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Matrix elements of r^q in relativistic quantum defect orbital theory

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Abstract. Formulae for the evaluation of the expectation values of r^q between the relativistic quantum defect orbital theory wavefunctions are derived. Their recursive structure leads to the development of explicit relations between the formulae for different values of q. The formulae may be considered as a relativistic quantum defect orbital theory generalization of the Kramers' relations for the hydrogenic wavefunctions.

1. Introduction

Quantum defect theories were formulated half a century ago by Bates and Damgaard [1], Ham [2], Seaton [3] and others (for a discussion of the early quantum defect theories see the review paper by Seaton [4]). A relativistic version of the quantum defect theory, constructed by Johnson and Cheng [5], has been generalized and applied, mainly to scattering phenomena, by Lee and Johnson [6] and by Chang [7], just to mention the earliest contributions.

The quantum defect method of Bates and Damgaard [1] was reformulated in the 1970s by Simons [8] and by Martin and Simons [9, 10] in such a way that the resulting equations are exactly solvable and the wavefunctions are also valid for $r \to 0$. This approach is referred to as the *quantum defect orbital* (QDO) method. Generalizations of the method to account for the effects of polarization of the atomic core [11] and to describe the behaviour of the molecular Rydberg electrons [12] have also been formulated. A relativistic generalization of the QDO theory is straightforward. One can simply replace the Schrödinger-type equation by its Dirac counterpart. Formally, while performing this procedure, any choice of the spinor representation is correct. However, it has already been noticed by Dirac [13] that the relativistic hydrogenic equation may be written in its second-order form resembling the corresponding non-relativistic equation. Biedenharn [14] introduced a representation in which the large- and the small-component equations are decoupled. Since then the hydrogenic Dirac second-order equation has become a standard textbook subject (see, e.g., [15]). Also in the case of QDO theory, using the Biedenharn representation appears to be the most natural way for its relativistic generalization. In the Biedenharn representation the radial second-order hydrogenic Dirac equations may be written in the same form as the hydrogenic Schrödinger equation except for differently defined constants [16]. From this observation a two-component relativistic

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version of the QDO method (RQDO) has been derived [17, 18]. Recently, a four-component generalization of the method has also been proposed [19].

QDO and RQDO methods proved to be most useful in studies of Rydberg systems. Both atomic and molecular Rydberg electrons may be very well described by the analytical quantum defect orbitals. Theoretical prediction of many properties of the Rydberg systems, such as, for example, of their long-range interactions or of their behaviour in external fields requires the knowledge of the expectation values of powers of the radial coordinate of the Rydberg electron. In this paper formulae for matrix elements of r^q between the RQDO wavefunctions are derived. Though, to our knowledge, expressions for RQDO matrix elements of r^q have never been published before, many papers were concerned with a related subject, namely with the evaluation of these elements for the hydrogenic wavefunctions. In the non-relativistic case, recurrent expressions for matrix elements of r^q, known as Kramers' formulae, have already been given in 1938 [20]. More recently, explicit expressions for wide ranges of integer [21, 22] and non-integer [23] values of q have been reported. For relativistic wavefunctions a closed-form expression for the expectation values of r^q was derived by Davies in 1939 [24]. Explicit expressions for several integer values of q were given, among others, by Burke and Grant [25]. Later the subject was discussed by numerous authors, including Goldman and Drake [26] and Shabaev [27]. The case of non-integer exponents has been solved by Salamin [28]. A simple recurrent algorithm valid for integer q values and a rather complete list of references may be found in a recent work by Andrae [29]. In this context one should also mention papers by Kaulakys [30] and by Kwato Njock *et al* [31] concerned with radial dipole matrix elements. The approach we have used in this paper is related to the one developed earlier for the case of the hydrogenic quasi-relativistic wavefunctions [32].

2. A general formulation

The relativistic QDO (RQDO) equation expressed as the second-order Dirac equation in the Biedenharn representation may be written as [18]

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{K}{r^2}-\frac{2z}{r}\right]\Psi_{nL}(r)=2\epsilon_{n\Lambda}\Psi_{nL}(r) \tag{1}$$

where

$$K=L(L+1) \qquad L=\varepsilon\Lambda \qquad \Lambda=\ell+|s|-|k|-\delta+c \qquad \varepsilon=\pm 1$$

$$s=\frac{k}{|k|}\sqrt{k^2-\zeta} \qquad \zeta=\alpha^2Z^2$$

$$k=\begin{cases} j+\frac{1}{2}=\ell+1 & \text{if} \quad j=\ell+\frac{1}{2} \\ -j-\frac{1}{2}=-\ell & \text{if} \quad j=\ell-\frac{1}{2} \end{cases}$$

where δ is the quantum defect, c is an integer chosen to ensure the correct number of nodes and the normalizability of $\Psi_{nL}(r)$,

$$\epsilon=E\left(1+\tfrac{1}{2}\alpha^2E\right) \qquad z=Z\left(1+\alpha^2E\right) \tag{2}$$

where E is the electron energy measured relative to the ionization limit, Z is the nuclear charge seen by the electron at large r and α is the fine structure constant. In equation (2), for simplicity, indices n and Λ have been omitted. Let us note that in spite of its similarity to the radial Schrödinger equation, equation (1) is the second-order Dirac equation and relations (2) link the eigenvalue $\epsilon_{n\Lambda}$ with the Sommerfeldt energy E (see [16] for details).

The relativistic quantum defect δ and the eigenvalue $\epsilon_{n\Lambda}$ are related by the formula [18]

$$\epsilon_{n\Lambda} = -\frac{z^2}{2(\tilde{n}-\delta)^2} \tag{3}$$

where $\tilde{n} = n + |s| - |k|$ and n is the principal quantum number. Equation (3), though it apparently resembles the Balmer formula, is equivalent to equation (1) in the paper of Johnson and Cheng [5] in which they introduced the notion of the relativistic quantum defect.

If the experimental binding energy of the electron, E^x, is substituted for E then the quantum defect becomes an empirical parameter and, according to equations (2) and (3), may be defined as

$$\delta = n + |s| - |k| - \nu \tag{4}$$

where

$$\nu = \frac{1-\zeta w}{\sqrt{w(2-\zeta w)}} = n - \delta_0 - \frac{3}{8}\frac{\zeta}{n-\delta_0} + \mathrm{O}(\zeta^4) \tag{5}$$

$$w = -\frac{E^x}{Z^2} \qquad \text{and} \qquad \delta_0 = n - \frac{1}{\sqrt{2w}} \tag{6}$$

is the non-relativistic quantum defect. From here,

$$\Lambda = \nu - n + l + c = \lambda - \frac{3}{8}\frac{\alpha^2 Z^2}{n-\delta_0} + \mathrm{O}(\zeta^4) \tag{7}$$

where

$$\lambda = l - \delta_0 + c \tag{8}$$

is the non-relativistic value of Λ. Equations (4) and (6) establish simple relations between the relativistic, δ, and non-relativistic, δ_0, quantum defects. After some simple algebra we obtain

$$\delta = \tilde{n} - \frac{2(n-\delta_0)^2 - \zeta}{\sqrt{4(n-\delta_0)^2 - \zeta}}. \tag{9}$$

A more detailed discussion of relations between δ and δ_0 is given in [18].

In this formulation, the RQDO theory is quasirelativistic, i.e. the radial parts of the orbitals are one-component functions. Two components of the Dirac spinor correspond to two signs of $L = \pm\Lambda$ in equation (1)—a detailed discussion of this point is given in [16]. It is customary to normalize solutions of equation (1) so that

$$\langle L|L\rangle = \langle \Lambda|\Lambda\rangle = \langle -\Lambda|-\Lambda\rangle = 1 \tag{10}$$

where $\langle L|L\rangle \equiv \langle \Psi_{nL}|\Psi_{nL}\rangle$. Then, equations (1) for $\pm\Lambda$ may be rewritten as a pair of first-order equations [16, 32] which are equivalent to the Dirac equation:

$$\hat{\mathbf{\Omega}}\,\mathbf{\Psi}_{nL}(r) = 0 \tag{11}$$

where

$$\hat{\mathbf{\Omega}} = \begin{bmatrix} -x & V(r) - \dfrac{\mathrm{d}}{\mathrm{d}r} \\ V(r) + \dfrac{\mathrm{d}}{\mathrm{d}r} & -x \end{bmatrix} \tag{12}$$

is a self-adjoint first-order differential operator,

$$\Psi_{nL}(r) = \begin{bmatrix} \Psi_{n\Lambda}(r) \\ \Psi_{n-\Lambda}(r) \end{bmatrix} \qquad V(r) = \frac{\Lambda}{r} - \frac{z}{\Lambda} \tag{13}$$

and

$$x = \frac{z}{\Lambda}\sqrt{1 - \left(\frac{\Lambda}{\nu}\right)^2}. \tag{14}$$

As one can easily see [16], the Dirac expectation values of an operator ω may be expressed in terms of $\langle\Lambda|\omega|\Lambda\rangle$, $\langle-\Lambda|\omega|-\Lambda\rangle$ and $\langle\Lambda|\omega|-\Lambda\rangle$. The quasirelativistic (i.e. evaluated using $\Psi_{nL}(r)$ only) and the Dirac expectation values are identical for the nodeless orbitals. In other cases, if $\omega = r^q$ and $|q| \leqslant 2$, the relative error for $Z = 90$ never exceeds 3% [16]—a difference entirely negligible in a semiempirical theory.

3. Matrix elements

If we denote

$$\hat{H} = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{K}{r^2} - \frac{2z}{r} \tag{15}$$

then

$$\hat{H}|L\rangle = 2\epsilon|L\rangle \tag{16}$$

and, as one can easily check,

$$\left[r^{q+1}, \hat{H}\right] = q(q+1)r^{q-1} + 2(q+1)r^q\frac{\mathrm{d}}{\mathrm{d}r} \tag{17}$$

and

$$\left[r^{q+1}\frac{\mathrm{d}}{\mathrm{d}r}, \hat{H}\right] = 2qKr^{q-2} + q(q+1)r^{q-1}\frac{\mathrm{d}}{\mathrm{d}r} - 2(2q+1)zr^{q-1} - 2(q+1)r^q\hat{H}. \tag{18}$$

Equations (11), (17) and (18) lead to a set of simple recurrent relations from which all matrix elements of r^q between the RQDO wavefunctions may be derived. In particular, equation (17) gives

$$\langle\Lambda|r^q\frac{\mathrm{d}}{\mathrm{d}r}|\Lambda\rangle = -\frac{q}{2}\langle\Lambda|r^{q-1}|\Lambda\rangle \tag{19}$$

and

$$2(q+1)\langle-\Lambda|r^q\frac{\mathrm{d}}{\mathrm{d}r}|\Lambda\rangle = -[2\Lambda + q(q+1)]\langle-\Lambda|r^{q-1}|\Lambda\rangle. \tag{20}$$

Equation (18) combined with equations (16) and (19) gives a recurrence relation coupling matrix elements of consecutive powers of r:

$$2(q+1)\epsilon\langle\Lambda|r^q|\Lambda\rangle + (2q+1)z\langle\Lambda|r^{q-1}|\Lambda\rangle + \tfrac{1}{4}q[q^2 - (2\Lambda+1)^2]\langle\Lambda|r^{q-2}|\Lambda\rangle = 0. \tag{21}$$

According to equation (11)

$$\langle\Lambda|r^q\frac{\mathrm{d}}{\mathrm{d}r}|\Lambda\rangle + \Lambda\langle\Lambda|r^{q-1}|\Lambda\rangle - \frac{z}{\Lambda}\langle\Lambda|r^q|\Lambda\rangle - x\langle\Lambda|r^q|-\Lambda\rangle = 0. \tag{22}$$

Combining equations (19) and (22) we have

$$(2\Lambda - q)\langle\Lambda|r^{q-1}|\Lambda\rangle = \frac{2z}{\Lambda}\langle\Lambda|r^q|\Lambda\rangle + 2x\langle\Lambda|r^q|-\Lambda\rangle. \tag{23}$$

Similarly, using equation (20) and the analogue of equation (22) with *bra* taken as equal to $\langle-\Lambda|$ rather than to $\langle\Lambda|$, we obtain

$$q(2\Lambda - q - 1)\langle-\Lambda|r^{q-1}|\Lambda\rangle - \frac{2z}{\Lambda}(q+1)\langle-\Lambda|r^q|\Lambda\rangle - 2x(q+1)\langle-\Lambda|r^q|-\Lambda\rangle = 0 \tag{24}$$

and, changing Λ to $-\Lambda$,

$$q(-2\Lambda - q - 1)\langle\Lambda|r^{q-1}|-\Lambda\rangle + \frac{2z}{\Lambda}(q+1)\langle\Lambda|r^q|-\Lambda\rangle + 2x(q+1)\langle\Lambda|r^q|\Lambda\rangle = 0. \tag{25}$$

The last two equations yield

$$q\langle\Lambda|r^{q-1}|-\Lambda\rangle = x\big[\langle\Lambda|r^q|\Lambda\rangle - \langle-\Lambda|r^q|-\Lambda\rangle\big]. \tag{26}$$

Finally, combining equations (24) and (26), we obtain a relation which couples different matrix elements of the same power of r:

$$(q+1)\frac{2z}{x\Lambda}\langle\Lambda|r^q|-\Lambda\rangle = (2\Lambda - q - 1)\langle\Lambda|r^q|\Lambda\rangle - (2\Lambda + q + 1)\langle-\Lambda|r^q|-\Lambda\rangle. \tag{27}$$

4. Explicit formulae

Similarly, as in the case of the hydrogenic wavefunctions, equation (21) may be used to determine all expectation values of r^q except for $q = -2$. Then, setting $q = 1, 2, 3$ one obtains

$$\langle L|r^{-1}|L\rangle = \frac{z}{\nu^2} \tag{28}$$

$$\langle L|r|L\rangle = \frac{3\nu^2 - K}{2z} \tag{29}$$

$$\langle L|r^2|L\rangle = \frac{\nu^2}{2z^2}\big(5\nu^2 + 1 - 3K\big) \tag{30}$$

$$\langle L|r^3|L\rangle = \frac{\nu^2}{8z^3}\big[5\nu^2(7\nu^2+5) + 4K(K - 10\nu^2 - 2)\big]. \tag{31}$$

Matrix elements between $\langle\Lambda|$ and $|-\Lambda\rangle$ may be easily derived from equation (26):

$$\langle\Lambda|r^{-2}|-\Lambda\rangle = 0 \tag{32}$$

$$\langle\Lambda|-\Lambda\rangle = -\frac{x\Lambda}{z} \tag{33}$$

$$\langle\Lambda|r|-\Lambda\rangle = -\frac{3x\Lambda\nu^2}{2z^2} \tag{34}$$

$$\langle\Lambda|r^2|-\Lambda\rangle = \frac{x\Lambda\nu^2}{2z^3}(\Lambda^2 - 5\nu^2 - 1). \tag{35}$$

For $q = -2$, equations (24) and (25) give the following relation:

$$(2L+1)\langle L|r^{-2}|L\rangle = (2L-1)\langle-L|r^{-2}|-L\rangle. \tag{36}$$

This implies that

$$\langle L|r^{-2}|L\rangle = \frac{1}{2\Lambda + \varepsilon}A \tag{37}$$

where A does not depend on the sign of L. A direct integration using the RQDO wavefunction gives

$$\langle L|r^{-2}|L\rangle = \frac{1}{(2L+\varepsilon)}\frac{2z^2}{\nu^3}. \tag{38}$$

Now, all the remaining matrix elements may be easily expressed in terms of the ones already evaluated. In particular, from equation (21)

$$\langle L|r^{-3}|L\rangle = \frac{z}{L(L+1)}\langle L|r^{-2}|L\rangle \tag{39}$$

from equation (25)

$$\langle \Lambda|r^{-3}|-\Lambda\rangle = \frac{2x}{2\Lambda-1}\langle \Lambda|r^{-2}|\Lambda\rangle \tag{40}$$

from equation (23)

$$\langle \Lambda|r^{-1}|-\Lambda\rangle = \frac{2\Lambda+1}{2x}\langle \Lambda|r^{-2}|\Lambda\rangle - \frac{z}{x\Lambda}\langle \Lambda|r^{-1}|\Lambda\rangle. \tag{41}$$

Matrix elements for any other power of r may readily be obtained from equations (21) and (27).

In the RQDO (as well as in the QDO) method all expectation values may be expressed in terms of Z, of the quantum numbers, and of the experimental energies. Instead of the experimental energies one can use, due to equations (4)–(6), either relativistic or non-relativistic quantum defect values, however, expressions in terms of the energies are both more general and more interesting. One should note that in the present formulation the relativistic effects are taken into account by the structure of the formulae and quantum defects compensate for the deviation of the atomic potential from the Coulombic form and for many-body effects (the electron correlation) only. In particular, for $|q| < 2$, we have

$$Z^2\langle L|r^{-2}|L\rangle^{-1} = p^2\left(t^2 - m_\varepsilon\, t\right) \tag{42}$$

$$Z\langle L|r^{-1}|L\rangle^{-1} = p\,t \tag{43}$$

$$Z\langle L|r|L\rangle = p(t+m_\varepsilon) - \frac{p}{2t}\,M \tag{44}$$

$$Z^2\langle L|r^2|L\rangle = p^2\left(t^2 + 3m_\varepsilon\, t - \tfrac{3}{2}M + \tfrac{1}{2}\right) \tag{45}$$

where $m = n - \ell - c$, $m_\varepsilon = m - \varepsilon/2$, $M = m(m-\varepsilon)$, $p = \{\zeta/[w(2-\zeta\, w)]\}^{1/2}$ and $t = p(1-\zeta w)$. Due to (6), equations (42)–(45) establish simple relations between the expectation values of r and the experimental term energies. For the negative powers of r the inverse of the expectation values are given because then the structure of the equations is simpler and more symmetric.

In order to see the relativistic corrections explicitly, it is convenient to express the expectation values as

$$\langle r^q\rangle = \langle r^q\rangle_0 + \zeta\,\Delta_q + \mathrm{O}(\zeta^2) \tag{46}$$

where $\langle r^q\rangle$ and $\langle r^q\rangle_0$ denote, respectively, the RQDO and the non-relativistic QDO expectation values of r^q. Matrix elements in the non-relativistic approximation may be easily obtained by the following substitutions (cf equations (5), (7) and (14)): $z \to Z$, $\nu \to n - \delta_0$, $\Lambda \to \lambda$, $K \to \lambda(\lambda+1)$, $x \to Z[1/\lambda^2 - 1/(n-\delta_0)^2]^{1/2}$. The relativistic corrections one can derive

using equations (5), (7), (14) and the appropriate expression for suitable matrix element. In particular, for $|q| \leqslant 2$, by transforming equations (42)–(45), one obtains

$$Z^2\langle L|r^{-2}|L\rangle^{-1} = \frac{1}{4w^2}\left(1 - m_\varepsilon\sqrt{2w}\right) - \frac{\zeta}{4w}\left(1 - \tfrac{1}{4}m_\varepsilon\sqrt{2w}\right) + \mathrm{O}(\zeta^2)$$

$$Z\langle L|r^{-1}|L\rangle^{-1} = \frac{1}{2w} - \frac{1}{4}\zeta + \mathrm{O}(\zeta^2)$$

$$Z\langle L|r|L\rangle = \frac{1}{2w}\left(1 + m_\varepsilon\sqrt{2w} - Mw\right) - \tfrac{1}{4}\zeta\left(1 - \tfrac{1}{2}m_\varepsilon\sqrt{2w} + 2Mw\right) + \mathrm{O}(\zeta^2)$$

$$Z^2\langle L|r^2|L\rangle = \frac{1}{4w^2}\left[1 + 3m_\varepsilon\sqrt{2w} - (3M-1)w\right] - \frac{\zeta}{4w}\left[1 + \tfrac{3}{4}m_\varepsilon\sqrt{2w}\,\tfrac{1}{2}(3M-1)w\right] + \mathrm{O}(\zeta^2).$$

As one can see, in all cases the relativistic corrections are negative. Since for $q < 0$ the corrections correspond to the inverse of the expectation values, the negative relativistic corrections reflect, in all cases, the relativistic contraction of the quantum defect orbitals.

5. Final remarks

Equations derived in this paper may be applied to an evaluation of the expectation values of various observables which are expressible in terms of polynomials in r. Particularly, they may be useful in studying an influence of external fields on systems described by the QDO wavefunctions. Relations between different expectation values are also useful for an easy checking of computer programs in which the QDO wavefunctions are used.

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