Relativistically extended Blanchard recurrence relation for hydrogenic matrix elements

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Abstract.

General recurrence relations for arbitrary non-diagonal, radial hydrogenic matrix elements are derived in Dirac relativistic quantum mechanics. Our approach is based on a generalization of the second hypervirial method previously employed in the non-relativistic Schrödinger case. A relativistic version of the Pasternack-Sternheimer relation is thence obtained in the diagonal (i.e. total angular momentum and parity the same) case, from such relation an expression for the relativistic virial theorem is deduced. To contribute to the utility of the relations, explicit expressions for the radial matrix elements of functions of the form $r^\lambda$ and $\beta r^\lambda$—where $\beta$ is a Dirac matrix—are presented.

Keywords: Relativistic hydrogen atom, recurrence relations, non-diagonal radial matrix elements, relativistic Pasternack-Sternheimer relation.

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I. Introduction

Recurrence relations for matrix elements are very useful tools in quantum calculations [1–5] since the direct computation of such elements is generally very cumbersome. An interesting example is the Blanchard’s relation which is a useful recurrence formula for arbitrary (i.e. not necessarily diagonal) non-relativistic matrix elements of the form \( \langle n_1 l_1 | r^\lambda | n_2 l_2 \rangle \), where the \(|nl\rangle\) stand for non-relativistic hydrogenic radial energy eigenstates; according to this relation, once any three successive matrix elements of powers of the radial coordinate, \( r \), are known, any other can be deduced in terms of the previously known ones. The Blanchard recurrence relation was derived more than twenty five years ago using a calculation-intensive method [6], which is not surprising since in general recurrence relations are rather difficult to obtain.

Trying to overcome such difficulties, different approaches have been proposed for obtaining general recurrence relations; some of them are based on algebraic methods, others use sum rules and hypervirial theorems [4,7–10]. In particular, a hypervirial result has been employed to obtain the Blanchard relation in a more compact way than in the original deduction [11]. In relativistic quantum mechanics, on the other hand, and despite its physical and its possible chemical interest [7,8,12,13], excepting for the results reported in [14], there are not as yet general recurrence relations which could be used for calculating matrix elements of powers of the radial coordinate in terms of previously known ones. We should mention though that there are previous efforts in such direction, in which closed forms for certain relativistic matrix elements have been evaluated [16,17] and certain, mostly diagonal, recurrence relations for relativistic and quasirelativistic states have been calculated [3,9,12,17].

In this paper we employ a relativistic calculation inspired on the hypervirial method [11] to deduce a recurrence relation 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 [18–20]— for relativistic hydrogenic states in the energy basis. The assumptions we use are that the nucleus is point-like and fixed in space, and that a description using the Dirac equation is 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, as we use the quantum number \( \epsilon \equiv (-1)^{j+l-1/2} \) instead of parity for labelling the hydrogenic eigenstates, where \( \epsilon_1 \neq \epsilon_2 \). 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 [Eqs. (6) and (7) of section II]. Given its special interest, we study in particular 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 rule [21] and to obtain an expression for the relativistic virial theorem [9,14,22].

This paper is organized as follows. In section II we review the second hypervirial scheme used for deriving the non-relativistic Blanchard relation. In section III, after obtaining the radial Hamiltonian useful for implementing the hypervirial result in relativistic quantum mechanics, we proceed to use it to deduce by a long but direct calculation the relativistic recurrence formulae. In section IV we study in particular the diagonal case \( (j_2 = j_1, \epsilon_2 = \epsilon_1) \) to derive the relativistic Pasternak-Sternheimer rule and use it \( (n_1 = n_2) \) to obtain a version of the relativistic virial theorem. In the Appendix, we obtain explicit expressions for diagonal and non-diagonal matrix elements for any power of \( r \) and of \( \beta r \) between radial relativistic hydrogenic states. 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 III of this article. Furthermore, these results can be of utility not only for relativistic atomic and molecular studies but also for evaluating matrix elements of interactions designed to test Lorentz and CPT invariance in hydrogen [14,29].

II. The non-relativistic recurrence relation

Both the Blanchard relation and its predecessor the Kramers selection rule, were originally obtained employing directly the Schrödinger equation together with appropriate boundary conditions and, at least in the former case, a great deal of computations [1,6]. A much simpler approach based on a generalized hypervirial result and certain Hamiltonian identities has been developed to simplify the computations leading to the Blanchard relation [11]. This technique seemed to us an appropriate starting point for deriving relativistic recurrence formulae. It is with such relativistic extension in mind that we review in this section the hypervirial method as it is applied in non-relativistic quantum mechanics. In this section, as in most of the paper, we employ atomic units \( \hbar = m = e = 1. \)

The idea is to start with the radial Schrödinger equation for a central potential \( V(r) \) written in the form

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

where \( |n_k l_k\rangle = \psi_{n_k l_k}(r) \) and \( E_{n_k l_k} \) are an energy eigenfunction and its corresponding energy eigenvalue with principal and angular momentum quantum numbers, \( n_k \) and \( l_k, \) respectively; \( k \) is just a label, and \( H_k, \) the non-relativistic radial Hamiltonian, is given by
\[ H_k = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{l_k (l_k + 1)}{2r^2} + V(r). \] (2)

Although we want to calculate the radial matrix elements of 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 choice we can readily show [11] that

\[
(E_i - E_k) \langle n_i l_i | f(r) | n_k l_k \rangle = \langle n_i l_i | \left( -\frac{1}{2} f'' - f' \frac{d}{dr} - \frac{1}{r} f' + \frac{\Delta_{l_k}^r f}{2r^2} \right) | n_k l_k \rangle,
\] (3)

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

\[
\langle n_i l_i | f(r) | n_k l_k \rangle = \int_0^\infty r^2 \psi_{n_i l_i}^*(r) f(r) \psi_{n_k l_k} (r) dr.
\] (4)

To establish the result we are after, we apply the previous result (3) to the radial function \( \xi(r) \equiv H_i f(r) - f(r) H_k \), to find

\[
2(E_i - E_k)^2 \langle n_i l_i | f(r) | n_k l_k \rangle = \langle n_i l_i | (H_i (H_i f(r) - f(r) H_k) - (H_i f(r) - f(r) H_k) H_k) | n_k l_k \rangle.
\] (5)

This is the generalized second hypervirial valid for arbitrary radial potential energy functions, \( V(r) \), introduced in Eq. (8) of Ref. 11.

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 [11], after a long—but much shorter than in [6]—direct calculation, the Blanchard relation

\[
\lambda (E_i - E_k)^2 \langle n_i l_i | r^{\lambda+2} | n_k l_k \rangle = c_0 \langle n_i l_i | r^\lambda | n_k l_k \rangle + c_1 \langle n_i l_i | r^{\lambda-1} | n_k l_k \rangle + c_2 \langle n_i l_i | r^{\lambda-2} | n_k l_k \rangle;
\] (6)

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

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

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

\[
c_2 = \frac{1}{2} (\lambda + 2) \left[ \lambda^2 - (l_k - l_i)^2 \right] [(l_k + l_i + 1)^2 - \lambda^2].
\] (7)
From this result we can also obtain, as special cases of the Blanchard recurrence relation (6), first the Pasternack-Sternheimer selection rule [21]:

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

(8)
saying that the matrix element of the potential \(1/r^2\) vanishes between radial states of central potentials when their angular momenta coincide and when the corresponding energy eigenvalues depend on the principal quantum number only. Second, in the completely diagonal case (\textit{i.e.} \(n_i = n_k, l_i = l_k\), we can further obtain the non-relativistic quantum virial theorem [9]

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

(9)

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

III. The relativistic recurrence relations.

In this section we apply the method sketched in section II to the relativistic Dirac case. We clearly need to start with a radial Dirac Hamiltonian analogous to (2). To obtain such Hamiltonian we start with the Dirac Hamiltonian \(H_D\) and the corresponding time-independent Dirac equation for a central potential

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

(10)

where we are using atomic units, \(\alpha\) and \(\beta\) are the \(4 \times 4\) Dirac matrices [18–20], which in the Dirac representation are given by

\[
\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

(11)

where the 1’s and 0’s stand respectively, for \(2 \times 2\) unit and zero matrices and the \(\sigma\) is the vector composed by the three \(2 \times 2\) Pauli matrices \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\). Please notice that, despite the selection of natural units we shall, where it aids interpretation, reinsert the appropriate dimensional factors in certain equations. The energy eigenvalues are given explicitly in Eq. (63) of section V. The Hamiltonian \(H_D\) is rotationally invariant, hence the solutions of the Dirac equation (10) can be written in the alternative but entirely equivalent forms [19,23]

\[
\Psi(r, \theta, \phi) = \frac{1}{r} \begin{pmatrix} F_{nj\epsilon}(r) Y_{jm_z}(\theta, \phi) \\ iG_{nj\epsilon}(r) Y'_{jm_z}(\theta, \phi) \end{pmatrix} = \frac{1}{r} \begin{pmatrix} F_{nn\kappa}(r) \chi_{km_z}(\theta, \phi) \\ iG_{nn\kappa}(r) \chi'_{km_z}(\theta, \phi) \end{pmatrix},
\]

(12)

where \(\chi_{km_z}\) and \(\chi_{-km_z}\), or \(Y_{jm}\) and \(Y'_{jm}\), 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 \( \Sigma \equiv \sigma \otimes I = \text{diag}(\sigma, \sigma) \)). The second form in (12) is the preferred in Ref. 18. 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 be

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

(13)

thus \( l = j + \epsilon/2 \) 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 (12) completely solves the angular part of the problem.

To construct the radial Hamiltonian, we use the relation

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

(14)

we then use \( J^2 = [L + (1/2)\Sigma]^2 = L^2 + \Sigma \cdot L + 3/4 \) but for expressing the term \( L \cdot \Sigma \), we also need an expression for \( L^2 \) acting on the eigenfunctions (12). 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,

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

(15)

for the big component, and

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

(16)

for the small one. The action of \( L^2 \) upon a solution of the form (12) is therefore always of the form

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

(17)

where \( \beta \) is the Dirac matrix (11). From this result we obtain the term \( L \cdot \Sigma \) and, substituting it into \( (\alpha \cdot p) \), we finally obtain

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

(18)

where
\[ \alpha_r \equiv \frac{1}{r} \alpha \cdot \mathbf{r}, \quad p_r = -\frac{i}{r} \left( 1 + r \frac{d}{dr} \right). \] \tag{19}

We are now ready to write the relativistic radial Hamiltonian, and the corresponding radial Dirac equation, as

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

\[ H_k \psi_k(r) = E_k \psi_k(r), \] \tag{20}

where we introduced the purely radial eigenfunctions

\[ \psi_k(r) = \frac{1}{r} \left( \frac{F_{n_k j_k \epsilon_k}(r)}{i G_{n_k j_k \epsilon_k}(r)} \right) \] \tag{21}

in a $2 \times 2$ representation where, $\beta = \text{diag}(+1, -1)$, $\alpha_r = \left( \begin{array}{cc} 0 & -1 \\ -1 & 0 \end{array} \right)$, and the radial Dirac equation becomes then [14,19]

\[ \begin{bmatrix} c^2 + (V_k(r) - E_k) & -c (-\epsilon_k (j_k + 1/2) / r + d/dr) \\ c (\epsilon_k (j_k + 1/2) / r + d/dr) & -c^2 + (V_k(r) - E_k) \end{bmatrix} \begin{bmatrix} F_{n_k j_k \epsilon_k}(r) \\ G_{n_k j_k \epsilon_k}(r) \end{bmatrix} = 0. \] \tag{22}

Though this explicit representation can be used for our problem [24,25], it is not really necessary since all our results are representation independent.

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

\[ (E_2 - E_1) \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \]

\[ = -ic \langle n_2 j_2 \epsilon_2 | \alpha_r \left( f'(r) + \frac{\Delta_{21}}{2r} \beta f(r) \right) | n_1 j_1 \epsilon_1 \rangle, \] \tag{23}

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 \( \Delta_{21} \equiv \epsilon_2 (2j_2 + 1) - \epsilon_1 (2j_1 + 1) \), and the matrix elements of radial functions are calculated as

\[ \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = \int f(r) (F_{2}^*(r)F_{1}(r) + G_{2}^*(r)G_{1}(r)) \, dr, \]

\[ \langle n_2 j_2 \epsilon_2 | \beta f(r) | n_1 j_1 \epsilon_1 \rangle = \int f(r) (F_{2}^*(r)F_{1}(r) - G_{2}^*(r)G_{1}(r)) \, dr. \] \tag{24}
where the subscripts stand for the 3 quantum numbers specifying the state.

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

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

and

\[
\xi H_1 = -e^2 \frac{1}{r} \left( f'(r) - \frac{\Delta_{21}}{2r} \beta f(r) \right) - e^2 \left( f'(r) - \frac{\Delta_{21}}{2r} \beta f(r) \right) \frac{d}{dr} + c^2 \epsilon_1 \frac{(2j_1 + 1)}{2r} \beta \left( f'(r) - \frac{\Delta_{21}}{2r} \beta f(r) \right) - ic\alpha_r \left( f'(r) + \frac{\Delta_{21}}{2r} \beta f(r) \right) (V(r) + \beta e^2).
\]

Then, we write down the difference of the matrix elements associated with Eqs. (25) and (26)

\[
(E_2 - E_1)^2 \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = 
\langle n_2 j_2 \epsilon_2 | - e^2 \frac{\Delta_{21}}{2r^2} \beta f(r) - e^2 f''(r) - e^2 \frac{\Delta_{21}}{2r} \beta f'(r) - e^2 \frac{\Delta_{21}}{r} \beta f(r) \frac{d}{dr} + c^2 \frac{\Delta_{21}^+}{2r} \beta f'(r) + c^2 \left( \frac{\Delta_{21}^-}{2r} \right)^2 f(r) + 2ic^3 \alpha_r \beta \left( f'(r) + \frac{\Delta_{21}^-}{2r} \beta f(r) \right) | n_1 j_1 \epsilon_1 \rangle.
\]

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 (27) is the direct relativistic equivalent of the generalized second hypervirial [Cf. Eq. (5) 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 [11]. Instead, let us calculate the following second order iteration for non-diagonal matrix elements

\[
\langle n_2 j_2 \epsilon_2 | H_2 \xi + \xi H_1 | n_1 j_1 \epsilon_1 \rangle = (E_2^2 - E_1^2) \langle n_2 j_2 \epsilon_2 | f(r) | n_1 j_1 \epsilon_1 \rangle = 
\langle n_2 j_2 \epsilon_2 | \left( - \frac{2e^2 f'(r)}{r} + c^2 \frac{\Delta_{21}^+}{2r^2} \beta f(r) - c^2 f''(r) - 2e^2 f'(r) \frac{d}{dr} + \right.
\left. \frac{c^2 \Delta_{21}^+ \Delta_{21}^-}{4r^2} f(r) - 2ic\alpha_r \left( f'(r) + \frac{\Delta_{21}^-}{2r} \beta f(r) \right) V(r) \right) | n_1 j_1 \epsilon_1 \rangle;
\]

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

\[
H_2 (\ldots) = \ldots
\]

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

and

\[
(-i\alpha_r f(r)) H_1 = \ldots
\]

\[
(-i\alpha_r f(r)) H_1 = -cf(r) \left[ \frac{1}{r} \left( 1 + r \frac{d}{dr} \right) + \epsilon_1 (2j_1 + 1) \beta \right] - ic^2 \alpha_r \beta f(r) - i\alpha_r V(r)f(r);
\]

adding up these two last expressions, we get

\[
(E_2 + E_1) \langle n_2 j_2 \epsilon_2 | -i\alpha_r f(r) | n_1 j_1 \epsilon_1 \rangle = \ldots
\]

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

From the matrix element of $H_2 (\ldots)$, we can obtain

\[
(E_2 - E_1) \langle n_2 j_2 \epsilon_2 | -i\alpha_r f(r) | n_1 j_1 \epsilon_1 \rangle = \ldots
\]

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

\[
(E_2 + E_1) \langle n_2 j_2 \epsilon_2 | \beta f(r) | n_1 j_1 \epsilon_1 \rangle = \ldots
\]

Equations (23–33) are the basic equations of our problem. To proceed, we consider, as in the non-relativistic case, radial functions of the form $f(r) = r^\lambda$ and 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 potentials [26].

Substituting $f(r) = r^\lambda$ in (28), it follows

\[
(E_2^2 - E_1^2) \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \ldots
\]
hence, we can eliminate the term containing the derivative operator in this last equation, using \( f(r) = r^\lambda \) in Eq. (31), to get the result

\[
\langle E_2^2 - E_1^2 \rangle \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \\
\langle n_2 j_2 \epsilon_2 | c^2 \frac{\Delta_{21}^+ \Delta_{21}^-}{4} r^{\lambda-2} + c^2 \frac{\Delta_{12}^+ \beta}{2} (1 - \lambda) r^{\lambda-2} - i c \alpha_r \beta \Delta_{21}^- r^{\lambda-1} V(r) + (E_2 + E_1) \lambda (-i c \alpha_r) r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle;
\]

in this last equation, we use Eq. (23) to eliminate the term with \(-i c \alpha_r \Delta_{21}^- \beta r^{\lambda-1}\), to get

\[
\langle E_2^2 - E_1^2 \rangle \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | c^2 \left[ \frac{\Delta_{21}^+ \Delta_{21}^-}{4} + \frac{\Delta_{12}^+}{2} (1 - \lambda) \beta \right] r^{\lambda-2} + 2Z \left[ i c \alpha_r r^{\lambda-2} (1 - \lambda) - (E_2 - E_1) r^{\lambda-1} \right] - (E_2 + E_1) \lambda i c \alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle.
\]

Now, from Eq. (32) with \( f(r) = r^\lambda \) we get

\[
(E_2 - E_1) \langle n_2 j_2 \epsilon_2 | - i c \alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle = \\
\langle n_2 j_2 \epsilon_2 | - c(\lambda - 1) r^{\lambda-2} + c \frac{\Delta_{12}^+ \beta}{2} r^{\lambda-2} + 2ic^2 \alpha_r \beta mr^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle
\]

and, using \( f(r) = r^\lambda \) in Eq. (33) to eliminate the term \( 2ic \alpha_r \beta mr^{\lambda-1} \) from the above equation, we obtain

\[
(E_2 - E_1) \langle n_2 j_2 \epsilon_2 | - i c \alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle = \\
\langle n_2 j_2 \epsilon_2 | - c(\lambda - 1) r^{\lambda-2} + c \frac{\Delta_{12}^+ \beta}{2} r^{\lambda-2} - \frac{2c}{\lambda} (E_2 + E_1) \beta r^\lambda + \frac{c^2}{\lambda} (-i c \alpha_r) \Delta_{21}^- r^{\lambda-1} + \\
+ \frac{4c^3}{\lambda} r^\lambda - \frac{4cZ}{\lambda} \beta r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle;
\]

which can be written as

\[
\left[ (E_2 - E_1) - \frac{\Delta_{21}^- c^2}{\lambda} \right] \langle n_2 j_2 \epsilon_2 | (-i c \alpha_r r^{\lambda-1}) | n_1 j_1 \epsilon_1 \rangle = \langle n_2 j_2 \epsilon_2 | - c(\lambda - 1) r^{\lambda-2} + \\
\frac{4c^3}{\lambda} r^\lambda + c \frac{\Delta_{12}^+ \beta}{2} r^{\lambda-2} - \frac{4Zc}{\lambda} \beta r^{\lambda-1} - \frac{2c}{\lambda} (E_2 + E_1) \beta r^\lambda | n_1 j_1 \epsilon_1 \rangle.
\]

We can also obtain a new relationship for the matrix elements of \(-i c \alpha_r r^{\lambda-1}\), using Eq. (23) with \( f(r) = r^\lambda \), and substitute the result in Eq. (37) to eliminate the term \( 2ic \alpha_r \beta mr^{\lambda-1} \)
\[ (E_2 - E_1)\langle n_2 j_2 \epsilon_2 | - i\alpha_r r^{\lambda-1} | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | - c (\lambda - 1) r^{\lambda-2} + c \frac{\Delta_{21}^+}{2} \beta r^{\lambda-2} + \frac{4c^2 \lambda}{\Delta_{21}} (-i\alpha_r) r^{\lambda-1} - \frac{4c}{\Delta_{21}} (E_2 - E_1) r^\lambda | n_1 j_1 \epsilon_1 \rangle. \]  
\hspace{1cm} (40)

Rearranging terms, we obtain
\[
\left[ (E_2 - E_1) - \frac{4c^2 \lambda}{\Delta_{21}} \right] \langle n_2 j_2 \epsilon_2 | (-i\alpha_r r^{\lambda-1}) | n_1 j_1 \epsilon_1 \rangle = \]
\[ \langle n_2 j_2 \epsilon_2 | - c(\lambda - 1)r^{\lambda-2} - \frac{4c}{\Delta_{21}} (E_2 - E_1) r^\lambda + c \frac{\Delta_{21}^+}{2} \beta r^{\lambda-2} | n_1 j_1 \epsilon_1 \rangle. \]  
\hspace{1cm} (41)

The relation we are looking for follows from this last result and Eq. (36). We use successively \( r^{\lambda-1} \) and \( r^{\lambda-2} \) from Eq. (41) to eliminate the terms \( 2(E_2 + E_1)\lambda ic\alpha_r r^{\lambda-1} \) and \( 2ic\alpha_r r^{\lambda-2}(1 - \lambda) \) that appear in Eq. (36) to finally get [14]

\[
c_0 \langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle = \sum_{i=1}^{3} c_i \langle n_2 j_2 \epsilon_2 | r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle + \sum_{i=2}^{3} d_i \langle n_2 j_2 \epsilon_2 | \beta r^{\lambda-i} | n_1 j_1 \epsilon_1 \rangle,
\]  
\hspace{1cm} (42)

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

\[
c_0 = \frac{(E_2^2 - E_1^2)(E_2 - E_1)\Delta_{21}^+}{(E_2 - E_1)\Delta_{21} - 4c^2 \lambda},
\]
\[
c_1 = \frac{-2Z(E_2 - E_1)^2\Delta_{21}^+}{(E_2 - E_1)\Delta_{21} - 4c^2 (\lambda - 1)},
\]
\[
c_2 = c^2 \frac{\Delta_{21}^+ \Delta_{21}^-}{4} - c^2 \lambda (\lambda - 1) \frac{(E_1 + E_2)\Delta_{21}^-}{(E_2 - E_1)\Delta_{21} - 4c^2 \lambda},
\]
\[
c_3 = \frac{-2Zc^2(\lambda - 1)(\lambda - 2)\Delta_{21}^-}{(E_2 - E_1)\Delta_{21}^- - 4c^2 (\lambda - 1)},
\]  
\hspace{1cm} (43)

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

\[
d_2 = c^2 \frac{\Delta_{21}^-}{2} \left[ (1 - \lambda) + \frac{\lambda(E_2 + E_1)\Delta_{21}^+}{(E_2 - E_1)\Delta_{21} - 4c^2 \lambda} \right],
\]
\[
d_3 = \frac{Zc^2(\lambda - 1)\Delta_{21}^-\Delta_{21}^+}{(E_2 - E_1)\Delta_{21} - 4c^2 (\lambda - 1)}. \]  
\hspace{1cm} (44)

As we may have expected, we need to know six matrix coefficients instead of only three as in the non-relativistic case. This is a consequence of the fact that, in
the Dirac case, we have to deal with the big and the small components in the state function, doubling in this sense the “degrees of freedom” of the system.

It does not seem to be possible to avoid the $\beta$-dependency in Eq. (44), and thus, taken on its own, Eq. (41) does not allow the computation of $\langle n_2 j_2 \epsilon_2 | r^\lambda | n_1 j_1 \epsilon_1 \rangle$ in terms of the $\langle n_2 j_2 \epsilon_2 | r^{\lambda-a} | n_1 j_1 \epsilon_1 \rangle$, $a = 1, 2, 3$. 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 $-i\alpha_r r^{\lambda-1}$ between Eqs. (39) and (41). 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

$$b_0 = 4\lambda \left[ (E_2 - E_1)^2 - 4\epsilon^4 \right],$$
$$b_2 = c^2 (1 - \lambda) \left[ (\Delta_{21}^-)^2 - 4\lambda^2 \right],$$
$$e_0 = 2(E_2 + E_1)[(E_2 - E_1)\Delta_{21}^- - 4c^2\lambda],$$
$$e_1 = 4\lambda [4c^2\lambda - (E_2 - E_1)\Delta_{21}^-],$$
$$e_2 = c^2 \Delta_{21}^+ \left[ (\Delta_{21}^-)^2 - 4\lambda^2 \right].$$

Equations (42) and (45) together are the useful recurrence relations in the relativistic Dirac case.

IV. The diagonal case $\Delta_{21}^- = 0$ ($j_2 = j_1$, $\epsilon_2 = \epsilon_1$).

In the results of the last section we always assume $\Delta_{21}^- \neq 0$, but in order to study the diagonal case we must have $\epsilon_1 = \epsilon_2$ and $j_1 = j_2$; this in turn imply $\Delta_{21}^- = 0$ and (as always!) $\Delta_{21}^+ \equiv \Delta^+ \neq 0$. To deal with the diagonal case we start all over again. The equation set for this case is particularly simple, first from Eq. (23) we have

$$(E_2 - E_1)(n_2 j \epsilon | f(r)| n_1 j \epsilon) = \langle n_2 j \epsilon | (-i\alpha_r f'(r))| n_1 j \epsilon \rangle,$$

then we can proceed to calculate the second order iteration by substituting, as in the previous section, $f(r) \rightarrow \xi_- = H_2 f(r) - f(r) H_1$ in (47) to obtain

$$(E_2 - E_1)^2 \langle n_2 j \epsilon | f(r)| n_1 j \epsilon \rangle = \langle n_2 j \epsilon | -c^2 f'''(r) + c^2 \frac{\Delta_{21}^+}{2r} f'(r) \beta + 2ic^3 \alpha_r \beta f'(r)| n_1 j \epsilon \rangle,$$

and then substitute $f(r) \rightarrow \xi_+ = H_2 f(r) + f(r) H_1$ again in (47) to get instead
\[ (E_2^2 - E_1^2) \langle n_2 j \epsilon | f(r) | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | - \frac{2c^2 f'(r)}{r} - c^2 f''(r) - 2c^2 f'(r) \frac{d}{dr} \]
\[- 2ic\alpha r f'(r)V(r) | n_1 j \epsilon \rangle. \tag{49} \]

The equations equivalent of Eqs. (31–33) are in this case

\[ (E_2 + E_1) \langle n_2 j \epsilon | ( - i \alpha r f(r)) | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | - \frac{2cf(r)}{r} - cf'(r) - 2cf(r) \frac{d}{dr} - 2i\alpha r V(f(r)) | n_1 j \epsilon \rangle, \tag{50} \]

and

\[ (E_2 - E_1) \langle n_2 j \epsilon | ( - i \alpha r f(r)) | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | - cf'(r) + \frac{c\Delta^{+}}{2r} \beta f(r) + 2i\alpha r \beta c^2 f(r) | n_1 j \epsilon \rangle. \tag{51} \]

We also have, for the matrix elements of \( \beta f(r) \),

\[ (E_2 + E_1) \langle n_2 j \epsilon | \beta f(r) | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | - i\alpha \beta f'(r) + 2 \left[ c^2 + \beta r \right] f(r) | n_1 j \epsilon \rangle. \tag{52} \]

These expressions are the basic equations for the case \( \Delta^{+}_{21} = 0 \).

We can now obtain a recurrence relation valid in the diagonal case. First, let us use \( f(r) = r^\lambda \) in Eq. (48) to get

\[ (E_2 - E_1)^2 \langle n_2 j \epsilon | r^\lambda | n_1 j \epsilon \rangle = \lambda \langle n_2 j \epsilon | - c^2 (\lambda - 1) r^{\lambda - 2} + c^2 \frac{\Delta^{+}}{2} \beta r^{\lambda - 2} + 2ic^3 \alpha \beta r^{\lambda - 1} | n_1 j \epsilon \rangle. \tag{53} \]

Evaluating now equation (52) with \( f(r) = r^\lambda \), we obtain

\[ (E_2 + E_1) \langle n_2 j \epsilon | \beta r^\lambda | n_1 j \epsilon \rangle = \langle n_2 j \epsilon | - ic\alpha \beta \lambda r^{\lambda - 1} + 2 \left( c^2 - \frac{Z \beta}{r} \right) r^\lambda | n_1 j \epsilon \rangle, \tag{54} \]

and eliminating the \( ic\alpha \beta \lambda r^{\lambda - 1} \) between Eqs. (53) and (54), we finally get

\[ \left( (E_2 - E_1)^2 - 4c^4 \right) \langle n_2 j \epsilon | r^\lambda | n_1 j \epsilon \rangle = \lambda c^2 \frac{\Delta^{+}_{21}}{2} \langle n_2 j \epsilon | \beta r^{\lambda - 2} | n_1 j \epsilon \rangle - 4Z c^2 \langle n_2 j \epsilon | \beta r^{\lambda - 1} | n_1 j \epsilon \rangle - 2c^2 (E_2 + E_1) \langle n_2 j \epsilon | \beta r^\lambda | n_1 j \epsilon \rangle - c^2 \lambda (\lambda - 1) \langle n_2 j \epsilon | r^{\lambda - 2} | n_1 j \epsilon \rangle. \tag{55} \]
This is the only recurrence relation we get in the diagonal case. To “close” the relation we can use the diagonal recurrence relations given in [9].

The special case when $\lambda = 0$ is of particular interest

$$[(E_2 - E_1)^2 - 4c^4] \delta_{n_1,n_2} = -4Zc^2 \langle n_2 \mid J \mid n_1 \rangle - 2c^2 (E_2 + E_1) \langle n_2 \mid J \mid n_1 \rangle. \tag{56}$$

This expression could be considered as a relativistic generalization of the Pasternak-Sternheimer rule of non relativistic quantum mechanics (Equation (8) of section II) [21], which 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, i.e. when $l_1 = l_2$. In the relativistic case the expectation value of the $\beta/r$ potential (which could be regarded as the square root of $1/r^2$ including both signs), does not necessarily vanish even when the total angular momenta of the two states coincide: i.e. it does not vanish when $j_1 = j_2$. Again, this 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 relativistic quantum mechanics [14].

Moreover, two special cases are immediately deduced from this last expression (56):

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

$$\langle n_2 \mid \frac{Z \beta}{r} \mid n_1 \rangle = -\frac{1}{2} (E_2 + E_1) \langle n_2 \mid \beta \mid n_1 \rangle. \tag{57}$$

2) The other case follows when $n_1 = n_2$

$$c^2 = -\langle \beta V(r) \rangle + E \langle \beta \rangle = Z \langle \frac{\beta}{r} \rangle + E \langle \beta \rangle, \tag{58}$$

which is the relativistic virial theorem [22]; from the relation $c^2 < \beta > = E$ [9], we can also put it in the alternative form

$$E^2 = c^2 \langle \beta V(r) \rangle + c^4 = -c^2 Z \langle \frac{\beta}{r} \rangle + c^4. \tag{59}$$

V. The values of $< r^{\lambda} >$ and $< \beta r^{\lambda} >$.  

The recurrence relations found above, involve in principle simple expressions (since they involve only matrix elements of Dirac hydrogenic states) that can be burdensome to handle. Given such situation, we have also calculated explicit formulas that are needed to evaluate the diagonal and the non-diagonal matrix elements of interest. The expressions are related to the hypergeometric function and can be deduced from the two differential equations that follow from the Hamiltonian (20),
as it is shown in the Appendix. In particular, from Eq. (A.15) we calculate $< r^\lambda >$ and $< \beta r^\lambda >$. We quote the results here and refer to the Appendix for the details.

$$< r^\lambda >= \frac{mc^2|C|^2}{(2k)^{\lambda+1}2s-1} \left[ I_{nn}^{2s}(\lambda) u^2 + I_{n-1n-1}^{2s}(\lambda) v^2 + E_{uv} I_{nn-1}^{2s}(\lambda) \right], \quad (60a)$$

and

$$< \beta r^\lambda >= \frac{E|C|^2}{(2k)^{\lambda+1}2s-1} \left[ I_{nn}^{2s}(\lambda) u^2 + I_{n-1n-1}^{2s}(\lambda) v^2 + mc^2 uv I_{nn-1}^{2s}(\lambda) \right]; \quad (60b)$$

in these expressions $n = 0, 1, 2, \ldots$, and $[23,27]$

$$k \equiv \frac{1}{\hbar c} \sqrt{m^2c^4 - E^2}, \quad \zeta \equiv \frac{Ze^2}{\hbar c} = Z\alpha_F, \quad \tau_j \equiv \epsilon(j + \frac{1}{2}),$$

$$\nu \equiv \sqrt{\frac{mc^2 - E}{mc^2 + E}}, \quad s \equiv \sqrt{\tau_j^2 - \zeta^2}, \quad (61)$$

where $\alpha_F \approx 1/137$ is the fine structure constant and the $I_{nn}(\lambda)$ symbols are defined in equation (A.15) of the Appendix. The numbers $u$ and $v$ are constants such that

$$u = (\tau_j + s + n - \zeta \nu^{-1})^{1/2}, \quad v = (n + 2s)(\tau_j + s + n - \zeta \nu^{-1})^{-1/2}; \quad (62)$$

in the Appendix we give a simple proof of this result. Notice that in this section we have explicitly written $\hbar, e,$ and $c$ in our results. Finally, to obtain $C$, we use relations (61) to get $(\tau_j + s + n - \zeta \nu^{-1})^{-1} = (n + s - \tau_j - \zeta \nu^{-1}) / n(n + 2s)$; we need also $(n + s) = \zeta E / \sqrt{m^2c^4 - E^2}$, which is obtained from the expression for the energy eigenvalues of the Dirac hydrogen atom:

$$E = mc^2 \left( 1 + \frac{Z^2\alpha_F^2}{(n - j - 1/2 + \sqrt{(j + 1/2)^2 - Z^2\alpha_F^2})^2} \right)^{-1/2}; \quad (63)$$

elementary algebra gives then the result

$$|C| = \frac{\hbar 2^{s-1}}{Z\alpha_F} \sqrt{\frac{n! k}{2m^3} \left[ \Gamma(n + 2s + 1) \right]^{-1/2}}. \quad (64)$$

where we have written explicitly the dimensional factors.
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Appendix. Explicit expressions for relativistic matrix elements of $r^\lambda$ and $\beta r^\lambda$

It is possible to obtain explicit expressions for the diagonal and non diagonal matrix elements in the case $V(r) = -Z/r$. The purpose of this appendix is to give the basic relation that is needed for such evaluation. As we heavily draw from results previously obtained, in this section we use the notation of Ref. 23, in particular $\hbar = c = e = 1$, though we sometimes write all the dimensional constants.

We are interested in the bound states of the problem, so the quantity $k \equiv \sqrt{m^2 - E^2}$ is positive. We can write the differential equations for the radial part of any central problem in terms of the dimensionless variable $\rho \equiv kr$ [23,25] and the symbols defined in (60)

\begin{align}
\left(-\frac{d}{d\rho} + \frac{\tau j}{\rho}\right) G(\rho) &= \left(-\nu + \zeta\right) F(\rho), \\
\left(+\frac{d}{d\rho} + \frac{\tau j}{\rho}\right) F(\rho) &= \left(\nu^{-1} + \zeta\right) G(\rho),
\end{align}

where we look for solutions of the form

\begin{align}
F(\rho) &= \sqrt{m + E} \left[\psi_-(\rho) + \psi_+(\rho)\right], \\
G(\rho) &= \sqrt{m - E} \left[\psi_-(\rho) - \psi_+(\rho)\right].
\end{align}

The solution to these coupled differential equations can be written in terms of the Laguerre polynomials of non-integer index [25,27,28]

\begin{align}
\psi_+(\rho) &= a \rho^s \exp(-\rho) \mathcal{L}^{2s}_{n-1}(2\rho), \\
\psi_-(\rho) &= b \rho^s \exp(-\rho) \mathcal{L}^{2s}_n(2\rho),
\end{align}

where the Laguerre polynomials $\mathcal{L}^{2s}_n(\rho)$ are related to both the hypergeometric function, $\mathcal{F}_1(-n, \alpha + 1; \rho)$, and the Sonine polynomials, $T^{(n)}_\alpha(\rho)$ [28], through the relation
\[ \mathcal{L}_n^\alpha(\rho) = \frac{\Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + 1)} F_1(-n; \alpha + 1; \rho) = (-1)^n \Gamma(\alpha + n + 1) T_\alpha^{(n)}(\rho), \quad (A5) \]

and \(a\) and \(b\) are constants. Substitution of these results in Eq. (A1) gives the condition

\[ \begin{align*}
a(\tau_j + s - \zeta \nu^{-1} + n) + b(n + 2s) &= 0, \\
(\tau_j - s + \zeta \nu^{-1} - n) - an &= 0.
\end{align*} \tag{A6} \]

Solving these last two equations gives us a relationship between \(n\) and \(\nu\). From Eq. (45) we see that we can solve for the energy \(E\) and obtain the relativistic energy spectrum (63), provided we first introduce the principal quantum number \(N \equiv j + 1/2 + n\). To proceed further, we take

\[ b = -a(\tau_j + s + n - \zeta \nu^{-1})/(n + 2s), \tag{A7} \]

and write the result in a symmetrized form:

\[ \begin{align*}
F(\rho) &= \frac{\sqrt{mc^2 + E C \rho^s e^{-\rho}} [u \mathcal{L}_n^{2s}(2\rho) + v \mathcal{L}_{n-1}^{2s}(2\rho)]}{\sqrt{n!}}, \\
G(\rho) &= \frac{-\sqrt{mc^2 - E C \rho^s e^{-\rho}} [u \mathcal{L}_n^{2s}(2\rho) - v \mathcal{L}_{n-1}^{2s}(2\rho)]}{\sqrt{n!}}, \tag{A8} \end{align*} \]

where

\[ u = (\tau_j + s + n - \zeta \nu^{-1})^{1/2}, \quad v = (n + 2s)(\tau_j + s + n - \zeta \nu^{-1})^{-1/2}. \tag{A9} \]

\(C\) is a normalization constant that can be obtained from

\[ \int_0^\infty e^{-x} x^\alpha \mathcal{L}_n^\alpha(x) \mathcal{L}_m^\alpha(x) dx = \delta_{mn} \frac{\Gamma(n + \alpha + 1)}{n!}; \tag{A10} \]

after some work we obtain

\[ |C| = \frac{\hbar^{2s-1}}{Z\alpha c^2 \sqrt{n!}} \sqrt{2m^3} (\Gamma(n + 2s + 1))^{-1/2}. \tag{A11} \]

We can also calculate the expectation values for diagonal and non-diagonal matrix elements. For diagonal, arbitrary power matrix elements of the form \(< r^\lambda >\) and \(< \beta r^\lambda >\), we need to calculate the expression

\[ \Gamma_{nm}^\alpha(\lambda) = \int_0^\infty e^{-x} x^{\alpha + \lambda} \mathcal{L}_n^\alpha(x) \mathcal{L}_m^\alpha(x) dx. \tag{A12} \]

This expression converges for \(\Re(\alpha + \lambda + 1) > 0\), 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 \((d^n/dx^n)x^{k+\lambda} = (-1)^m[-k - \lambda]_m x^{k+\lambda-m}\), where \([n]_n\) is a Pochhammer symbol [28], we find, after a \(m\)-times partial integration,

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

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

\[
[-\lambda]_{m-n+k} = [-\lambda]_{m-n} [-\lambda + m - n]_k,
\]
\[
\Gamma(n + \alpha + 1) = (-1)^k \Gamma(\alpha + n - k + 1) [-\alpha - n]_k,
\]
\[
\Gamma(\alpha + \lambda + n + 1) = (-1)^k \Gamma(\alpha + \lambda + n - k + 1) [-\alpha - \lambda - n]_k,
\]
\[
[k - n - \lambda]_{n-k} = (-1)^n \frac{\Gamma(\lambda + n + 1)}{\Gamma(\lambda + 1)} \frac{1}{[-\lambda - n]_k};
\]
to obtain that

\[
I_{nm}^\alpha(\lambda) = \frac{\Gamma(\alpha + \lambda + n + 1)\Gamma(\lambda + n + 1)}{m! n! \Gamma(\lambda + 1)} 3F_2(-\alpha - n, -\lambda + m - n, -n; -\lambda - n, -\alpha - \lambda - n; 1).
\]

We consider two cases for the general matrix elements \(\langle n_2 j_2 \epsilon_2 | r^{\lambda} | n_1 j_1 \epsilon_1 \rangle\) and \(\langle n_2 j_2 \epsilon_2 | \beta r^{\lambda} | n_1 j_1 \epsilon_1 \rangle\); the first one, when \(k_1 = k_2\), where we need to evaluate

\[
K_{nm}^{s_1 s_2}(\lambda) = \int_0^{\infty} x^{s_1+s_2+\lambda} e^{-x} L_n^{(2s_1)}(x) L_m^{(2s_2)}(x) \, dx,
\]

and the second one, when \(k_1 \neq k_2\), where we need

\[
K_{nm}^{s_1 s_2}(\lambda) = \int_0^{\infty} r^{s_1+s_2+\lambda} e^{-(k_1+k_2)r} L_n^{(2s_1)}(2k_1 r) L_m^{(2s_2)}(2k_2 r) \, dr.
\]

In the first case, we see that integral (A16) is convergent if \(Re(s_1 + s_2 + \lambda + 1) > 0\), and vanishes when \(s_1 - s_2 + \lambda\) is an integer such that \(m - n > s_1 - s_2 + \lambda \geq 0\). Using a similar reasoning as in the diagonal case, we get

\[
K_{nm}^{s_1 s_2}(\lambda) = \frac{\Gamma(s_1 + s_2 + \lambda + n + 1)\Gamma(\lambda + s_1 - s_2 + n + 1)}{m! n! \Gamma(\lambda + s_1 - s_2 + 1)} 3F_2(-2s_1 - n, -\lambda + s_2 - s_1 + m - n, -n; -\lambda + s_2 - s_1 - n, -\lambda - s_1 - s_2 - n; 1).
\]
In the second case, the integral converges for $\text{Re}(s_1 + s_2 + \lambda + 1) > 0$, and is not zero provided $k_1 \neq k_2$. A straightforward calculation by parts shows that

$$K_{nm}^{s_1 s_2}(\lambda) = \sum_{j=0}^{n} \sum_{i=0}^{m} \frac{(-1)^j (k_2 - k_1)^{m-i} (k_1 + k_2)^{(i-m-s_1-s_2-\lambda-1)}}{i! j! (m-i)! (n-j)!} \frac{\Gamma(n+2s_1+1)[s_2-s_1-\lambda-j]_i \Gamma(m+s_2+s_1+\lambda-i+1)}{\Gamma(2s_1+j+1)}$$

(A19)

where $k_1 \neq k_2$. Although less practical than the other expressions found here, we still can rewrite Eq. (A19) in a different form using the well known identities [28]

$$[p]_{m-i} = (-1)^{m-i} \frac{\Gamma(-p+1)}{[-p-m+1]_i \Gamma(-p-m+1)}$$

$$\Gamma(-p-m+i+1) = [-p-m+1]_i \Gamma(-p-m+1),$$

$$\Gamma(p+1) = [p-m+1]_m \Gamma(p-m+1).$$

(A20)

for any number $p$ and $m$ and $i$ integers. After some algebra, we finally get

$$K_{nm}^{s_1 s_2}(\lambda) = \frac{(-1)^m \Gamma(n+2s_1+1)\Gamma(s_1+s_2+\lambda+1)}{m! (k_2 + k_1)^{s_1+s_2+\lambda+1}} \sum_{j=0}^{n} \frac{(-1)^j [s_1-s_2+\lambda+j-m+1]_m}{j! (n-j)! \Gamma(2s_1+j+1)}$$

$$\times \text{$_2F_1$}(-m, s_1 + s_2 + \lambda + 1; s_1 - s_2 + \lambda + j - m + 1; \frac{k_2 - k_1}{k_2 + k_1}),$$

(A21)
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