypervirial result

The relativistic recurrence relation we are after, can be deduced using a similar reasoning as the used in section 2 for the non-relativistic case, that is we need a hypervirial result. Let us first calculate the non-diagonal matrix element of an arbitrary radial function $f(r)$

$$(E_2 - E_1) \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | H_2 f(r) - f(r) H_1 | n_1 j_1 \epsilon_1 \rangle =$$

$$-ic \langle n_2 j_2 \epsilon_2 | \alpha_r \left( f'(r) + \frac{\Delta_{21}}{2r} \beta f(r) \right) | n_1 j_1 \epsilon_1 \rangle,$$

(26)

where from now on the labelling in the kets stand for the three quantum numbers $n_k$, $j_k$, and $\epsilon_k$, we have defined $\Delta_{21} \equiv \epsilon_2 (2 j_2 + 1) - \epsilon_1 (2 j_1 + 1)$, and the matrix elements of radial functions are calculated as

$$\langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \int f(r) \left( F_2^*(r) F_1(r) + G_2^*(r) G_1(r) \right) dr,$$

(27)

$$\langle n_2 j_2 \epsilon_2 | \beta f(r) | n_1 j_1 \epsilon_1 \rangle = \int f(r) \left( F_2^*(r) F_1(r) - G_2^*(r) G_1(r) \right) dr.$$

(28)
The subscripts stand for the 3 quantum numbers specifying the state.

We next proceed to calculate a “second order iteration” by substituting \( f(r) \rightarrow \xi(r) = H_2f(r) - f(r)H_1 \) in the last expression. Let us calculate first \( H_2\xi \) and \( \xi H_1 \),

\[
H_2\xi = -c^2 \left( f'/r - f'' - f' \frac{d}{dr} - (\Delta_{21}/2r\beta) f' - (\Delta_{21}/2r) \beta f \frac{d}{dr} \right) + \epsilon_2 c^2 (2j_2 + 1)/2r \beta \left[ f' + \frac{\Delta_{21}}{2r} \beta f \right] - ic\alpha_r \left[ f' + \frac{\Delta_{21}}{2r} \beta f \right] [V(r) - c^2 \beta],
\]

and

\[
\xi H_1 = -(1/r) \left[ c^2 f' - c^2 (\Delta_{21}/2r) \beta f \right] - \left[ c^2 f' - c^2 (\Delta_{21}/2r) \beta f \right] \frac{d}{dr} + c^2 (2j_1 + 1) \frac{\Delta_{21}}{2r} \beta \left( f' - \frac{\Delta_{21}}{2r} \beta f \right) - ic\alpha_r \left( f' + \frac{\Delta_{21}}{2r} \beta f \right) (V(r) + \beta c^2);
\]

and then, we write down the difference of the matrix elements associated with Eqs. (29) and (30)

\[
(E_2 - E_1)^2 \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | c^2 (-\Delta_{21}/2r^2) \beta f - c^2 f'' - c^2 (\Delta_{21}/2r) \beta f' - c^2 (\Delta_{21}/r) \beta f \frac{d}{dr} + c^2 (\Delta_{21}/2r) \beta f' + c^2 (\Delta_{21}/2r)^2 f + 2ic\alpha_r \beta \left( c^2 f' + (\Delta_{21}/2r) \beta f \right) | n_1 j_1 \epsilon_1 \rangle.
\]

where we have defined \( \Delta_{21} \equiv \epsilon_2 (2j_2 + 1) + \epsilon_1 (2j_1 + 1) \). Please notice that here and in what follows we are always assuming \( \Delta_{21} \neq 0 \).

This last expression (31) is the direct relativistic equivalent of the generalized second hypervirial \([\text{Cf. Eq. (31)}]\) above. The expression involves the operator \( d/dr \), but here, due to the presence of Dirac matrices in the result, we cannot use the trick employed in the non-relativistic case where we took advantage of the Hamiltonian to simplify the calculation. Instead, let us calculate the following second order iteration for non-diagonal matrix elements

\[
\langle n_2 j_2 \epsilon_2 | H_2\xi + \xi H_1 | n_1 j_1 \epsilon_1 \rangle = (E_2^2 - E_1^2) \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | -2c^2 f'(r)/r + c^2 (\Delta_{21}/2r^2) \beta f(r) - c^2 f''(r) - 2c^2 f'(r) \frac{d}{dr} + c^2 (\Delta_{21}/2r) \beta f(r) - 2ic\alpha_r \left( f'(r) + \frac{\Delta_{21}}{2r} \beta f(r) \right) V(r) \rangle | n_1 j_1 \epsilon_1 \rangle.
\]

Due to the presence of Dirac matrices in our results, we also require to calculate non-diagonal matrix elements for expressions involving \( \alpha_r f(r) \) and \( \beta f(r) \), namely

\[
H_2 (-ic\alpha_r f(r)) = [-c^2 f/r - c^2 f' - c^2 f \frac{d}{dr} + c^2 (\epsilon_2/2r) (2j_2 + 1) \beta f] + ic^2 \alpha_r \beta f = -ic\alpha_r V(r)f,
\]

and

\[
8
\]
\[ (-ica_r f(r)) H_1 = \]
\[-f \left[ c^2 (1/r) \left( 1 + r \frac{d}{dr} \right) + c^2 (\epsilon_1/2r) (2j_1 + 1) \beta \right] - ic^3 \alpha \beta f - ic \alpha V(r) f; \]  
(34)

adding up these two last expressions, we get

\[ (E_2 + E_1) \langle n_2 j_2 \epsilon_2 | (-ica_r f(r)) | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | c^2 \left( -2f/r - f' - 2f \frac{d}{dr} \right) + c^2 (\Delta_{21}^+/2r) \beta f - 2ic \alpha V(r) f | n_1 j_1 \epsilon_1 \rangle. \]

(35)

From the matrix element of \( H_2 (-ica_r f(r)) - (-ica_r f(r)) H_1 \), we can obtain

\[ -ic(E_2 - E_1) \langle n_2 j_2 \epsilon_2 | \alpha f | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | -c^2 f'(r) + c^2 (\Delta_{21}^+/2r) \beta f(r) + 2ic \alpha \beta m(r) | n_1 j_1 \epsilon_1 \rangle; \]  
(36)

proceeding in a similar way for \( H_2 (\beta f(r)) + (\beta f(r)) H_1 \), we get

\[ (E_2 + E_1) \langle n_2 j_2 \epsilon_2 | \beta f(r) | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | \left[ c_{\beta} f - ic \alpha \alpha \left( \Delta_{21}^+/2r \right) f + 2 (c^2 + \beta V(r)) f(r) \right] | n_1 j_1 \epsilon_1 \rangle. \]  
(37)

Equations (35)–(37) are the basic equations of our problem.

### 3.3 The relativistic recurrence relations

To proceed from (37), we now consider, as in the non-relativistic case, only radial functions of the form \( f(r) = r^\lambda \) and we insert the explicit expression for the Coulomb potential: \( V(r) = -Z/r \). Let us mention though that our results can be generalized to other power of potentials, such as the Lennard-Jones potential \[42\]. Substituting \( f(r) = r^\lambda \) in (32), it follows that

\[ (E_2^2 - E_1^2) \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | \left[ (1/4)c^2 \Delta_{21}^+ \Delta_{21}^- - c^2 \lambda (\lambda + 1) \right] r^{\lambda-2} + (c^2/2) \Delta_{21}^+ \beta r^{\lambda-2} - 2c^2 \lambda r^{\lambda-1} d \frac{d}{dr} \]
\[ -2ic \alpha \beta \left( \lambda + (1/2) \Delta_{21}^+ \right) r^{\lambda-1} V(r) | n_1 j_1 \epsilon_1 \rangle; \]  
(38)

hence, we can eliminate the term containing the derivative operator in this last equation using \( f(r) = r^{\lambda-1} \) in Eq. (35), to get the result

\[ (E_2^2 - E_1^2) \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | \left( c^4/4 \right) \Delta_{21}^+ \Delta_{21}^- r^{\lambda-2} + (c^2/2) \Delta_{21}^+ \beta (1 - \lambda) r^{\lambda-2} - ic \alpha \beta \Delta_{21}^+ r^{\lambda-1} V(r) \]
\[ + (E_2 + E_1) \lambda (-ic \alpha) r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle; \]  
(39)
we can, in this last equation, eliminate the term with \(-ica_r\Delta_{21}^-\beta r^{\lambda-1}\) by using Eq. \textbf{26} with \(f(r) = r^\lambda\), to get

\[
(E_2^2 - E_1^2)\langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | \left[ c^2 \Delta_{21}^-/\lambda + c^2 \Delta_{21}^- (1 - \lambda) \beta \right] r^{\lambda-2} + 2Z \left[ ic\alpha_r r^{\lambda-2} (1 - \lambda) - (E_2 - E_1) r^{\lambda-1} \right] - (E_2 + E_1) ic\alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle. \tag{40}
\]

Now, from Eq. \textbf{36} with \(f(r) = r^\lambda\) we get

\[
(E_2 - E_1)\langle n_2 j_2 \epsilon_2 | -ic\alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | -c^2 (\lambda - 1) r^{\lambda-2} + (c^2 / 2) \Delta_{21}^+ \beta r^{\lambda-2} + 2ic\beta c\alpha r mr^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle \tag{41}
\]

and using \(f(r) = r^\lambda\) in Eq. \textbf{37} to eliminate the term \(2ic\beta c\alpha r mr^{\lambda-1}\) of the above equation, we obtain

\[
(E_2 - E_1)\langle n_2 j_2 \epsilon_2 | (-ic\alpha_r r^{\lambda-1}) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | \left[ -c^2 (\lambda - 1) r^{\lambda-2} + (c^2 / 2) \Delta_{21}^+ \beta r^{\lambda-2} - (2 / \lambda) (E_2 + E_1) c^2 \beta r^\lambda + (c^2 / \lambda) (-ic\alpha_r) \Delta_{21}^- r^{\lambda-1} + c^2 ((4/\lambda)r^\lambda - (4Z/\lambda) r^{\lambda-1}) \right] | n_1 j_1 \epsilon_1 \rangle; \tag{42}
\]

which can be written as

\[
\left[ (E_2 - E_1) - c^2 \Delta_{21}^- / \lambda \right] \langle n_2 j_2 \epsilon_2 | (-ic\alpha_r r^{\lambda-1}) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | [(1 - \lambda)r^{\lambda-2} + \frac{4c^2}{\lambda} r^\lambda + \frac{c^2}{2} \Delta_{21}^+ \beta r^{\lambda-2} - \frac{4c^2 Z}{\lambda} \beta r^{\lambda-1} - \frac{2}{\lambda} (E_2 + E_1) \beta r^\lambda] | n_1 j_1 \epsilon_1 \rangle. \tag{43}
\]

We can also obtain a new relationship for the matrix elements of \(-ic\alpha_r r^{\lambda-1}\), using Eq. \textbf{26} with \(f(r) = r^\lambda\), and substitute the result in Eq. \textbf{41} to eliminate the term \(2ic\beta c\alpha r mr^{\lambda-1}\)

\[
(E_2 - E_1)\langle n_2 j_2 \epsilon_2 | -ic\alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | [-c^2 (\lambda - 1) r^{\lambda-2} + (c^2 / 2) \Delta_{21}^+ \beta r^{\lambda-2} + (4\lambda / \Delta_{21}) (-ic\alpha_r) r^{\lambda-1} - (c^2 / \Delta_{21}) (E_2 - E_1) r^\lambda] | n_1 j_1 \epsilon_1 \rangle. \tag{44}
\]

Rearranging terms, we obtain

\[
\left[ (E_2 - E_1) - \frac{4c^2}{\Delta_{21}} \right] \langle n_2 j_2 \epsilon_2 | (-ic\alpha_r r^{\lambda-1}) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | c^2 (1 - \lambda) r^{\lambda-2} - \left( \frac{4c^2}{\Delta_{21}} \right) (E_2 - E_1) r^\lambda + \left( \frac{c^2}{2} \right) \Delta_{21}^+ \beta r^{\lambda-2} | n_1 j_1 \epsilon_1 \rangle. \tag{45}
\]

The relation we are looking for follows from this last result and Eq. \textbf{11}. We use successively \(r^{\lambda-1}\) and \(r^{\lambda-2}\) from Eq. \textbf{15} to eliminate the terms \(2(E_2 + E_1) ic\alpha_r r^{\lambda-1}\) and \(2ic\alpha r^{\lambda-2}(1 - \lambda)\) that appear in Eq. \textbf{40} to finally get

\[
c_0 \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \]

10
\[
\sum_{i=1}^{3} c_i \langle n_2 j_2 \epsilon_2 | r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle + \sum_{i=2}^{3} d_i \langle n_2 j_2 \epsilon_2 | \beta r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle,
\]

where the numbers \(c_i, i = 0, \ldots, 3\) are given by

\[
c_0 = \frac{(E_2^2 - E_1^2)(E_2 - E_1)\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4\lambda c^2},
\]

\[
c_1 = -\frac{2Z(E_2 - E_1)^2\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4(\lambda - 1)c^2},
\]

\[
c_2 = \frac{c^2\Delta_{21}^+\Delta_{21}^-}{4} - \lambda(\lambda - 1) - \frac{c^2(E_1 + E_2)\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4\lambda c^2},
\]

\[
c_3 = \frac{-2c^2Z(\lambda - 1)(\lambda - 2)\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4(\lambda - 1)c^2},
\]

and the numbers \(d_i, i = 2\) and \(3\), by

\[
d_2 = \frac{c^2\Delta_{21}^-}{2} \left[ (1 - \lambda) + \frac{\lambda(E_2 + E_1)\Delta_{21}^+}{(E_2 - E_1)\Delta_{21}^- - 4\lambda c^2} \right],
\]

\[
d_3 = \frac{Zc^2(\lambda - 1)\Delta_{21}^+\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4(\lambda - 1)c^2},
\]

It seems to be natural that we obtained six matrix coefficients instead of only three as in the non-relativistic case. This is to be so, because in the Dirac case we have to deal at the same time with the big and the small components in the state function of the system, doubling the ‘degrees of freedom’ we need to know to determine completely a state in the relativistic realm.

Unfortunately it is not easy to avoid the \(\beta\)-dependency in Eq. \(46\), and thus, taken on its own, Eq. \(45\) does not allow the computation of \(<2 | r^\lambda | 1>\) in terms of the \(<2 | r^{\lambda-a} | 1>\), \(a = 1, 2, 3\). The situation is not hopeless though, because it is still possible to obtain another recurrence relation for non-diagonal matrix elements of \(\beta r^\lambda\) simply by eliminating the term \(-ic\alpha_r r^{\lambda-1}\) between Eqs. \(43\) and \(45\). In such a way we get

\[
e_0 \langle n_2 j_2 \epsilon_2 | \beta r^\lambda | n_1 j_1 \epsilon_1 \rangle = b_0 \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle + b_2 \langle n_2 j_2 \epsilon_2 | r^{\lambda-2} | n_1 j_1 \epsilon_1 \rangle + e_1 \langle n_2 j_2 \epsilon_2 | \beta r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle + e_2 \langle n_2 j_2 \epsilon_2 | \beta r^{\lambda-2} | n_1 j_1 \epsilon_1 \rangle,
\]

where the numbers \(b_i\) and \(e_i, i = 1, 2, 3\) are given by

\[
b_0 = 4\lambda [(E_2 - E_1)^2 - 4c^4],
\]

\[
b_2 = c^2(1 - \lambda) [(\Delta_{21}^-)^2 - 4\lambda^2],
\]

\[
e_0 = 2(E_2 + E_1)[(E_2 - E_1)\Delta_{21}^- - 4\lambda c^2],
\]

\[
e_1 = 4c^2 Z [4\lambda c^2 - (E_2 - E_1)\Delta_{21}^-],
\]

\[
e_2 = c^2\frac{\Delta_{21}^+}{2} [(\Delta_{21}^-)^2 - 4\lambda^2].
\]
We consider Eqs. (46) - (58) as the equivalent of the Blanchard relation for the relativistic case. The reason appears to be evident in the next section, but let us mention that these equations produce the relativistic virial theorem, as happens to be also the case in the non-relativistic Blanchard sum rule (see subsection 2.2).

To end this subsection, we should say that the relativistic recurrence relations can be, juggling with all the relations used (see [14, 15] for details), put in the uncoupled (and possibly the simplest) form

\[ \nu_0 \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \sum_{i=1}^{5} \nu_i \langle n_2 j_2 \epsilon_2 | r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle, \quad (59) \]

where

\[ \nu_0 = \frac{2(E^+)^2(E^-)^2 J}{c^2 Z(\lambda - 1)}, \quad (60) \]
\[ \nu_1 = -8E^+(E^-)^2 \frac{J + 6c^2}{c^2(\lambda - 1)}, \quad (61) \]
\[ \nu_2 = \frac{2LF}{Z} \left[ \frac{\lambda E^+}{(\lambda - 1)H} - J - E^+ - \frac{4c^2(\lambda - 2)}{S} \right] - \frac{E^+ D}{Z} \left[ \frac{G}{2} - \frac{2c^2}{K} \right] \frac{J}{c^2 Z(\lambda - 1)} \left[ 8Z^2(E^-)^2 H + \frac{c^2 E^+(E^-)^2 L}{2HJ} \right], \quad (62) \]
\[ \nu_3 = - \left[ D \left( G - \frac{4c^2}{K} \right) + 4E^+(\lambda - 2)HJ + \frac{(E^-)^2 L}{(\lambda - 1)} \right], \quad (64) \]
\[ \nu_4 = \frac{c^2(\lambda - 1)L}{2Z} \left[ \frac{\lambda E^+}{(\lambda - 1)H} - J - E^+ - \frac{4c^2(\lambda - 2)}{S} \right] - 8Z(\lambda - 2)HJ \frac{c^2 \Delta_{21}^+ L}{8Z} \left( G - \frac{4c^2}{K} \right), \quad (66) \]
\[ \nu_5 = c^2(\lambda - 2)L \quad (67) \]

and

\[ \eta_0 \langle n_2 j_2 \epsilon_2 | \beta r^\lambda | n_1 j_1 \epsilon_1 \rangle = \sum_{i=1}^{3} \eta_i \langle n_2 j_2 \epsilon_2 | \beta r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle, \quad (68) \]

where

\[ \eta_0 = \frac{E^+ D}{2\lambda F} - \frac{KE^+}{2c^2} - \frac{2\lambda}{\Delta_{21}^+}, \quad (69) \]
\[ \eta_1 = Z \left[ \frac{K}{c^2} - \frac{D}{\lambda F} \right], \quad (70) \]
\[ \eta_2 = \frac{(\lambda - 1)L}{2\lambda F} \left[ \frac{E^+ K}{4} + \frac{c^2(\lambda - 2)}{\Delta_{21}^+} - \frac{c^2 \Delta_{21}^+}{4(\lambda - 1)} \right], \quad (71) \]
\[ \eta_3 = \frac{(\lambda - 1)ZKL}{4\lambda F}. \] (72)

The symbols defined in order to write the above recursion relations are, \( M = \lambda(\lambda - 1)E^+, \)
\( D = \Delta_{21}E^+ - 4c^2, \) \( F = -(E^+)^2 - 4c^2, \)
\( S = \Delta_{21}^+ + \Delta_{21}^{-}, \)
\( K = S/\Delta_{21}^+, \)
\( L = 4\lambda^2 - (\Delta_{21}^-)^2, \)
\( J = (D + 4c^2)/\Delta_{21}^+, \)
\( G = [J(2M - \Delta_{21}D)/(\lambda - 1)D], \) and \( H = D/(D + 4c^2). \) One more thing is worth mentioning, all the relativistic sum rules we have discussed are valid whenever the following condition holds \( \omega_1 + \omega_2 + |\lambda| + 1 > 0 \) where \( \omega_a \) defined by the quantities 
\( +\sqrt{(j_a + 1/2)^2 - (Z\alpha_F)^2}, \) \( a = 1, 2 \) are real numbers, and you must keep in mind that the \( \lambda \)'s are even allowed to be complex [8 [12 [13 [19].

### 3.4 The diagonal case

In the calculations of the last section we always assumed that \( \Delta_{21}^- \neq 0, \) but some interesting results are also obtained when this quantity vanishes. In order to study the diagonal case we put \( \epsilon_1 = \epsilon_2 \) and \( j_1 = j_2; \) this in turn imply \( \Delta_{21}^- = 0. \) We remark that in all cases \( \Delta_{21}^+ \equiv \Delta^+ \neq 0. \)

We start from Eq. \( \text{(26)} \) and put
\[
(E_2 - E_1)\langle n_2 j \epsilon \mid f(r)\rangle_{n_1 j \epsilon} = \langle n_2 j \epsilon \mid (-ic\alpha_f)\rangle_{n_1 j \epsilon}. \] (73)

We proceed to calculate the second order iteration by substituting \( f(r) \rightarrow \xi_+ = H_2f(r) - f(r)H_1, \) as was done in the previous section, in the above equation to obtain
\[
(E_2 - E_1)^2\langle n_2 j \epsilon \mid f\rangle_{n_1 j \epsilon} = c^2\langle n_2 j \epsilon \mid [- f'' + \frac{\Delta^+}{2r}f'\beta + 2ic\alpha_f\beta f']\rangle_{n_1 j \epsilon}; \] (74)

and then substitute \( f(r) \rightarrow \xi_+ = H_2f(r) + f(r)H_1 \) again in \( \text{(58)} \) to get
\[
(E_2^2 - E_1^2)\langle n_2 j \epsilon \mid f(r)\rangle_{n_1 j \epsilon} = -\langle n_2 j \epsilon \mid [c^2(2f'(r)/r + f''(r) + 2f'(r)\frac{\Delta^+}{dr})
+ 2ic\alpha_f f'(r)V(r)]\rangle_{n_1 j \epsilon}. \] (75)

So, the relevant equations for the diagonal case are now
\[
(E_2 + E_1)\langle n_2 j \epsilon \mid (-ic\alpha_f)\rangle_{n_1 j \epsilon} = -\langle n_2 j \epsilon \mid [c^2(2f'(r)/r + f''(r) + 2f(r)\frac{\Delta^+}{dr})
- 2ic\alpha_f V(r)f(r)]\rangle_{n_1 j \epsilon}, \] (76)

and
\[
(E_2 - E_1)\langle n_2 j \epsilon \mid (-ic\alpha_f)\rangle_{n_1 j \epsilon} = \langle n_2 j \epsilon \mid [- c^2f'(r) + c^2(\Delta^+/2r)f + 2ic^3\alpha_f f(r)]\rangle_{n_1 j \epsilon}. \] (77)

We also have, for the matrix elements of \( \beta f(r), \)
\[
(E_2 + E_1)\langle n_2 j \epsilon \mid \beta f\rangle_{n_1 j \epsilon} = \langle n_2 j \epsilon \mid [- ic\alpha_f f' + 2\left(c^2 + \beta V(r)\right)f]\rangle_{n_1 j \epsilon}. \] (78)
We can now obtain a recurrence relation valid in the diagonal case. First, let us use \( f(r) = r^\lambda \) in Eq. (74) to get

\[
(E_2 - E_1)^2 \langle n_2 j \epsilon | r^\lambda | n_1 j \epsilon \rangle = \lambda \langle n_2 j \epsilon | [- c^2(\lambda - 1)r^{\lambda - 2} + (c^2/2)\Delta + \beta r^{\lambda - 2} + 2ic^3\alpha_r \beta r^{\lambda - 1}] | n_1 j \epsilon \rangle. \tag{79}
\]

Evaluating now equation (78) with \( f(r) = r^\lambda \), we obtain

\[
(E_2 + E_1) \langle n_2 j \epsilon | \beta r^\lambda | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | [- ic\alpha_r \beta \lambda r^{\lambda - 1} - 2Z(\beta/r) r^\lambda + 2c^2 r^\lambda] | n_1 j \epsilon \rangle, \tag{80}
\]

and eliminating the \( ic\alpha_r \beta \lambda r^{\lambda - 1} \) between the last two equations, we finally get

\[
[(E_2 - E_1)^2 - 4c^4] \langle n_2 j \epsilon | r^\lambda | n_1 j \epsilon \rangle = -(c^2/2)\lambda \Delta \langle n_2 j \epsilon | \beta r^{\lambda - 2} | n_1 j \epsilon \rangle - 4c^2Z \langle n_2 j \epsilon | \beta r^{\lambda - 1} | n_1 j \epsilon \rangle - 2c^2(E_2 + E_1) \langle n_2 j \epsilon | \beta r^\lambda | n_1 j \epsilon \rangle - c^2\lambda(\lambda - 1) \langle n_2 j \epsilon | r^{\lambda - 2} | n_1 j \epsilon \rangle. \tag{81}
\]

This is the only recurrence relation we get in the diagonal case.

### 3.5 The relativistic Pasternack-Sternheimer rule and the relativistic virial theorem

The special case when \( \lambda = 0 \) in (81) is of particular interest

\[
[(E_2 - E_1)^2 - 4c^4] \delta_{n_1 n_2} = -4Zc^2 \langle n_2 j \epsilon | \left( \frac{\hat{\alpha}}{\hat{r}} \right) | n_1 j \epsilon \rangle - 2c^2(E_2 + E_1) \langle n_2 j \epsilon | \beta | n_1 j \epsilon \rangle. \tag{82}
\]

What we have obtained in this last expression is the relativistic generalization of the Pasternack-Sternheimer rule of non relativistic quantum mechanics \cite{30}. This rule says that the expectation value between hydrogenic states of the \( 1/r^2 \) potential, vanishes when the orbital angular momenta of the states 1 and 2 coincide, that is when \( l_1 = l_2 \). We want to remark in this point that in the relativistic case, the expectation value of the \( 1/r \) potential (which could be regarded as the square root of \( 1/r^2 \)) times \( \beta \), does not necessarily vanish even when the total angular momenta of the two states coincide: \( j_1 = j_2 \). This point agrees with the fact that the non-relativistic Pasternack-Sternheimer rule is applicable to eigenfunctions of potentials whose energy eigenvalues depend only on the principal quantum number—which is not the case for the hydrogen atom in Dirac quantum mechanics \cite{12}.

Furthermore, two special cases are immediately deduced from this last expression:

1) The first case, when \( n_1 \neq n_2 \), is

\[
2\langle n_2 j \epsilon | \frac{Z\beta}{r} | n_1 j \epsilon \rangle = -(E_2 + E_1) \langle n_2 j \epsilon | \beta | n_1 j \epsilon \rangle. \tag{83}
\]

2) The other case follows when \( n_1 = n_2 \)
\[ c^2 = - \langle \beta V(r) \rangle + E \langle \beta \rangle = Z \left\langle \frac{\beta}{r} \right\rangle + E \langle \beta \rangle, \] (84)

which is the relativistic virial theorem \[31\]. Also, from the relation \( c^2 < \beta >= E \) \[3\], we can also write an interesting result for the average value of the Coulomb potential and the \( \beta \) matrix.

\[ E^2 = c^2 \langle \beta V(r) \rangle + c^4 = -Zc^2 \left\langle \frac{\beta}{r} \right\rangle + c^4. \] (85)

4 Analytic results for \( r^\lambda \) and \( \beta r^\lambda \)

The recurrence relations found above involve expressions that can be burdensome to handle, excepting perhaps in the diagonal case. Given such situation, before we generalize the relations above to the case of two-potentials, we calculate explicit formulas to evaluate the diagonal and the non-diagonal matrix elements of interest in the particular case of the Coulomb potential \( V(r) = -Z/r \). The results obtained are based on properties of the hypergeometric function and can be deduced directly from the two differential equations that follow directly from the Hamiltonian (23). In this section we mostly use ideas from \[43\]. First of all we must say that we are interested in the bound states of the problem, so the quantity \( k \equiv \sqrt{c^4 - E^2} \) is positive. We can write the differential equations for the radial part of any central problem in terms of the dimensionless variable \( \rho \equiv kr \). We also define the following quantities \[43\]:

\[ k \equiv \frac{1}{\hbar c} \sqrt{c^4 - E^2}, \quad \zeta \equiv Z/c = Z\alpha_F, \quad \tau_j \equiv \epsilon(j + \frac{1}{2}), \]
\[ \nu \equiv \sqrt{(c^2 - E)/(c^2 + E)}, \quad s \equiv \sqrt{\tau_j^2 - \zeta^2}, \] (86)

where \( \alpha_F \approx 1/137 \) is the fine structure constant.

It is proven in \[43\], that the radial Dirac equation with potential \( V(r) = -Z/r \) is completely equivalent to

\[ \left\{ \begin{array}{l} \left( -\frac{d}{d\rho} + \frac{\tau_j}{\rho} \right) G(\rho) = (-\nu + \zeta/\rho) F(\rho), \\ \left( +\frac{d}{d\rho} + \frac{\tau_j}{\rho} \right) F(\rho) = (\nu^{-1} + \zeta/\rho) G(\rho); \end{array} \right. \] (87)

where \( F(\rho) \) and \( G(\rho) \) are the radial solutions of the big and small components respectively. Now, to solve these two equations, we look for solutions of the form

\[ F(\rho) = \sqrt{c^2 + E} \left[ \psi_+(\rho) - \psi_-(\rho) \right], \] (88)

and

\[ G(\rho) = \sqrt{c^2 - E} \left[ \psi_+(\rho) + \psi_-(\rho) \right]. \] (89)
The solution to these coupled differential equations can be written in terms of the Laguerre polynomials of non-integer index \[13, 44, 45\]

\[
\psi_+^{(\rho)} = a\rho^s e^{-\rho} L_{n-1}^{2s}(2\rho),
\psi_-^{(\rho)} = b\rho^s e^{-\rho} L_{n}^{2s}(2\rho),
\]

where the Laguerre polynomials \(L_n^\alpha(\rho)\) are related to both the hypergeometric function, \(_1F_1(-n, \alpha + 1; \rho)\), and the Sonine polynomials, \(T_n^{(n)}(\rho)\) \[45\], through the relation

\[
L_n^\alpha(\rho) = \frac{\Gamma(\alpha + n + 1)}{n!\Gamma(\alpha + 1)} _1F_1(-n; \alpha + 1; \rho) = (-1)^n \Gamma(\alpha + n + 1) T_n^{(n)}(\rho),
\]

and \(a\) and \(b\) are constants. Substitution of these results in Eq. (87) gives the condition

\[
a(\tau_j + s - \zeta\nu^{-1} + n) + b(n + 2s) = 0,
\]

\[
b(\tau_j - s + \zeta\nu^{-1} - n) - an = 0.
\]

When we solve the above equations we obtain a relationship between \(n\) and \(\nu\). From Eq. (86) we see that this in turn gives us an expression for the energy, which coincides with the correct value provided we define the principal quantum number \(N \equiv j + 1/2 + n\), where \(n = 0, 1, 2, \cdots 46\)

\[
E = mc^2 \left(1 + \frac{Z^2\alpha_F^2}{(N - j - 1/2 + \sqrt{(j + 1/2)^2 - Z^2\alpha_F^2})^2}\right)^{-1/2};
\]

To proceed further, we take

\[
b = -a(\tau_j + s + n - \zeta\nu^{-1})/(n + 2s),
\]

and write the result in a symmetrized form:

\[
F(\rho) = \sqrt{mc^2 + \xi E} C\rho^s e^{-\rho} \left[u L_n^{2s}(2\rho) + v L_{n-1}^{2s}(2\rho)\right],
G(\rho) = -\sqrt{mc^2 - \xi E} C\rho^s e^{-\rho} \left[u L_n^{2s}(2\rho) - v L_{n-1}^{2s}(2\rho)\right],
\]

where

\[
u = (n + 2s)(\tau_j + s + n - \zeta\nu^{-1})^{-1/2},
\]

The \(C\) in Eq. \[95\] is a normalization constant that can be obtained from

\[
\int_0^\infty e^{-x} x^\alpha L_n^\alpha(x) L_m^\alpha(x) = \frac{\Gamma(n + \alpha + 1)}{n!};
\]

To obtain \(C\), we use relations \[96\] to get \((\tau_j + s + n - \zeta\nu^{-1})^{-1} = (n + s - \tau_j - \zeta\nu^{-1})/n(n + 2s)\); we need also \((n + s) = \xi E/\sqrt{m^2c^4 - \xi E^2}\), which is obtained from the expression for the energy eigenvalues of the Dirac hydrogen atom: after some work we obtain.
The calculation of diagonal, arbitrary power matrix elements of the form $<r^\lambda>$ and $<\beta r^\lambda>$, are obtained from

$$I_{nm}^\alpha(\lambda) \equiv \int_0^\infty e^{-x} x^{\alpha + \lambda} \mathcal{L}_n^\alpha(x) \mathcal{L}_m^\alpha(x) dx.$$  \hspace{1cm} (99)

This expression converges for $\text{Re}(\alpha + \lambda + 1) > 0$, and is zero if $\lambda$ is an integer such that $m - n > \lambda \geq 0$, where without loss of generality, we assume that $m > n$. From Rodrigues formula and $(d^m/dx^m)x^{k+\lambda} = (-1)^m[-k - \lambda]_m x^{k+\lambda-m}$, where $[n]$, $n$ an integer, is a Pochhammer symbol, we find, after a $m$-times partial integration,

$$I_{nm}^\alpha(\lambda) = \frac{1}{m!} \sum_{k=0}^n (-1)^k \frac{\Gamma(n + \alpha + 1) \Gamma(\alpha + k + \lambda + 1) [-k - \lambda]_m}{k! (n-k)! \Gamma(\alpha + k + 1)}.$$ \hspace{1cm} (100)

We now use the identity $[-k - \lambda]_m = [-k - \lambda]_k [-\lambda]_{m-k}$, change the order of summation $k \to n - k$ and use the identities

$$\begin{align*}
[-\lambda]_{m-n+k} &= [-\lambda]_{m-n} [-\lambda + m-n]_k, \\
\Gamma(n + \alpha + 1) &= (-1)^k \Gamma(\alpha + n - k + 1) [-\alpha - n]_k, \\
\Gamma(\alpha + \lambda + n + 1) &= (-1)^k \Gamma(\alpha + \lambda + n - k + 1) [-\alpha - \lambda - n]_k, \\
[k - n - \lambda]_{n-k} &= (-1)^n \frac{\Gamma(\alpha + n + 1)}{\Gamma(\lambda + 1)} \frac{1}{[-\lambda - n]_k},
\end{align*}$$

(101)

to deduce that

$$I_{nm}^\alpha(\lambda) = [-\lambda]_{m-n} \frac{\Gamma(\alpha + \lambda + n + 1) \Gamma(\lambda + n + 1)}{m! \Gamma(\lambda + 1)} \times {}_3 F_2\left(-\alpha - n, -\lambda + m - n, -n; -\lambda - n, -\alpha - \lambda - n; 1\right).$$ \hspace{1cm} (102)

Now, we are going to consider two cases for the matrix elements $\langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle$ and $\langle n_2 j_2 \epsilon_2 | \beta r^\lambda | n_1 j_1 \epsilon_1 \rangle$; in the first one $k_1 = k_2$, where we need to evaluate

$$K_{nm}^{s_1 s_2}(\lambda) \equiv \int_0^\infty x^{s_1 + s_2 + \lambda} e^{-x} \mathcal{L}_n^{(2s_1)}(x) \mathcal{L}_m^{(2s_2)}(x) dx, \hspace{1cm} (103)$$

and the second one, when $k_1 \neq k_2$, we need

$$K_{nm}^{s_1 s_2}(\lambda) \equiv \int_0^\infty r^{s_1 + s_2 + \lambda} e^{-(k_1 + k_2) r} \mathcal{L}_n^{(2s_1)}(2k_1 r) \mathcal{L}_m^{(2s_2)}(2k_2 r) dr. \hspace{1cm} (104)$$

In the first case, we see that integral (103) is convergent if $\text{Re}(s_1 + s_2 + \lambda + 1) > 0$, and vanishes when $s_1 - s_2 + \lambda$ is an integer such that $m - n > s_1 - s_2 + \lambda \geq 0$. With a similar reasoning as in the diagonal case, we get

$$K_{nm}^{s_1 s_2}(\lambda) = [w]_{m-n} \frac{\Gamma(s_1 + s_2 + \lambda + n + 1) \Gamma(\lambda + s_1 - s_2 + n + 1)}{m! \Gamma(\lambda + s_1 - s_2 + 1)}.$$
\[ \times_{3}F_{2}(-2s_{1} - n, w + m - n, -n; w - n, -\lambda - s_{1} - s_{2} - n; 1). \] (105)

where \( w \equiv -\lambda + s_{2} - s_{1} \). In the second case we see that the integral converges for \( Re(s_{1} + s_{2} + \lambda + 1) > 0 \), and is not zero provided \( k_{1} \neq k_{2} \). A calculation by parts shows that

\[
K_{nm}^{s_{1}s_{2}}(\lambda) = \sum_{i=0}^{m} \sum_{j=0}^{n} \frac{(-1)^{i}(k_{2} - k_{1})^{m-i}(k_{1} + k_{2})(i-m-s_{1}-s_{2}-\lambda-1)}{i! (m-i)! (n-j)!} \Gamma(n + 2s_{1} + 1)\Gamma(m + s_{2} + s_{1} + \lambda - i + 1),
\]

(106)

where \( k_{1} \neq k_{2} \). This expression can be simplified a little bit by eliminating the double sum in terms of a single one using the identities.

\[
[p]_{m-i} = (-1)^{m-i} \frac{\Gamma(-p+1)}{[-p-m+1]i \Gamma(-p-m+1)}, \tag{107}
\]

\[
\Gamma(-p-m+i+1) = [-p-m+1]i \Gamma(-p-m+1), \tag{108}
\]

\[
(m-i)! = m! (-1)^{i}, \tag{109}
\]

\[
\Gamma(p+1) = [p-m+1]m \Gamma(p-m+1). \tag{110}
\]

This expression is valid provided \( p, m \) and \( i \) are integers. After some algebra, we finally get

\[
K_{nm}^{s_{1}s_{2}}(\lambda) = \frac{(-1)^{m} \Gamma(n + 2s_{1} + 1)\Gamma(s_{1} + s_{2} + \lambda + 1)}{m!(k_{2} + k_{1})^{i+1} + s_{2} + \lambda + 1)} \sum_{j=0}^{n} \frac{(-1)^{j} [s_{1} - s_{2} + \lambda + j - m + 1]}{j! (n-j)! \Gamma(2s_{1} + j + 1)} \times_{2}F_{1}(-m, s_{1} + s_{2} + \lambda + 1; s_{1} - s_{2} + \lambda + j - m + 1; k_{2} - k_{1} k_{2} + k_{1}). \tag{111}
\]

We are now in the position to calculate the values of \( < r^{\lambda} > \) and \( < \beta r^{\lambda} > \), using the expression (99) for \( I_{nm}^{\alpha}(\lambda) \), with \( \alpha = 2s \). After some algebra we obtain from Eq. (99) and our previous definitions the following expressions

\[
< r^{\lambda} > = \frac{mc^{2}|C|^{2}}{(2k)^{\lambda+1}2^{s-1}} \left[ I_{nm}^{2s}(\lambda)u^{2} + I_{n-1n-1}^{2s}(\lambda)v^{2} + EuwI_{nm}^{2s}(\lambda) \right] \tag{112}
\]

and

\[
< \beta r^{\lambda} > = \frac{E|C|^{2}}{(2k)^{\lambda+1}2^{s-1}} \left[ I_{nm}^{2s}(\lambda)u^{2} + I_{n-1n-1}^{2s}(\lambda)v^{2} + mc^{2}uwI_{nm}^{2s}(\lambda) \right]. \tag{113}
\]

The numbers \( u \) and \( v \) are the constants defined in Eq. (96)

\section{5 Generalized recurrence relations for two potentials}

In this section we exhibit that the hypervirial techniques suffice to obtain relations between relativistic matrix elements of an arbitrary radial function between eigenstates corresponding
to two different potentials. We obtain four recursion relations between the matrix elements of arbitrary radial functions, \( f(r) \) and \( \beta f(r) \), with the matrix elements of their first and second derivatives, taken between eigenstates of different potential functions, \( V_1(r) \) and \( V_2(r) \) — both behaving as the fourth component of a 4-vector. We call these relations between matrix elements generalized recurrence relations because they led to relations relating successive powers of the radial coordinate when the arbitrary function \( f(r) \) is chosen to be \( r^\lambda \) where \( \lambda \) is a constant number. The recursions between matrix elements we deal with in this section are calculated under the further assumption that the two potentials, \( V_1(r) \) and \( V_2(r) \), have a common minimum, that is, that they are referred to the same origin. The relations lead to explicit recursions when specific forms of the radial functions are used and particular potentials are substituted. The recursions can be useful for studying radiative transitions in Rydberg atoms, in analysing atomic photorecombination and photoionization processes, 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 in any other atomic processes involving highly excited electrons which need to be studied using multichannel spectroscopy or quantum defect theory \[23, 47, 48, 49\]. It can be also useful 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 rather crude manner \[50, 23, 51, 52, 53\].

Let us mention that analogous relations for matrix elements between eigenstates of two potentials were obtained some years ago in nonrelativistic atomic physics also with the help of hypervirial results \[9, 55\].

Let us consider two radial Dirac Hamiltonians with two possibly different radial potentials (each behaving as the temporal component of a fourvector) \( V_1(r) \) and \( V_2(r) \). We further assume that these potentials have the same equilibrium position which, furthermore, is coincident with the origin of coordinates. That is, the recurrence relations correspond to the so-called unshifted case \[9\]. The main difficulty for not dealing with the general (so called, shifted) case is the angular couplings introduced by the relative displacement of one of the potentials respect the other in the otherwise purely radial interactions.

These two Dirac Hamiltonians can be written as

\[
H_1 = c\alpha_r[p_r - i\beta \epsilon_1(j_1 + 1/2)/r] + M_1\beta c^2 + V_1(r),
\]

and

\[
H_2 = c\alpha_r[p_r - i\beta \epsilon_2(j_2 + 1/2)/r] + M_2\beta c^2 + V_2(r),
\]

where we are assuming \( M_1 \neq M_2 \) as it is convenient for our calculations. The eigenstates of these radial Hamiltonians correspond to a definite value of the total angular momentum \( J = L + S \) and of the quantum number \( \epsilon \). The Dirac equations are \( H_k\psi_k(r) = E_k\psi_k(r) \) where the energy eigenvalues \( E_{nkjs_k} \equiv E_k \) and the corresponding eigenfunctions \( \psi_{nkjs_k}(r) \equiv \psi_k(r) \) are assumed known.
5.1 The first generalized recurrence relation for the case of two potentials

Taking the difference between the radial Hamiltonians $H_1$ and $H_2$ in [114] and [115], we obtain

$$H_1 = H_2 + i\alpha_r\beta \frac{\Delta^+}{2r} - c^2\beta M^+ - (V_2(r) - V_1(r)).$$  \hspace{1cm} (116)

where $M^± \equiv M_2 ± M_1$, and $\Delta^± \equiv \epsilon_2(2j_2 + 1) ± \epsilon_1(2j_1 + 1)$ and, in general, if $X$ is any symbol we define $X^± \equiv X_2 ± X_1$. We can directly evaluate the commutator

$$[H_1, f(r)] = -i\alpha_r \frac{df(r)}{dr}$$ \hspace{1cm} (117)

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 (116), to get the alternative form

$$[H_1, f(r)] = H_2f(r) - f(r)H_1 + \left(i\alpha_r\beta \frac{\Delta^+}{2r} - c^2\beta M^+ - V^-\right)f(r).$$ \hspace{1cm} (118)

It is now simple to obtain, from equations (117) and (118), the relation

$$(E_2 - E_1)\langle 2|f|1 \rangle = \langle 2| \left(c^2\beta M^- + V^-\right)f|1 \rangle - ic\langle 2| \alpha_r \left(f' + \beta f \frac{\Delta^+}{2r}\right)|1 \rangle;$$ \hspace{1cm} (119)

where we have additionally taken matrix elements between the eigenstates $\langle 1 \rangle \equiv \langle n_1 j_1 \epsilon_1 \rangle$ and $|n_2 j_2 \epsilon_2 \rangle \equiv |2 \rangle$, and we have defined

$$V^± \equiv V_2(r) ± V_1(r).$$ \hspace{1cm} (120)

Equation (119) leads to recursions between relativistic matrix elements of radial functions between hydrogenic states [14, 13, 15], and generalizes a nonrelativistic expression useful for similar purposes [6]. On the other hand, it is an exact relation for the calculation of any matrix elements of $f(r)$ between eigenstates of two potentials in relativistic quantum mechanics.

Taking the potentials as equal, i.e. $V_1(r) = V_2(r)$, we recover a relation which has been useful for obtaining recurrence relations between atomic matrix elements in relativistic quantum mechanics [14, 15]. Albeit exact, equation (119) is not entirely convenient due to the presence of the operator $\alpha_r \beta$. To get rid of this term, we found it convenient to work directly in terms of operators and not in terms of the matrix elements themselves. The matrix elements will be evaluated at the end of the operator calculations.

Let us first establish that

$$H_2f - fH_1 = \left(c^2\beta M^- + V^-\right)f - ic\alpha_r \left(f' + \beta f \frac{\Delta^+}{2r}\right),$$ \hspace{1cm} (121)
notice that equation (119) above can be obtained from (121) just by taking matrix elements. The following result is also easily established

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

(122)

Then, it can be seen that

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

(123)

and that

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

(124)

It is also readily apparent that

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

(125)

Let us define \( \psi(r) \equiv H_2 f(r) + f(r) H_1 \), and evaluate

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

(126)

In this way, working with all the previous equations, in the way we have exhibited in the previous sections, we can get

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

(127)
Evaluating the matrix elements between the Dirac eigenstates $\langle 2 |$ and $| 1 \rangle$ and rearranging, we finally obtain the relation

$$a_0 \langle 2 | f | 1 \rangle + a_2 \langle 2 | \frac{f}{r^2} | 1 \rangle - 2E^- \langle 2 | V^- f | 1 \rangle + \langle 2 | \left(V^-\right)^2 f | 1 \rangle + c^2 \langle 2 | f'' | 1 \rangle =$$

$$b_0 \langle 2 | \beta f | 1 \rangle + b_1 \langle 2 | \frac{\beta f}{r^2} | 1 \rangle - c^2 M^- \langle 2 | V^+ \beta f | 1 \rangle + c^2 M^+ \langle 2 | V^- \beta f | 1 \rangle + b_4 \langle 2 | \frac{\beta f}{r} | 1 \rangle,$$  

(128)

where

$$a_0 = \left(E^-\right)^2 - \left(c^2 M^-\right)^2$$

$$a_2 = -\frac{c^2}{4} \Delta^- \Delta^+$$

$$b_0 = c^2 \left(M^- E^+ - M^+ E^-\right)$$

$$b_1 = c^2 \Delta^-$$

$$b_4 = \frac{c^2}{2} \left(\Delta^+ - \Delta^-\right)$$  

(129)

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.

### 5.2 More generalized recurrence relations for the case of two potentials

Given that the radial eigenstates have two components in relativistic quantum mechanics, it should be clear that we need more relations. We can obtain at least three more, following a path similar to the one outlined above and in previous papers to get

$$c_0 \langle 2 | f | 1 \rangle + a_2 \langle 2 | \frac{f}{r^2} | 1 \rangle - E^+ \langle 2 | V^- f | 1 \rangle - E^- \langle 2 | V^+ f | 1 \rangle + \langle 2 | V^+ V^- f | 1 \rangle$$

$$-c^2 \langle 2 | \frac{f'}{r} | 1 \rangle + c^2 \langle 2 | f'' | 1 \rangle = \frac{b_2}{2} \langle 2 | \frac{\beta f}{r^2} | 1 \rangle + b_4 \langle 2 | \frac{\beta f'}{r} | 1 \rangle,$$  

(130)

where the only newly defined coefficient is

$$c_0 = E^+ E^- - c^4 M^+ M^-.$$  

(131)

We also get

$$c_0 \langle 2 | f | 1 \rangle = g_0 \langle 2 | \beta f | 1 \rangle - \langle 2 | \left(V^+ - V^-\right) \beta f | 1 \rangle,$$  

(132)
where

\[ e_0 = c^2 (M^+ - M^-) \]
\[ g_0 = E^+ - E^- . \] (133)

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 (132) into (128) to obtain the new relation

\[
A_0 \langle 2 | \beta f | 1 \rangle + A_1 \langle 2 | \beta \frac{f}{r^2} | 1 \rangle + A_2 \langle 2 | V^- \beta f | 1 \rangle + A_3 \langle 2 | (V^-)^2 \beta f | 1 \rangle
+ \langle 2 | (V^-)^3 \beta f | 1 \rangle + A_5 \langle 2 | V^+ \beta f | 1 \rangle + 2 E^- \langle 2 | V^- V^+ \beta f | 1 \rangle
- \langle 2 | (V^-)^2 V^+ \beta f | 1 \rangle + a_2 \langle 2 | (V^+ - V^-) \beta \frac{f}{r^2} | 1 \rangle - c^2 \langle 2 | (V^+ - V^-)^\prime \beta f | 1 \rangle
= A_9 \langle 2 | \beta f' | 1 \rangle + 2 c^2 \langle 2 | (V^+ - V^-)^\prime \beta f' | 1 \rangle - c^2 g_0 \langle 2 | \beta f'' | 1 \rangle
- c^2 \langle 2 | (V^+ - V^-) \beta f'' | 1 \rangle. \] (134)

where the newly defined coefficients are

\[
A_0 = \left( E^- \right)^2 (E^+ - E^-) + c^2 E^- \left[ (M^-)^2 + (M^+)^2 \right] - c^4 M^+ M^- (E^+ + E^-)
A_1 = -\frac{c^2}{4} \left( E^+ - E^- \right) \Delta^+ \Delta^- - c^4 \Delta^- \left( M^+ - M^- \right)
A_2 = -2 E^- \left( E^+ - E^- \right) + \left( E^- \right)^2 - (c^2 M^-)^2 - c^4 M^+ \left( M^+ - M^- \right)
A_3 = E^+ - 3 E^- 
A_5 = c^4 M^+ M^- - \left( E^- \right)^2
A_9 = \frac{c^4}{2} \left( M^+ - M^- \right) \left( \Delta^+ - \Delta^- \right). \] (135)

Equation (134) is the fourth recurrence relation for the calculation of relativistic \( f(r) \) matrix elements between states of different potentials in terms of their energy eigenvalues. Notice that, at difference of the previous relations [equations (128), (130) and (132)], equation (134) relates among themselves matrix elements of \( \beta f \) and its derivatives times a certain function of \( r \).

In summary, in this section we have obtained generalized recurrence relations for the calculation of matrix elements of a radial function between states of two different radial potentials sharing a common origin. The obtained sum rules are given in the most general case of an arbitrary function taken between any non-necessarily diagonal radial eigenstates
of the two radial potentials. Such relations have, as particular cases, sum rules between one-potential integrals or, in other particular cases, between overlap and one centre integrals in Dirac relativistic quantum mechanics. We expect the obtained formulas, together with the previous relations we have obtained \[13, 14, 15\], to be useful in atomic or molecular physics calculations as they may simplify calculation of matrix elements in the range of applicability of Dirac's relativistic quantum mechanics \[54, 19\]. For most uses of the relations we first have to set \(M_1 = M_2\), i.e. \(M^- = 0\) and \(M^+ = 2\) —assuming the particles are electrons— since the use of unequal masses is basically a recourse of our calculational method.

From a more practical angle, there is little that can be done for the analytical evaluation of these integrals beyond the Coulomb and the few similarly exactly solvable potentials. However, there are relativistic theoretical techniques \[56\] and 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 \[57\]. 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 \[23, 54, 34, 58, 59\]. On the other hand, our results may be also of some 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 recently explicitly solved and its eigenfunctions can be expressed in terms of hypergeometric functions \[60\].

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