PHYSICAL REVIEW A **66**, 052503 (2002)

Expectation values of r^q between Dirac and quasirelativistic wave functions in the quantum-defect approximation

L. C. Owono Owono*
Département de Physique, Ecole Normale Supérieure, Université de Yaoundé, I, Boîte Postale 47, Yaoundé, Cameroon

M. G. Kwato Njock†
Centre de Physique Atomique Moléculaire et Optique Quantique, Faculté des Sciences, Université de Douala, Boîte Postale 24157, Douala, Cameroon

B. Oumarou
Département de Physique, Faculté des Sciences, Université de Ngaoundéré, Boîte Postale 454, Ngaoundéré, Cameroon

(Received 2 April 2002; revised manuscript received 12 July 2002; published 18 November 2002)

A search is conducted for the determination of expectation values of r^q between Dirac and quasirelativistic radial wave functions in the quantum-defect approximation. The phenomenological and supersymmetry-inspired quantum-defect models, which have proven so far to yield accurate results, are used. The recursive structure of formulas derived on the basis of the hypervirial theorem enables us to develop explicit relations for arbitrary values of q. Detailed numerical calculations concerning alkali-metal-like ions of the Li, Na, and Cu isoelectronic sequences confirm the superiority of supersymmetry-based quantum-defect theory over quantum-defect orbital and exact orbital quantum number approximations. It is also shown that relativistic rather than quasirelativistic treatment may be used for consistent inclusion of relativistic effects.

DOI: 10.1103/PhysRevA.66.052503 PACS number(s): 31.15.−p

I. INTRODUCTION

Expectation values of powers of the radius have deservedly received continued attention since the beginning of the study of quantum mechanics because they are central to countless problems in this field. It suffices to point out that many properties of interest, such as, for example, the long-range interactions with the ionic core or the behavior in external fields of the Rydberg electrons [1–4], require the knowledge of the expectation values of powers of the radial coordinate. Indeed, a power of r may be a well-defined function, such as in the London or Lennard-Jones potentials, or a term in the multipolar expansion of the electromagnetic field. Also, other well-known subjects, namely, the nuclear quadrupole coupling in polar molecules [5] and shielding and antishielding effects pertaining to the hyperfine structure of various ions and atomic species [6,7], lead to expansions involving matrix elements of powers of r to allow for a clear understanding of the asymptotic behavior of the property studied. It should be noted that many derivations are frequently concerned with expectation values for q covering a certain range. Hence, it is advantageous to use recurrence relations for the evaluation of these quantities instead of closed-form expressions that become cumbersome with increasing magnitude of q. Owing to the above highlighted importance of expectation values of r^q and making reference to the fact that relativistic quantum-defect models proved to be most useful in studies of Rydberg systems where analytical quantum-defect wave functions accurately describe Rydberg electrons as well as in many other problems with numerous applications [8–10], it then becomes obvious that writing these expectation values in terms of quantum-defect parameters may provide an important tool both for theoretical derivations as well as for the corresponding computational calculations. We have thus been working at obtaining recurrence relations between matrix elements of r^q by using relativistic and quasirelativistic quantum-defect radial wave functions.

The first formulation of the quantum-defect method using the Coulomb approximation technique was presented by Bates and Damgaard [11]. During the last three decades, this theory has been reformulated in the nonrelativistic context by Martin and Simons [12–14], Gruzdev and Sherstyuk [15–17], and Kostelecky and Nieto [8,9,18–20] who, respectively, worked out the quantum-defect orbital (QDO) method, the semiempirical effective orbital quantum number (EOQN) method, and the supersymmetry-inspired (SUSY-inspired) quantum-defect theory (SQDT) or the exact quantum-defect method. These theories have been applied to determine alkali-metal-like elements' transition probabilities and oscillator strengths. The above three quantum-defect models are related to the QDT developed by Burgess and Seaton [21–24], and Greene, Fano, and Strinati [25–27]. However, they essentially differ from QDT since the resulting equations are exactly solvable and the wave functions obtained are valid also in the core region.

Owing to the good accuracy observed in the above cited transition probabilities and f values predicted by nonrelativistic approaches, especially for low stages of ionization, we reformulated these works in order to include a major part of the relativistic effects of multicharged ions [10,28], by using

---

*Present address: Laboratoire de Spectroscopie Atomique Moléculaire et Applications, Département de Physique, Faculté des Sciences, Campus Universitaire 1060 Tunis, Tunisia. Email address: lcowono@yahoo.fr

†Email address: mkwato@yahoo.com

1050-2947/2002/66(5)/052503(16)/$20.00

Dirac wave functions. This led, respectively, in the fully relativistic scheme to the DQDO and DSQDT models, while in the quasirelativistic (QR) approach, we worked out the quasirelativistic REOQN and RSQDT models. It should be noted that the DEOQN method has been worked out by Gruzdev and Sherstyuk [29]. The quasirelativistic RQDO method has been formulated by Martin and co-workers [30–32] and has been applied in extensive calculations of transition probabilities for many isoelectronic sequences [33–47]. It is important to mention that there are two types of quasirelativistic approaches [48–51]. The first one, presented by Cowan and Griffin [52], is based on the scalar equation obtained from that of Dirac by a direct elimination of the small component. In the second approach, resulting from an application of Martin and Glauber's transformation [53] to a Dirac radial equation and formulated by Barthelat, Pelissier, and Durand [54], the scalar wave function is derived from the second-order equation obtained by transforming the first-order Dirac equation. This approach, referred to as the scalar second-order Dirac approach, was used to formulate the RQDO method.

In this paper, we apply the hypervirial theorem (HVT) [55–62] to deduce recurrence formulas for expectation values of successive powers of r for relativistic quantum-defect states. This HVT originates from the work of Löwdin on the virial theorem in quantum mechanics [55] and has been formulated by Hirschfelder [56] in the early 1960s. As a first application, the theorem has been used successfully in the calculation of expectation values [57] deserving separate places in the literature [58,59]. Since then the use of HVT has become a subject of great interest in two main ways concerning the determination of accurate energy eigenvalues and eigenfunctions (see Refs. [60–62] for detailed informations), and the calculation of radial matrix elements. Our interest in the present work lies within this second aspect.

The determination of expectation values may be traced back to around 1929 [63]. The hydrogenic radial matrix elements for the nonrelativistic case were derived by Gordon soon after he obtained the solutions of the corresponding Schrödinger equation. After this pioneering work, many authors tried to overcome the difficulty of evaluating these matrix elements by a direct integration for all values of q until Kramers [64] developed a recurrent relation for the calculation of the quantities in question in the hydrogenic context for neutral atoms. In a recent work, Morales, Peña, and Lopez-Bonilla [65], combining the HVT and Kramers' rules successfully determined expectation values of r^q with wave functions of central potential approximation. The procedure they used leads to a generalization of the usual $l=l'$ diagonal three-dimensional and $l=0$ one-dimensional hypervirial relations of first and second class. Another derivation of matrix elements of powers of r with improvement to the WKB approximation has been performed by Marxer [66]. Although there are several simple nonrelativistic procedures for generating expectation values [67], accurate determination sometimes has to resort to numerical technique using the Hartree-Fock (HF) equation. A compilation of HF results may be found in Ref. [68].

In the relativistic case, the problem is more complicated and has recently attracted some renewed attention [69]. Using the second-order Dirac equation with a standard Hartree-Fock-Roothan technique, Barthelat, Pelissier, and Durand [54] have determined the expectation values of r^q ($q=-1,1,2$) for Rn (s^2p^6) atom within the *jj*-coupling scheme, with satisfactory accuracy. Applying the QR formulation as derived, respectively, by Cowan and Griffin [52], Wood and Boring [70], and Mott and Massey [71], using a model potential introduced by Green, Sellin, and Zachor [72] to simulate a Hartree-Fock potential, Karwowsky and Kobus [49] obtained good numerical results in the calculation of expectation values, orbital energies, and electron density. Among other recent developments, we should mention an application of the Dirac second-order equation in a very interesting generalization of the decoupling procedure of Biedenharn [73] to account for a general atomic spherical potential for the calculation of hydrogenic matrix elements between Dirac and quasirelativistic wave functions [50]. In addition, Salamin has performed a derivation of diagonal matrix elements of arbitrary powers of r with Dirac hydrogenic wave functions [74]. This work has further been extended to the off-diagonal case by the same author [75]. The results of Ref. [74] have been rederived in a more suitable form by Andrae [76] for integer exponents. Formulas of expectation values were casted in a single recurrence relation, which results in a simple algorithm in terms of generalized hypergeometric ${}_3F_2$ series. Some months ago, Martinez-y-Romero, Núñez-Yépez, and Salas-Brito [77] reported recursion relations between relativistic atomic matrix elements of radial powers by using relativistic hydrogenic eigenstates.

In the nonhydrogenic scheme, there seem to be very few studies on the subject in the literature. A recent attempt in this realm was made by Martin and co-workers [78] who reported recurrence relations for matrix elements in the RQDO approximation. In the present paper, we extend the above work to derive a set of useful recurrence formulas that allow the determination of radial expectation values between Dirac and QR effective wave functions. It is obvious from the QR treatment that the formulas obtained are to be considered as a direct implementation of the Kramers' relations for the matrix elements of r^q in the eigenstates of the nonrelativistic hydrogen atom Hamiltonian. In this respect, the nonrelativistic formulas obtained earlier by Bockasten [79] are easely retrived. We apply the formulas worked out to the one electron alkali-metal-like ions of the Li, Na, and Cu isoelectronic sequences as an illustrative example to test the inclusion of relativistic effects in our treatment.

Our paper is organized as follows. In Sec. II, we review the relevant features related to the Dirac and QR effective radial wave functions and parameters. In Sec. III, we establish our notations concerning expectation values. Section IV is devoted to the presentation and discussion of our numerical results. Our conclusions are presented in Sec. V. Notice that relativistic atomic units [10] are used throughout this paper, unless otherwise stated explicitly.

II. BACKGROUND

A. Fully relativistic approach

The wave function for a relativistic state of the Dirac electron in the central field approximation may be written as [80]

$$\Psi=\begin{pmatrix} \varphi(r)|ljm\rangle \\ i\phi(r)|\bar{l}jm\rangle \end{pmatrix}, \tag{1}$$

where $\bar{l}=2j-l$, $|ljm\rangle$ are the spherical harmonics, $\varphi(r)$ and $\phi(r)$ are, respectively, the large-and small-component radial wave functions. For the particular case of the Coulomb potential $-z/r$, we introduce the following transformation [10,28,81]:

$$\Psi_r=P\Phi_r, \tag{2}$$

where

$$\Psi_r=\begin{pmatrix} \varphi(r) \\ \phi(r) \end{pmatrix}, \quad \Phi_r=\begin{pmatrix} u(r) \\ v(r) \end{pmatrix}, \quad P=\rho\begin{pmatrix} 1 & \gamma \\ \gamma & 1 \end{pmatrix}, \tag{3}$$

with

$$\gamma=\frac{z}{\kappa-s}, \quad z=Z\alpha, \quad \kappa=\epsilon(j+1/2), \quad j=l-\epsilon/2,$$

$$\epsilon=\pm 1, \quad s=\sqrt{\kappa^2-z^2}, \quad \rho=\frac{1}{2s}. \tag{4}$$

The subscript r refers to the radial part of the wave function. The quantities α, Z, and j are, respectively, the fine-structure constant, the charge of the ionic core, and the total angular momentum quantum number of the valence electron.

From the well-known Dirac-Coulomb equation [82–85] we get the following pair of first-order differential equations:

$$\left[\frac{d}{dr}-\left(\frac{s}{r}-\frac{\sigma}{s}\right)\right]u(r)=\left[1-\frac{\kappa E}{s}\right]v(r), \tag{5}$$

$$\left[\frac{d}{dr}+\left(\frac{s}{r}-\frac{\sigma}{s}\right)\right]v(r)=\left[1+\frac{\kappa E}{s}\right]u(r), \tag{6}$$

where $\sigma=zE$ and E is the total energy.

Taking now into account nonhydrogenic contributions in connection with the previously mentioned quantum-defect approaches, the hydrogenic parameters s, κ, and n are replaced by the effective parameters s^*, κ^*, and n^*. It is then easy to deduce from Eqs. (5) and (6) the Dirac effective second-order radial equations [10],

$$\tilde{H}^*_+ v^*(r)=2e^* v^*(r), \tag{7}$$

$$\tilde{H}^*_- u^*(r)=2e^* u^*(r), \tag{8}$$

with

$$\tilde{H}^*_\pm=\left[-\frac{d^2}{dr^2}-\frac{2\sigma}{r}+\frac{s^*(s^*\pm 1)}{r^2}\right], \quad e^*=-\frac{\sigma^2}{2\tilde{n}^{*2}}. \tag{9}$$

Equations (7) and (8) present a supersymmetric structure that was studied in detail in Ref. [81].

From Eqs. (2), (7), and (8), we get the effective generalized Dirac radial wave function,

$$\begin{pmatrix} \varphi^*(r) \\ \phi^*(r) \end{pmatrix}=\frac{a^2}{s^*}\sqrt{\frac{(\kappa^* E-s^*)\Gamma(\overline{n}^*+1)}{z(\kappa^*-s^*)\Gamma(\overline{n}^*+2s^*)}}\,x^{s^*-1}e^{-x/2}$$
$$\times\mathbf{M}\begin{pmatrix} xL^{(2s^*+1)}_{\overline{n}^*-1}(x) \\ L^{(2s^*-1)}_{\overline{n}^*}(x) \end{pmatrix}, \tag{10}$$

where

$$\mathbf{M}=\begin{pmatrix} \dfrac{az}{\kappa^* E-s^*} & \kappa^*-s^* \\ \dfrac{a(\kappa^*-s^*)}{\kappa^* E-s^*} & z \end{pmatrix}, \quad \overline{n}^*=n^*-|\kappa^*|,$$

$$x=2ar, \quad a=\sqrt{1-E^2}, \quad E=[1+(z/\tilde{n}^*)^2]^{-1/2}. \tag{11}$$

B. Quasirelativistic approach

Let us consider the projection operator for positive mass [53]

$$P^+=\tfrac{1}{2}[\gamma^\nu(p_\nu-A_\nu)+1-\gamma^0 U]. \tag{12}$$

The Dirac second-order bispinor ψ is related to Ψ by

$$\Psi=P^+\psi, \tag{13}$$

and obeys the following equation in the Coulomb approximation picture:

$$\frac{1}{2}\left[P_r^2+1-E^2+\frac{\mathcal{L}(\mathcal{L}+1)}{r^2}-\frac{2\sigma}{r}\right]\psi=0, \tag{14}$$

where

$$P_r=-i\frac{\partial}{\partial r} \tag{15}$$

is the radial momentum and

$$\psi=\Phi(r)\mathcal{Y}_{jlm}(\hat{r}), \quad \hat{r}=\frac{\vec{r}}{r}. \tag{16}$$

$\mathcal{Y}_{jlm}(\hat{r})$ are eigensolutions of the Kramers-Dirac operator [53,54],

$$\mathcal{L}=-\mathcal{K}\gamma^0-i\alpha_r z, \tag{17}$$

with

$$\mathcal{K}=-\gamma^0(\vec{\Sigma}\cdot\vec{L}+I). \tag{18}$$

ϵs and κ are, respectively, the eigenvalues of $\mathcal{L}$ and $\mathcal{K}$. The Dirac second-order radial equation that accounts for effective parameters is then derived from what precedes,

$$\left[\frac{d^2}{dr^2}+2e^*+\frac{2\sigma}{r}-\frac{s^*(s^*+\epsilon)}{r^2}\right]\phi(r)=0. \tag{19}$$

This quasirelativistic or Dirac scalar radial equation is identical to that obtained in Ref. [10] using the nonrelativistic limit. Its solution is then simply inferred, i.e.,

$$\phi(r)=\sqrt{\frac{a\Gamma(N+1)}{\overline{n}^{*}\Gamma(\overline{n}^{*}+\Lambda+1)}}\,x^{\Lambda+1}e^{-x/2}L_{N}^{(2\Lambda+1)}(x), \tag{20}$$

where

$$\Lambda=s^{*}+\frac{\epsilon-1}{2},\quad N=\overline{n}^{*}-\frac{\epsilon+1}{2}. \tag{21}$$

C. Effective parameters

The key element in each of the three quantum-defect approaches involved is the determination of the effective parameters. Subsequent informations concerning this derivation are found in our previous paper [10]. To make our text self-contained we recall them below.

1. Quantum-defect orbital approach

QDO procedure ensures phenomenological modifications in nonhydrogenic systems through the sequential determination of effective parameters [30–32],

$$\tilde{n}^{*}=\frac{Z'(1+\alpha^{2}\varepsilon)}{\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}},\quad \delta''=n-\tilde{n}^{*},\quad \delta'=\delta''+s-|\kappa|, \tag{22}$$

$$\overline{n}^{*}=\overline{n}-c,\quad s^{*}=|\kappa|-\delta'+c,\quad \kappa^{*}=\epsilon\sqrt{s^{*2}+z^{2}},$$
$$a=\alpha\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}, \tag{23}$$

and

$$c=|\delta'|, \tag{24}$$

i.e., the nearest integer value to the quantum defect δ' [12–14]. ε, the binding energies in a.u. are taken from experiments.

2. Effective orbital quantum number approach

For EOQN procedure, the effective parameters write [86]

$$\tilde{n}^{*}=\frac{Z(1+\alpha^{2}\varepsilon)}{\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}},\quad \overline{n}^{*}=\overline{n},s^{*}=\tilde{n}^{*}-\overline{n},$$
$$\kappa^{*}=\epsilon\sqrt{s^{*2}+z^{2}}. \tag{25}$$

It is then clear that EOQN parameters are identical to QDO's with $c=0$, i.e., EOQN orbitals retain the hydrogenic nodal structure.

3. Supersymmetry-based quantum-defect approach

The SUSY-based quantum-defect parameters result in the combination of SUSY ideas with the notion of quantum-defect [8,9,18–20,87–89]. The effective parameters are obtained as follows:

$$l^{*}=l-\delta(l,j)+I(l,j),\quad j^{*}=l^{*}-\epsilon/2=j-\delta(l,j)+I(l,j), \tag{26}$$

$$\kappa^{*}=\epsilon(j^{*}+\tfrac{1}{2}),\quad s^{*}=\sqrt{\kappa^{*2}-z^{2}},\quad n^{*}=n-\delta(l,j),$$
$$\overline{n}^{*}=n^{*}-|\kappa^{*}|,\quad \tilde{n}^{*}=\overline{n}^{*}+s^{*}. \tag{27}$$

$\delta(l,j)$ is the exact quantum-defect, i.e., for a given (l,j), $\delta(l,j)$ is exactly constant for all n. Therefore DSQT eigenfunctions form a complete and orthogonal set. $I(l,j)$ is a phenomenological non-negative integer playing the role of the supersymmetric shift.

III. MATRIX ELEMENTS

A. General formulation

Starting from Eqs. (5) and (6) and taking into account the effective parameters, it is easy to obtain the Dirac expectation values of r^{q} in the following form:

$$\langle r^{q}\rangle_{D}=\frac{1}{2s^{*2}(\kappa^{*}-s^{*})}[\kappa^{*}(\langle s^{*}|r^{q}|s^{*}\rangle+\langle\tilde{s}^{*}|r^{q}|\tilde{s}^{*}\rangle)$$
$$+2z\langle s^{*}|r^{q}|\tilde{s}^{*}\rangle]. \tag{28}$$

The corresponding quantities in the quasirelativistic approach write

$$\langle r^{q}\rangle_{QR}=\langle\Lambda|r^{q}|\Lambda\rangle. \tag{29}$$

For convenience, we introduce Dirac's notations with $|s\rangle\equiv rv(r)$, $|\tilde{s}\rangle\equiv ru(r)$, and $|\Lambda\rangle\equiv\Phi(r)$.

Applying the well-known HVT [56] to Eqs. (9) gives the following commutation rules:

$$[r^{q+1},\tilde{H}_{+}^{*}]=q(q+1)r^{q-1}+2(q+1)r^{q}\frac{d}{dr}, \tag{30}$$

$$\left[r^{q+1}\frac{d}{dr},\tilde{H}_{+}^{*}\right]=2Sqr^{q-2}+q(q+1)r^{q-1}\frac{d}{dr}$$
$$-2\sigma(2q+1)r^{q-1}-2(q+1)r^{q}\tilde{H}_{+}^{*}. \tag{31}$$

where $S=s^{*}(s^{*}+1)$.

From Eqs. (5), (6), (30), and (31), it is easy to obtain recurrence relations from which expectation values of r^{q} between effective radial wave functions may be derived.

Using Eq. (30), we get

$$\langle s^{*}|r^{q}\frac{d}{dr}|s^{*}\rangle=-\frac{q}{2}\langle s^{*}|r^{q-1}|s^{*}\rangle \tag{32}$$

and

$$2(q+1)\langle s^{*}|r^{q}\frac{d}{dr}|\tilde{s}^{*}\rangle=-[2s^{*}+q(q+1)]\langle s^{*}|r^{q-1}|\tilde{s}^{*}\rangle. \tag{33}$$

If we combine Eqs. (7), (31), and (32), we obtain a recurrence relation coupling matrix elements of consecutive powers of r,

$$2(q+1)e^*\langle s^*|r^q|s^*\rangle+(2q+1)\sigma\langle s^*|r^{q-1}|s^*\rangle+\frac{q}{4}[q^2-(2s^*+1)^2]\langle s^*|r^{q-2}|s^*\rangle=0. \tag{34}$$

According to Eqs. (5) and (6)

$$\langle s^*|r^q\frac{d}{dr}|s^*\rangle+s^*\langle s^*|r^{q-1}|s^*\rangle-\frac{\sigma}{s^*}\langle s^*|r^q|s^*\rangle-\xi\langle s^*|r^q|\tilde{s}^*\rangle=0, \tag{35}$$

where

$$\xi=\frac{(\kappa^{*2}E^2-s^{*2})^{1/2}}{s^*}. \tag{36}$$

Combining Eqs. (32) and (35) gives

$$(2s^*-q)\langle s^*|r^{q-1}|s^*\rangle=\frac{2\sigma}{s^*}\langle s^*|r^q|s^*\rangle+2\xi\langle s^*|r^q|\tilde{s}^*\rangle. \tag{37}$$

Setting actually the "bra" of Eq. (35) to $\langle\tilde{s}^*|$ instead of $\langle s^*|$ and using Eq. (33), we obtain the following equation:

$$q(2s^*-q-1)\langle\tilde{s}^*|r^{q-1}|s^*\rangle-\frac{2\sigma}{s^*}(q+1)\langle\tilde{s}^*|r^q|s^*\rangle-2\xi(q+1)\langle\tilde{s}^*|r^q|\tilde{s}^*\rangle=0, \tag{38}$$

in which on changing s^* into $-s^*$ results in

$$q(-2s^*-q-1)\langle s^*|r^{q-1}|\tilde{s}^*\rangle+\frac{2\sigma}{s^*}(q+1)\langle s^*|r^q|\tilde{s}^*\rangle+2\xi(q+1)\langle s^*|r^q|s^*\rangle=0. \tag{39}$$

Equations (38) and (39) yield

$$q\langle s^*|r^{q-1}|\tilde{s}^*\rangle=\xi[\langle s^*|r^q|s^*\rangle-\langle\tilde{s}^*|r^q|\tilde{s}^*\rangle]. \tag{40}$$

Equation (40) holds for all values of q only in a quasirelativistic treatment [78] where the normalization condition is given by

$$\langle s^*|s^*\rangle=\langle\tilde{s}^*|\tilde{s}^*\rangle=1. \tag{41}$$

We may also obtain a relation coupling different matrix elements of the same power of r with Eqs. (38) and (40),

$$\frac{2\sigma}{\xi s^*}(q+1)\langle s^*|r^q|\tilde{s}^*\rangle=(2s^*-q-1)\langle s^*|r^q|s^*\rangle-(2s^*+q+1)\langle\tilde{s}^*|r^q|\tilde{s}^*\rangle. \tag{42}$$

B. Explicit formulas

1. Relativistic case

A direct integration performed with the effective radial wave functions gives

$$\langle s^*|s^*\rangle=E(\kappa^*-s^*)(\kappa^*E+s^*), \tag{43}$$

$$\langle\tilde{s}^*|\tilde{s}^*\rangle=E(\kappa^*-s^*)(\kappa^*E-s^*), \tag{44}$$

$$\langle s^*|\tilde{s}^*\rangle=-\frac{1}{z}(\kappa^*-s^*)(\kappa^{*2}E^2-s^{*2}). \tag{45}$$

To construct some of the terms needed in the determination of the Dirac expectation values, we set $q=0$, 1, 2, 3 in Eq. (34). This leads to

$$\langle s^*|r^{-1}|s^*\rangle=\frac{\sigma E}{\tilde{n}^{*2}}(\kappa^*-s^*)(\kappa^*E+s^*), \tag{46}$$

$$\langle s^*|r|s^*\rangle=\frac{E}{2\sigma}[3\tilde{n}^{*2}-S](\kappa^*-s^*)(\kappa^*E+s^*), \tag{47}$$

$$\langle s^*|r^2|s^*\rangle=\frac{\tilde{n}^{*2}E}{2\sigma^2}[5\tilde{n}^{*2}+1-3S](\kappa^*-s^*)(\kappa^*E+s^*), \tag{48}$$

$$\langle s^*|r^3|s^*\rangle=\frac{\tilde{n}^{*2}E}{8\sigma^3}[5\tilde{n}^{*2}(7\tilde{n}^{*2}+5)+3S(S-10\tilde{n}^{*2}-2)]\times(\kappa^*-s^*)(\kappa^*E+s^*). \tag{49}$$

Using the above results, we find for $|\tilde{s}^*\rangle$,

$$\langle\tilde{s}^*|r^{-1}|\tilde{s}^*\rangle=\frac{\sigma E}{\tilde{n}^{*2}}(\kappa^*-s^*)(\kappa^*E-s^*), \tag{50}$$

$$\langle\tilde{s}^*|r|\tilde{s}^*\rangle=\frac{E}{2\sigma}[3\tilde{n}^{*2}-S'](\kappa^*-s^*)(\kappa^*E-s^*), \tag{51}$$

$$\langle\tilde{s}^*|r^2|\tilde{s}^*\rangle=\frac{\tilde{n}^{*2}E}{2\sigma^2}[5\tilde{n}^{*2}+1-3S'](\kappa^*-s^*)(\kappa^*E-s^*), \tag{52}$$

$$\langle\tilde{s}^*|r^3|\tilde{s}^*\rangle=\frac{\tilde{n}^{*2}E}{8\sigma^3}[5\tilde{n}^{*2}(7\tilde{n}^{*2}+5)+3S'\times(S'-10\tilde{n}^{*2}-2)](\kappa^*-s^*)(\kappa^*E-s^*), \tag{53}$$

where $S'=s^*(s^*-1)$.

Performing an integration with explicit relativistic radial wave functions gives

$$\langle s^*|r^{-2}|s^*\rangle=\frac{2\sigma^2}{(2s^*+1)\tilde{n}^{*3}}E(\kappa^*-s^*)(\kappa^*E+s^*), \tag{54}$$

$$\langle \tilde{s}^*|r^{-2}|\tilde{s}^*\rangle = \frac{2\sigma^2}{(2s^*-1)\tilde{n}^{*3}} E(\kappa^*-s^*)(\kappa^* E - s^*), \tag{55}$$

$$\langle s^*|r^{-2}|\tilde{s}^*\rangle = 0. \tag{56}$$

According to Eqs. (34) and (37) with $q=-1$, we obtain

$$\langle s^*|r^{-3}|s^*\rangle = \frac{\sigma}{s^*(s^*+1)}\langle s^*|r^{-2}|s^*\rangle, \tag{57}$$

$$\langle s^*|r^{-1}|\tilde{s}^*\rangle = \frac{2s^*+1}{2\xi}\langle s^*|r^{-2}|s^*\rangle - \frac{\sigma}{\xi s^*}\langle s^*|r^{-1}|s^*\rangle, \tag{58}$$

while using Eq. (40) results in

$$\langle s^*|r|\tilde{s}^*\rangle = -\frac{3\tilde{n}^{*2}}{2z\sigma}(\kappa^*-s^*)(\kappa^{*2}E^2-s^{*2}), \tag{59}$$

$$\langle s^*|r^2|\tilde{s}^*\rangle = \frac{\tilde{n}^{*2}}{2z\sigma^2}[s^{*2}-5\tilde{n}^{*2}-1](\kappa^*-s^*) \times(\kappa^{*2}E^2-s^{*2}). \tag{60}$$

If we set $q=-2$ in Eq. (39) we derive

$$\langle s^*|r^{-3}|\tilde{s}^*\rangle = \frac{\xi}{2s^*-1}\langle s^*|r^{-2}|s^*\rangle. \tag{61}$$

With this set of relations, all the remaining terms needed in the construction of relativistic matrix elements of any power of r may easily be obtained from Eqs. (34) and (42).

2. *Quasirelativistic case*

Since our quasirelativistic radial wave functions obey the same recurrence relations for the Hamiltonian $\tilde{H}_+^*$, it is obvious that matrix elements in this case may derive from what precedes under the substitution of s^* by Λ, thus giving $S=\Lambda(\Lambda+1)$, in all recurrence formulas where only $|s^*\rangle$ is available. Thus Eqs. (21)–(27) of Ref. [78] are straightforward. It is important to mention that while performing these equations, their authors assumed normalization condition given in Eq. (41), which copes with a quasirelativistic treatment. The following explicit formulas are then easily worked out:

$$\langle \Lambda|r^{-1}|\Lambda\rangle = \frac{\sigma}{\tilde{n}^{*2}}, \tag{62}$$

$$\langle \Lambda|r|\Lambda\rangle = \frac{1}{2\sigma}[3\tilde{n}^{*2}-S], \tag{63}$$

$$\langle \Lambda|r^2|\Lambda\rangle = \frac{\tilde{n}^{*2}}{2\sigma^2}[5\tilde{n}^{*2}+1-3S], \tag{64}$$

$$\langle \Lambda|r^3|\Lambda\rangle = \frac{\tilde{n}^{*2}}{8\sigma^3}[5\tilde{n}^{*2}(7\tilde{n}^{*2}+5)+3S(S-10\tilde{n}^{*2}-2)], \tag{65}$$

From Eq. (65), it is clear that there is a misprint in Eq. (31) of Ref. [78]. In addition, a direct integration using effective quasirelativistic radial wave functions leads to

$$\langle \Lambda|r^{-2}|\Lambda\rangle = \frac{2\sigma^2}{(2\Lambda+1)\tilde{n}^{*3}}. \tag{66}$$

Then all the remaining matrix elements of any power of r for quasirelativistic approach may actually be derived without any difficulty.

C. Nonrelativistic limit

Setting $\alpha\to 0$, we achieve the nonrelativistic limit [90] in the above expressions by the following substitutions: $\sigma\to Z$, $\tilde{n}^*\to n^*=n-\delta_0$, $s^*\to l^*$, $\Lambda\to l^*$, $l^*=l-\delta_0+i(l)$ $[i(l)\equiv c(l)$ or $I(l)]$, where δ_0 is the nonrelativistic quantum defect. We then retrieve the nonrelativistic formulas given by Bockasten [79] and modified accordingly to account for the quantum defect. We report hereafter some of these formulas,

$$\langle r^{-2}\rangle = \frac{2Z^2}{n^{*3}(2l^*+1)}, \tag{67}$$

$$\langle r^{-1}\rangle = \frac{Z}{n^{*2}}, \tag{68}$$

$$\langle r\rangle = \frac{1}{2Z}[3n^{*2}-l^*(l^*+1)], \tag{69}$$

$$\langle r^2\rangle = \frac{n^{*2}}{2Z^2}[5n^{*2}+1-3l^*(l^*+1)]. \tag{70}$$

The explicit relativistic corrections in the expectation values may be obtained as coefficients of the expansion of the corresponding formulas as

$$\langle r^q\rangle_{R_r\mathrm{QR}} = \langle r^q\rangle_{\mathrm{NR}} + \alpha^2\Delta_q + \alpha^4\tilde{\Delta}_q + O(\alpha^6), \tag{71}$$

where the subscripts R, QR, and NR stand, respectively, for relativistic, quasirelativistic, and nonrelativistic approaches. The results we present below for some terms Δ_q and $\tilde{\Delta}_q$ are obtained making use of MAPLE.

TABLE I. Quantum-defect numbers δ and δ' and integers c and I used in the computation of ns radial expectation values for neutral alkali-metal atoms.

			QDO		SQDT	
Z	Element	Level	δ'	c	δ	I
3	Li	2s	0.404 173	0	0.419 824	0
11	Na	3s	1.344 037	1	1.352 339	1
19	K	4s	2.162 127	2	2.099 634	2
29	Cu	4s	2.570 756	3	2.655 832	2
37	Rb	5s	3.110 459	3	3.090 318	3
47	Ag	5s	3.547 971	4	3.534 622	3
55	Cs	6s	4.025 407	4	4.015 407	4
87	Fr	7s	5.058 967	5	5.045 967	5
119	E-119	8s	7.865 041	8	6.166 705	6

1. Relativistic treatment

$$\Delta_{-2}=\frac{Z^{10}\{[(n-\delta_0)^2+\lambda Z^2][3(n-\delta_0)(12\lambda^2-1)+\lambda(4\lambda^2-1)]\}}{32\lambda(2\lambda+1)^2(2\lambda-1)^2(n-\delta_0)^{13}}, \tag{72}$$

$$\tilde{\Delta}_{-2}=\frac{Z^2[(n-d)^2+\lambda Z^2]}{512\lambda(2\lambda-1)^3(2\lambda+1)^3(n-d)^{15}}[11\lambda(n-d)(1-16\lambda^2+48\lambda^4)+18(n-d)^2(1-12\lambda^2+96\lambda^4) \\ +11\lambda^2(1-8\lambda^2+16\lambda^4)], \tag{73}$$

$$\Delta_1=\frac{1}{8}\left[\frac{6(n-\delta_0)^2}{Z}+\frac{Z\lambda[Z^2\lambda-2(n-\delta_0)^2]}{(n-\delta_0)^4}\right], \tag{74}$$

$$\tilde{\Delta}_1=\frac{Z}{16}\left[3+\frac{Z^2\lambda[Z^2\lambda-2(n-\delta_0)^2]}{(n-\delta_0)^6}\right], \tag{75}$$

$$\Delta_2=-\frac{1}{8Z^4}\{4(n-\delta_0)^4(\lambda[\lambda-3(n-\delta_0)]-1+10(n-\delta_0)^2)-\lambda Z^2[4(n-\delta_0)^2-\lambda Z^2]\}, \tag{76}$$

$$\tilde{\Delta}_2=-\left[\frac{(n-\delta_0)^2}{32Z^2}\{\lambda[4\lambda-17(n-\delta_0)]-4+29(n-\delta_0)^2\}-\lambda\left(\frac{1}{8}-\frac{\lambda Z^2}{32(n-\delta_0)^2}\right)\right], \tag{77}$$

$$\lambda=l^*.$$

2. Quasirelativistic treatment

$$\Delta_{-2}=\frac{Z^4[6(n-\delta_0)+2\lambda+1]}{(n-\delta_0)^5(2\lambda+1)^2}, \tag{78}$$

$$\tilde{\Delta}_{-2}=\frac{Z^6[72(n-\delta_0)^2+22(n-\delta_0)(2\lambda+1)+44\lambda(\lambda+1)]}{64(n-\delta_0)^T(2\lambda+1)^3}, \tag{79}$$

$$\Delta_{-1}=\frac{Z^3}{4(n-\delta_0)^4}, \tag{80}$$

$$\tilde{\Delta}_{-1}=\frac{Z^5}{8(n-\delta_0)^6}, \tag{81}$$

$$\Delta_1=-\frac{3Z}{16(n-\delta_0)}\left[2(n-\delta_0)-Z(2\lambda+1)+\frac{4\lambda(\lambda+1)}{3(n-\delta_0)}\right], \tag{82}$$

$$\tilde{\Delta}_1=-\frac{Z^3}{256(n-\delta_0)^3}\left[42(n-\delta_0)-(24-5Z)(2\lambda+1)+\frac{32\lambda(\lambda+1)}{(n-\delta_0)}\right], \tag{83}$$

$$\Delta_2=-\tfrac{1}{8}[(n-\delta_0)^2-1+3\lambda(\lambda+1)+9(n-\delta_0)(n-\delta_0-\lambda-\tfrac{1}{2})], \tag{84}$$

$$\tilde{\Delta}_2=-\frac{Z^2}{256(n-\delta_0)^2}\left[8(n-\delta_0)^2-8+24\lambda(\lambda+1)+102(n-\delta_0)\left(n-\delta_0-\lambda-\frac{1}{2}\right)\right]. \tag{85}$$

IV. NUMERICAL ILLUSTRATION

As underlined in the Introduction, analytical expressions of matrix elements of powers of r are very useful in problems in which one is interested in obtaining explicit formulas of physical quantities expanded as polynomials of $\langle r^q\rangle$. Also, the need for such expressions in the study of Rydberg problems has been established quite a long time ago. Given such importance, matrix elements of r^q and particularly those expressed in terms of relativistic quantum-defect radial wave functions then become a meaningful tool. It is, therefore, natural to test our formulas on ions of the Li, Na, and

TABLE II. Phenomenological and SUSY-based quantum-defect radial expectation values for *ns* levels of neutral alkali-metal atoms (see Table I) compared with HF and DF calculations. Results are given in a.u.

Z		q	RQDO $\langle r^q \rangle$	%	RSQDT $\langle r^q \rangle$	%	DQDO $\langle r^q \rangle$	%	DSQDT $\langle r^q \rangle$	%	HF[a] $\langle r^q \rangle$	DP[b] $\langle r^q \rangle$
3	Li	−1	0.392 679	13.7	0.400 506	15.9	0.392 699	13.7	0.400 527	15.9	0.345 392	0.345 437
		1	3.940 318	1.7	3.867 046	0.4	3.940 419	1.7	3.867 157	0.1	3.873 674	3.873 326
		2	18.406 22	3.8	17.746 19	0.0	18.406 73	3.8	17.746 75	0.0	17.738 39	17.735 56
		4	602.9645	6.6	563.0782	0.4	602.9835	6.6	563.0978	0.4	565.8824	565.7127
11	Na	−1	0.364 677	20.8	0.368 368	22.0	0.364 691	20.8	0.368 382	22.0	0.301 397	0.301 910
		1	4.226 070	0.5	4.186 123	0.4	4.226 138	0.5	4.186 194	0.4	4.208 760	4.203 247
		2	21.097 87	2.1	20.710 32	0.3	21.098 25	2.1	20.710 72	0.3	20.685 03	20.633 11
		4	779.2158	4.5	752.4970	1.0	779.2323	4.5	752.5139	1.0	748.7983	745.3314
19	K	−1	0.295 948	24.5	0.285 201	20.0	0.296 064	24.5	0.285 215	20.0	0.236 688	0.237 719
		1	5.134 425	1.7	5.176 246	0.9	5.134 480	1.7	5.176 287	0.9	5.243 751	5.224 035
		2	30.898 75	1.3	31.006 70	1.0	30.899 43	1.3	31.006 92	1.0	31.545 03	31.317 28
		4	1603.796	0.3	1604.879	0.3	1603.830	0.3	1604.969	0.3	1631.287	1609.314
29	Cu	−1	0.489 551	25.0	0.486 189	24.1	0.489 551	25.0	0.486 189	24.1	0.382 210	0.391 723
		1	2.757 305	15.4	2.773 394	14.9	2.757 305	15.4	2.773 894	14.9	3.331 147	3.261 527
		2	9.573 150	23.7	9.683 605	22.8	9.573 150	23.7	9.683 605	22.8	13.084 39	12.552 12
		4	196.4305	31.4	200.6958	29.9	196.4305	31.4	200.6958	29.9	310.3446	286.3643
37	Rb	−1	0.280 093	26.2	0.269 680	21.5	0.280 094	26.2	0.269 681	21.5	0.217 757	0.221 905
		1	5.404 560	2.5	5.451 283	1.7	5.404 562	2.5	5.451 286	1.7	5.631 897	5.544 997
		2	34.178 86	2.6	34.499 01	1.7	34.178 86	2.6	34.499 02	1.7	36.176 02	35.109 93
		4	1943.217	2.2	1954.872	1.6	1943.217	2.2	1954.873	1.6	2103.154	1987.670
47	Ag	−1	0.474 307	28.9	0.474 328	28.9	0.474 308	28.9	0.474 376	28.9	0.344 253	0.367 966
		1	2.834 347	17.9	3.286 212	4.8	2.834 346	17.9	3.286 455	4.8	3.656 488	3.451 177
		2	10.091 28	27.4	12.949 16	6.8	10.091 28	27.4	12.950 16	6.8	15.586 67	13.900 35
		4	216.8101	36.0	312.9301	7.6	216.8101	36.0	312.9558	7.6	424.3125	338.8263
55	Cs	−1	0.256 480	27.9	0.253 902	26.6	0.256 484	27.9	0.253 905	26.6	1.192 167	0.200 579
		1	5.860 801	3.7	5.915 390	2.8	5.860 793	3.7	5.915 381	2.8	6.305 878	6.084 542
		2	40.098 75	4.5	40.839 06	2.7	40.098 73	4.5	40.839 03	2.7	44.989 39	41.983 65
		4	2635.814	4.9	2729.642	1.5	2635.817	4.9	2729.645	1.5	3159.881	2772.448
87	Fr	−1	0.265 426	28.0	0.261 906	26.3	0.265 430	28.0	0.261 910	26.3	0.181 544	0.207 325
		1	5.679 051	4.1	5.749 179	2.9	5.679 047	4.1	5.749 173	2.9	6.629 696	5.922 042
		2	37.683 20	5.3	38.606 26	3.0	37.683 20	5.3	38.606 25	3.0	49.553 19	39.794 19
		4	2340.806	6.1	2451.523	1.6	2340.811	6.1	2451.527	1.6	3785 468	2492 920
119	E-119	−1	0.317 692	32.2	0.297 541	23.8	0.317 700	32.2	0.297 547	23.8		0.240 269
		1	4.808 963	7.6	5.110 784	1.8	4.808 989	7.6	5.110 797	1.8		5.202 889
		2	27.169 34	11.5	30.619 62	0.3	27.169 53	11.5	30.619 73	0.3		30.714 54
		4	1256.381	15.2	1576.335	6.3	1256.393	15.2	1576.344	6.3		1482.349

[a] Data from Ref. [68].

[b] Data from Ref. [91].

Cu isoelectronic sequences to enable a comparison of the level of achievement in accounting for relativistic effects in the fully relativistic and quasirelativistic procedures. But before presenting below our numerical results, we start with a few introductory statements relative to our database.

A. Database

The computation of expectation values requires prior determination of precise input data. This concerns energy values for QDO and EOQN methods while for SQDT, the free parameters δ and I are of interest. For the first two approaches, we have used for *s* orbitals of neutral alkali-metal-like atoms the energies obtained earlier by Desclaux [91]. These energies were derived by solving a multiconfiguration Dirac-Fock equation which includes the classical Coulomb repulsion and the Breit interaction in the *LS* coupling scheme. The corresponding parameters δ' and c are listed in Table I.

Concerning SQDT parameters of the above cited *s* orbitals of neutral alkali-metal-like atoms, the search was conducted in the DSQDT approach. This concerns precisely K I, Rb I, Ag I, Cs I, Fr I, and E-199 I. Values of δ and I obtained are also reported in Table I. In the same table, parameters for Li I, Na I, and Cu I [10] for QDO and SQDT procedures are also listed. Expectation values derived for these *s* orbitals are

TABLE III. Radial expectation values for $2s$, $2p_{1/2}$, and $2p_{3/2}$ levels for ions of Li isoelectronic sequence. Results are given in a.u.

			$\langle 2s_{1/2}\rangle$				$\langle 2p_{1/2}\rangle$				$\langle 2p_{3/2}\rangle$			
Z	Ion	q	RQDO	RSQDT	DQDO	DSQDT	RQDO	RSQDT	DQDO	DSQDT	RQDO	RSQDT	DQDO	DSQDT
4	Be^{1+}	-1	0.669 26	0.671 45	0.669 33	0.671 52	0.523 78	0.526 23	0.523 81	0.526 26	0.523 75	0.526 20	0.523 75	0.526 20
		1	2.290 71	2.283 71	2.290 70	2.283 70	2.397 73	2.387 69	2.397 67	2.387 63	2.397 86	2.387 81	2.397 86	2.387 81
		2	6.176 62	6.139 71	6.176 63	6.139 71	6.920 48	6.864 78	6.920 20	6.864 50	6.921 17	6.865 48	6.921 17	6.865 48
		4	65.599 18	64.860 06	65.600 03	64.860 91	90.228 11	88.864 16	90.223 16	88.859 25	90.245 00	88.881 25	90.245 00	88.881 25
10	Ne^{7+}	-1	2.197 18	2.200 75	2.199 44	2.203 03	2.051 14	2.057 25	2.052 98	2.059 10	2.049 26	2.055 40	2.049 26	2.055 40
		1	0.687 93	0.686 90	0.687 86	0.686 83	0.610 99	0.609 36	0.610 75	0.609 12	0.611 50	0.609 86	0.611 50	0.609 86
		2	0.553 47	0.551 84	0.553 44	0.551 81	0.448 75	0.446 44	0.448 47	0.446 16	0.449 46	0.447 14	0.449 46	0.447 14
		4	0.507 89	0.505 04	0.507 93	0.505 08	0.377 81	0.374 16	0.377 49	0.373 84	0.378 94	0.375 26	0.378 94	0.375 26
24	Cr^{21+}	-1	5.759 96	5.759 38	5.800 69	5.800 10	5.611 39	5.611 60	5.649 03	5.649 25	5.573 60	5.574 34	5.573 60	5.574 34
		1	0.261 48	0.261 50	0.261 27	0.261 29	0.223 28	0.223 28	0.222 62	0.222 61	0.224 64	0.224 62	0.224 64	0.224 62
		2	0.079 87	0.079 88	0.079 83	0.079 85	0.059 92	0.059 92	0.059 64	0.059 64	0.060 63	0.060 61	0.060 63	0.063 61
		4	0.010 50	0.010 50	0.010 50	0.010 51	0.006 73	0.006 73	0.006 69	0.006 69	0.006 88	0.006 88	0.006 88	0.006 88
36	Kr^{33+}	-1	8.918 84	8.911 38	9.070 08	9.062 23	8.763 60	8.756 21	8.907 01	8.899 26	8.622 12	8.616 59	8.622 12	8.616 59
		1	0.168 96	0.169 09	0.168 63	0.168 76	0.143 19	0.143 30	0.142 16	0.142 27	0.145 30	0.145 38	0.145 30	0.145 38
		2	0.033 35	0.033 40	0.033 32	0.033 37	0.024 57	0.024 70	0.024 39	0.024 43	0.025 37	0.025 40	0.025 37	0.025 40
		4	0.001 83	0.001 84	0.001 83	0.001 84	0.001 14	0.001 15	0.001 13	0.001 13	0.001 21	0.001 21	0.001 21	0.001 21
42	Mo^{39+}	-1	10.557 66	10.560 63	10.808 60	10.811 78	10.397 67	10.400 23	10.637 26	10.640 01	10.163 88	10.168 52	10.163 88	10.168 52
		1	0.142 84	0.142 80	0.142 46	0.142 42	0.120 83	0.120 80	0.119 61	0.119 58	0.123 32	0.123 27	0.123 32	0.123 27
		2	0.023 84	0.023 83	0.023 81	0.023 80	0.017 58	0.017 57	0.017 30	0.017 80	0.018 28	0.018 27	0.018 28	0.018 27
		4	0.000 94	0.000 94	0.000 94	0.000 94	0.000 58	0.000 58	0.000 57	0.000 57	0.000 63	0.000 63	0.000 63	0.000 63
74	W^{71+}	-1	20.522 84	20.546 21	22.378 75	22.408 67	20.317 33	20.333 14	22.116 26	22.136 41	18.723 95	18.695 53	18.723 95	18.695 53
		1	0.074 08	0.074 00	0.073 43	0.073 36	0.062 55	0.062 51	0.060 29	0.060 24	0.067 27	0.067 36	0.067 27	0.067 36
		2	0.006 43	0.006 42	0.006 41	0.006 40	0.004 75	0.004 74	0.004 48	0.004 48	0.005 46	0.005 47	0.005 46	0.005 47
		4	0.000 07	0.000 07	0.000 07	0.000 07	0.000 04	0.000 04	0.000 04	0.000 04	0.000 06	0.000 06	0.000 06	0.000 06
92	U^{89+}	-1	27.777 84	27.797 84	32.446 54	32.477 25	27.495 99	27.535 18	32.015 63	32.075 32	23.862 24	23.831 69	23.862 24	23.831 69
		1	0.055 14	0.055 10	0.054 40	0.054 37	0.046 76	0.046 70	0.043 84	0.043 78	0.053 01	0.053 07	0.053 01	0.053 07
		2	0.003 58	0.003 57	0.003 56	0.003 56	0.002 67	0.002 67	0.002 42	0.002 41	0.003 40	0.003 41	0.003 40	0.003 41
		4	0.000 02	0.000 02	0.000 02	0.000 02	0.000 01	0.000 01	0.000 01	0.000 01	0.000 02	0.000 02	0.000 02	0.000 02

TABLE IV. Radial expectation values for $3p_{1/2}$ and $3p_{3/2}$ levels for ions of Na isoelectronic sequence. Results are given in a.u.

			$\langle 3p_{1/2}\rangle$				$\langle 3p_{3/2}\rangle$			
Z	Ion	Q	RQDO	RSQDT	DQDO	DSQDT	RQDO	RSQDT	DQDO	DSQDT
12	Mg^{1+}	−1	0.389 60	0.459 78	0.389 61	0.459 80	0.389 60	0.459 76	0.389 60	0.459 76
		1	3.133 16	2.696 36	3.133 11	2.696 30	3.133 16	2.696 47	3.133 16	2.696 47
		2	11.591 42	8.676 29	11.591 12	8.676 00	11.591 42	8.676 97	11.591 42	8.676 97
		4	238.961 98	138.224 02	238.953 31	138.217 72	238.961 98	138.244 52	238.961 98	138.244 52
17	Cl^{3+}	−1	1.039 07	0.967 17	1.040 42	0.968 18	1.036 61	0.966 37	1.036 86	0.966 57
		1	1.375 75	1.467 60	1.375 43	1.467 30	1.378 70	1.468 70	1.378 62	1.468 62
		2	2.188 39	2.488 04	2.187 63	2.487 29	2.197 72	2.491 74	2.197 60	2.491 61
		4	7.317 10	9.390 51	7.313 40	9.386 46	7.377 77	9.417 68	7.377 62	9.417 47
24	Cr^{13+}	−1	1.859 46	1.713 94	1.866 39	1.719 05	1.850 46	1.706 46	1.851 92	1.707 63
		1	0.760 41	0.818 29	0.759 83	0.817 75	0.763 73	0.821 52	0.763 58	0.821 36
		2	0.667 60	0.772 32	0.666 86	0.771 58	0.673 42	0.778 38	0.673 28	0.778 23
		4	0.673 57	0.894 74	0.672 51	0.893 52	0.685 05	0.908 49	0.684 98	0.908 40
29	Co^{18+}	−1	2.437 64	2.287 63	2.452 84	2.299 65	2.420 17	2.271 53	2.423 45	2.274 29
		1	0.578 08	0.612 09	0.577 32	0.611 38	0.581 84	0.616 00	0.581 62	0.615 78
		2	0.385 67	0.432 05	0.384 93	0.431 31	0.390 66	0.437 53	0.390 52	0.437 38
		4	0.224 08	0.279 60	0.223 47	0.278 93	0.229 77	0.286 57	0.229 73	0.286 52
34	Se^{23+}	−1	3.018 17	2.830 02	3.046 61	2.852 48	2.988 02	2.803 97	2.994 24	2.809 19
		1	0.465 99	0.493 79	0.465 05	0.492 90	0.470 22	0.497 91	0.469 95	0.497 64
		2	0.250 55	0.281 10	0.249 81	0.280 36	0.255 09	0.285 78	0.254 94	0.285 63
		4	0.094 40	0.118 15	0.094 01	0.117 71	0.097 77	0.122 02	0.097 74	0.121 99
45	Rh^{34+}	−1	4.315 84	4.191 81	4.397 97	4.265 62	4.237 94	4.119 13	4.255 78	4.135 63
		1	0.325 31	0.333 96	0.323 97	0.332 65	0.330 69	0.339 26	0.330 29	0.338 86
		2	0.122 08	0.128 61	0.121 34	0.127 87	0.126 12	0.132 69	0.125 96	0.132 53
		4	0.022 38	0.024 77	0.022 19	0.024 57	0.023 84	0.026 33	0.023 83	0.026 31
51	Sb^{40+}	−1	5.047 16	4.871 33	5.178 50	4.986 69	4.928 13	4.760 71	4.956 23	4.786 26
		1	0.278 17	0.287 18	0.276 61	0.285 67	0.284 20	0.293 18	0.283 75	0.292 72
		2	0.089 26	0.095 10	0.088 53	0.094 36	0.093 15	0.099 08	0.092 99	0.098 92
		4	0.011 96	0.013 54	0.011 82	0.013 39	0.013 00	0.014 66	0.012 99	0.014 65
74	W^{33+}	−1	8.064 07	7.844 09	8.612 02	8.338 29	7.618 83	7.431 77	7.722 73	7.528 78
		1	0.174 65	0.179 05	0.172 20	0.176 65	0.183 80	0.187 95	0.183 09	0.187 24
		2	0.035 20	0.036 98	0.034 48	0.036 26	0.038 96	0.040 72	0.038 80	0.040 57
		4	0.001 87	0.002 05	0.001 81	0.002 00	0.002 27	0.002 48	0.002 27	0.002 47
92	U^{81+}	−1	10.837 60	10.594 42	12.232 17	11.871 37	9.887 82	9.641 47	10.113 80	9.852 24
		1	0.130 70	0.133 39	0.127 50	0.130 25	0.141 92	0.145 18	0.141 02	0.144 27
		2	0.019 73	0.020 54	0.019 03	0.019 84	0.023 23	0.024 80	0.023 08	0.024 15
		4	0.000 59	0.000 64	0.000 56	0.000 61	0.000 81	0.000 88	0.000 81	0.000 88

summarized in Table II which contains, when available, HF [68] and Dirac-Fock (DF) [91] results for comparative purposes.

For the various ions of the Li, Na, and Cu isoelectronic sequences, the data input are those presented exhaustively in Ref. [10] (see references therein). The radial matrix elements computed with these data are given in Tables III, IV, and V. Additional results concerning a particular ion of the isoelectronic sequences covered are available upon request from the authors.

B. Results and discussions

Radial expectation values have been computed without any difficulty from the above formulas and data. We remind the reader that EOQN procedure coincides with QDO when $c=0$ and their results in this case are identical [10]. In other cases, the EOQN outputs are in error compared to QDO and EQDT. For these reasons, we have not included them in the tables. Before discussing the results of ions of the Li, Na, and Cu isoelectronic sequences, we present hereafter some important features related to radial matrix elements for neutral alkali-metal atoms.

In Table II, we compare our predicted quantum-defect values for neutral atoms to those obtained with highly refined numerical techniques by Fischer [68] and Desclaux [91]. As one can see from this table, quasirelativistic results are within at least three to five digits practically identical to the corresponding relativistic values. This has already been no-

TABLE V. Radial expectation values for $4p_{1/2}$ and $4p_{3/2}$ levels for ions of Cu isoelectronic sequence. Results are given in a.u.

			$\langle 4p_{1/2}\rangle$				$\langle 4p_{3/2}\rangle$			
Z	Ion	Q	RQDO	RSQDT	DQDO	DSQDT	RQDO	RSQDT	DQDO	DSQDT
30	Zn^{1+}	-1	0.439 29	0.348 78	0.439 31	0.348 79	0.435 31	0.344 43	0.435 31	0.344 43
		1	2.809 85	3.465 82	2.809 79	3.465 77	2.833 11	3.505 78	2.833 11	3.505 78
		2	9.394 12	14.086 77	9.393 83	14.086 45	9.544 69	14.402 52	9.544 69	14.402 52
		4	160.611 26	345.641 85	160.60 438	345.631 07	165.508 72	360.467 13	165.508 72	360.467 13
33	As^{4+}	-1	0.743 63	0.585 78	0.744 13	0.585 98	0.736 14	0.579 37	0.736 23	0.579 42
		1	1.922 67	2.383 61	1.922 44	2.383 42	1.940 31	2.407 33	1.940 25	2.407 28
		2	4.274 33	6.549 52	4.273 57	6.548 78	4.352 51	6.679 64	4.352 39	6.679 48
		4	27.919 44	64.095 69	27.912 21	64.085 45	28.920 07	66.604 68	28.919 76	66.603 82
40	Zr^{11+}	-1	1.291 45	0.815 56	1.293 49	0.817 09	1.274 42	0.806 99	1.274 92	0.807 44
		1	1.072 06	1.775 32	1.071 65	1.774 83	1.084 95	1.792 57	1.084 82	1.792 39
		2	1.323 49	3.574 63	1.322 75	3.573 22	1.355 28	3.644 46	1.355 11	3.644 10
		4	2.598 81	17.716 90	2.596 75	17.706 83	2.722 22	18.406 80	2.722 02	18.405 78
48	Cd^{19+}	-1	1.857 68	1.604 07	1.863 42	1.619 58	1.823 93	1.579 76	1.825 46	1.583 17
		1	0.734 47	0.914 85	0.733 84	0.913 85	0.746 69	0.927 83	0.746 48	0.927 54
		2	0.620 03	0.949 31	0.619 26	0.947 76	0.640 69	0.976 42	0.640 49	0.976 14
		4	0.563 90	1.260 42	0.562 93	1.257 35	0.601 30	1.332 26	0.601 18	1.332 11
53	I^{24+}	-1	2.206 01	1.955 68	2.215 49	1.982 30	2.157 54	1.919 00	2.160 12	1.925 09
		1	0.615 38	0.748 94	0.614 62	0.747 74	0.627 82	0.762 12	0.627 56	0.761 75
		2	0.434 98	0.636 20	0.434 20	0.634 69	0.452 60	0.658 77	0.452 39	0.658 47
		4	0.276 50	0.565 29	0.275 82	0.563 31	0.298 89	0.605 48	0.298 80	0.605 36
70	Yb^{41+}	-1	3.410 13	3.211 90	3.564 74	3.325 04	3.277 61	3.096 67	3.308 05	3.122 17
		1	0.430 84	0.455 29	0.428 74	0.453 37	0.446 88	0.470 85	0.446 26	0.470 22
		2	0.210 54	0.235 10	0.209 02	0.233 65	0.226 50	0.251 44	0.226 21	0.251 12
		4	0.062 05	0.077 11	0.061 39	0.076 41	0.071 65	0.088 03	0.071 62	0.087 97
82	Pb^{53+}	-1	4.319 84	4.143 63	4.624 79	4.389 33	4.080 72	3.926 44	4.139 24	3.978 36
		1	0.339 78	0.353 07	0.337 20	0.350 63	0.358 08	0.370 99	0.357 28	0.370 19
		2	0.130 95	0.141 39	0.129 48	0.139 95	0.145 43	0.156 10	0.145 12	0.155 77
		4	0.023 99	0.027 90	0.023 59	0.027 48	0.029 49	0.033 91	0.029 46	0.033 87
88	Ra^{59+}	-1	4.800 69	4.553 83	5.220 86	4.873 84	4.487 44	4.277 60	4.565 18	4.344 64
		1	0.305 79	0.321 02	0.302 94	0.318 36	0.325 39	0.340 02	0.324 50	0.339 13
		2	0.106 06	0.116 89	0.104 60	0.115 47	0.120 08	0.131 12	0.119 77	0.130 79
		4	0.015 74	0.019 06	0.015 42	0.018 72	0.020 10	0.023 90	0.020 07	0.023 87
92	U^{63+}	-1	5.134 20	5.002 43	5.652 73	5.454 12	4.760 02	4.651 34	4.852 75	4.737 67
		1	0.286 01	0.292 94	0.282 98	0.290 01	0.306 64	0.313 22	0.305 70	0.312 27
		2	0.092 78	0.097 33	0.091 33	0.095 91	0.106 65	0.111 27	0.106 33	0.110 94
		4	0.012 05	0.013 24	0.011 77	0.012 95	0.015 85	0.017 23	0.015 83	0.017 20

ticed by Karwowski and co-workers [49,78]. They pointed out that for neutral elements, relativistic and quasirelativistic results are practically identical for nodeless orbitals up to $Z=90$, which stands in their work as an illustrative example.

In order to show how closely our results agree with those obtained by means of DF calculations [91] and which serve as reference data for our neutral elements, we have plotted the percent errors

$$d=\frac{|\langle r^q\rangle_D-\langle \mathrm{DF}\rangle|}{\langle \mathrm{DF}\rangle}\times 100 \tag{86}$$

of our computations in Figs. 1–4. d has also been calculated for HF numbers and inserted in the figures. The following clearly arises. It is obvious that DSQDT procedure which accounts for SUSY quantum-defect features is more effective and efficient than the phenomenological DQDO approach which, however, remains substantially better than DEOQN. Focussing our attention on Fig. 1 (i.e., for $q=-1$), we see that HF results are more close to DF values than the others. In the available domain, the HF results experience at the most a 12% divergence while for DSQDT and DQDO, the agreement lies between 14 and 32 % with increasing Z.

Switching our attention to Figs. 2–4 which correspond to $q=1$, 2, and 4, it is easy to notice that except for Cu and Ag, our results are reasonably in agreement with DF numbers. The calculated errors lie under 10% in the range $Z\leqslant 19$ and $Z\geqslant 55$. Only two values of E-119 corresponding to $q=2$ and $q=4$ in the QDO approximation are slightly above this gap, i.e., the differences are, respectively, 11.5 and 15.2 %. Simi-

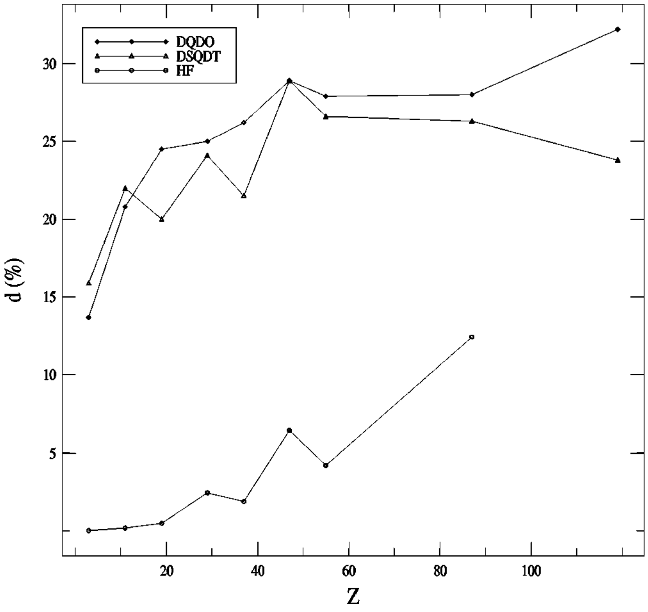

FIG. 1. Plot of the percentage difference *d* between DQDO, DSQDT, HF (Ref. [68]) values, and DF (Ref. [91]) reference data vs the nuclear charge for *ns* levels of neutral alkali-metal atoms (see Table I) for $q=-1$. Curves are drawn to guide the eye.

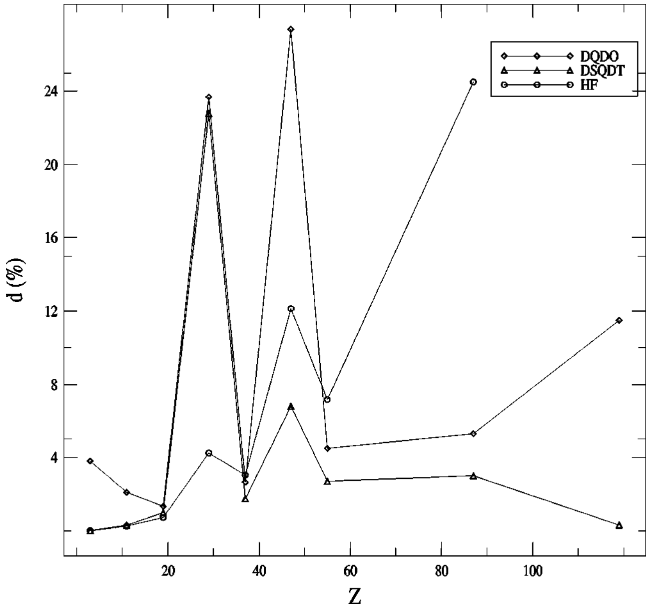

FIG. 3. Plot of the percentage difference *d* between DQDO, DSQDT, HF (Ref. [68]) values, and DF (Ref. [91]) reference data vs the nuclear charge for *ns* levels of neutral alkali-metal atoms (see Table I) for $q=2$. Curves are drawn to guide the eye.

lar reasonable agreement also occurs for Rb. Returning to Cu and Ag, it is important to stress that HF DQDO, and DSQDT procedures diverge almost strongly but with different scales. This may be explained as a manifestion of a large amount of polarization effects over relativistic ones. Kostelecky, Nieto, and Truax [19] pointed out that polarization effects are automatically taken into account in the effective parameters. Nevertheless, these effects remain important for some members of alkali-metal-like isoelectronic sequences. It should be noted that the general trends of our curves are relevant to the fact that relativistic effects increase with the nuclear charge Z [92,93]. In this respect, one may easily understand why HF results are in fatal error as Z grows larger. Their difference with DF data ranges up to 80% and above. It then becomes worth commenting that an adequate technique has to include relativistic effects in the treatment of atomic characteristics.

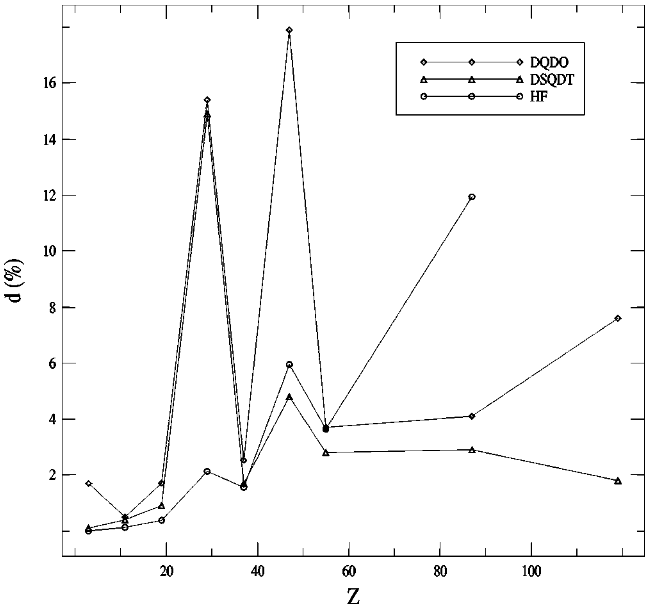

FIG. 2. Plot of the percentage difference *d* between DQDO, DSQDT, HF (Ref. [68]) values, and DF (Ref. [91]) reference data vs the nuclear charge for *ns* levels of neutral alkali-metal atoms (see Table I) for $q=1$. Curves are drawn to guide the eye.

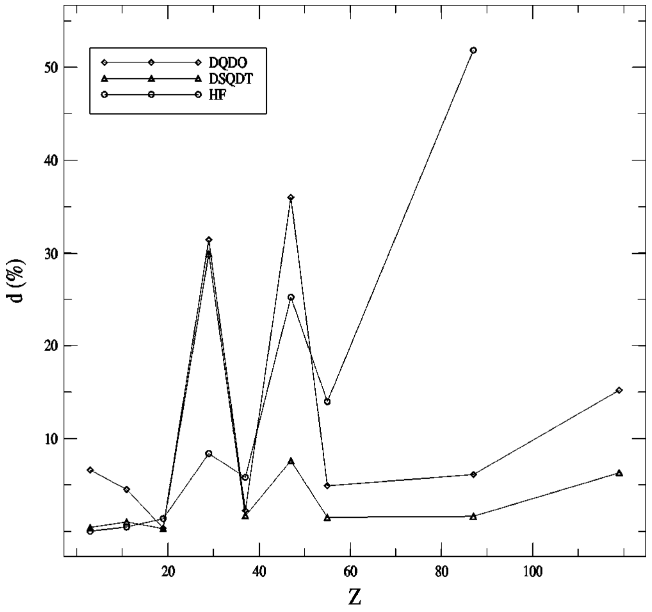

FIG. 4. Plot of the percentage difference *d* between DQDO, DSQDT, HF (Ref. [68]) values, and DF (Ref. [91]) reference data vs the nuclear charge for *ns* levels of neutral alkali-metal atoms (see Table I) for $q=4$. Curves are drawn to guide the eye.

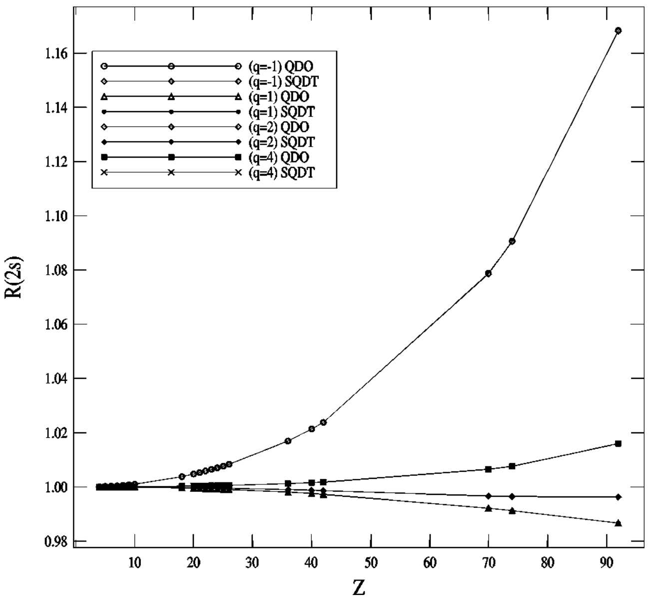

FIG. 5. Plot of the ratio values vs the nuclear charge for $2s$ energy level of the Li isoelectronic sequence. Curves are drawn to guide the eye.

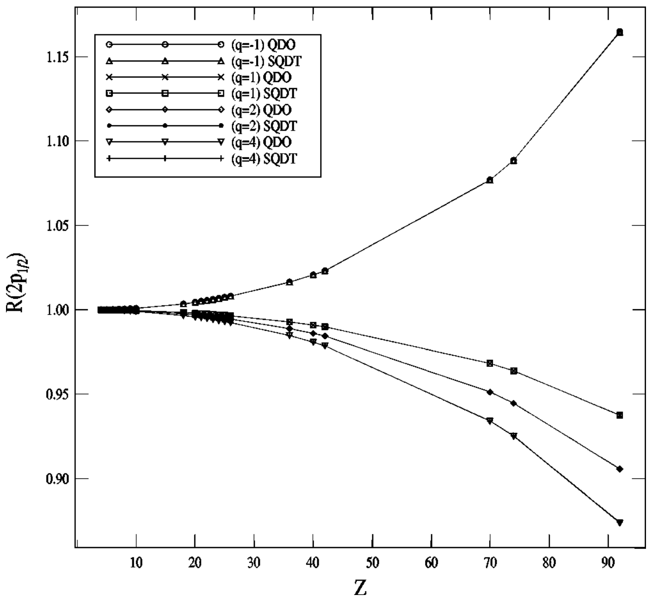

FIG. 6. Plot of the ratio values vs the nuclear charge for $2p_{1/2}$ energy level of the Li isoelectronic sequence. Curves are drawn to guide the eye.

An additional feature that may explain to some extent part of the above discrepancies is the picture change correction that arises in the transformation of the original Dirac Hamiltonian to approximate Hamiltonians, thus affecting the operators to use. This problem has been discussed by many authors and detailed informations may be found in the papers by Baerends *et al.* [94], Kellö and Sadlej [95], and Barysz [96]. It has been proved from their works that approximate relativistic calculations of expectation values may gain insight if picture change is taken into account. But in the case of concern, Kellö and Sadlej [95] observed that the correction would be large for high inverse powers of the radial distance. Additionally, Barysz [96] mentioned that apart from the general improvement provided by the picture change effects on matrix elements of the radial powers, there are some arguments showing that the nonrelativistic form of the electron-nucleus distance operator and its functions r^q may be used in both relativistic and nonrelativistic theories. A more general discussion of picture change effects in relativistic quantum-defect treatments is under investigation and will be reported in a forthcoming paper.

In Tables III, IV, and V are listed the results of the computation of radial matrix elements for the ions of the Li, Na, and Cu isoelectronic sequences. In addition to this, Figs. 5–10 display as illustrative examples plots of the ratio

$$R(nlj)=\frac{\langle r^q\rangle_D}{\langle r^q\rangle_{QR}} \tag{87}$$

of relativistic to quasirelativistic radial expectation values versus the nuclear charge Z. Such ratios have some insight when comparing two different approaches that attempt to account for the same effects. Their behavior along a level can help to build confidence on whether or not relativistic and quasirelativistic procedures effectively include relativistic effects at the same scale. As already noticed for neutral alkali-metal elements this is actually the case, but for ions the two approaches diverge from each other with increasing nuclear charge. As one can see, all our curves start from the value 1 and very quickly, they pull apart as Z increases. The deviation may be upward or downward depending on whether q is negative or positive. The general trends of our curves are in quite good agreement with the ones obtained by Desclaux [91] in the comparison of DF radial expectation values with HF. Since the ratio is not equal to unity along a series, this clearly shows as observed elsewhere [10] that relativistic and

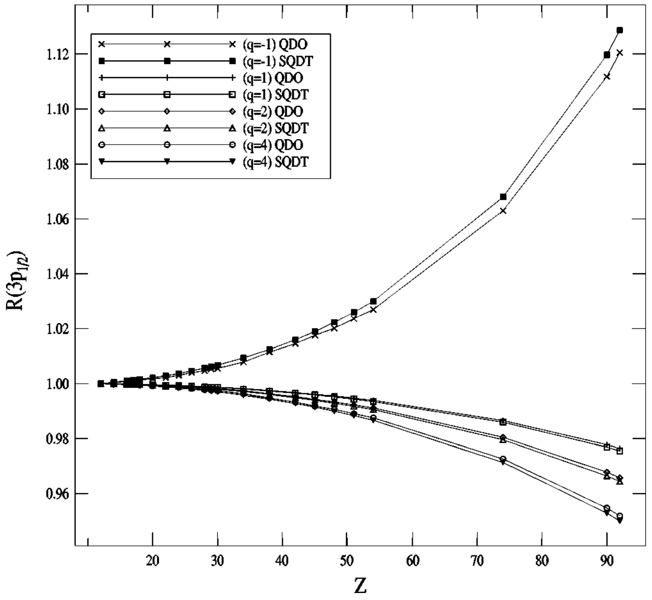

FIG. 7. Plot of the ratio values vs the nuclear charge for $3p_{1/2}$ energy level of the Na isoelectronic sequence. Curves are drawn to guide the eye.

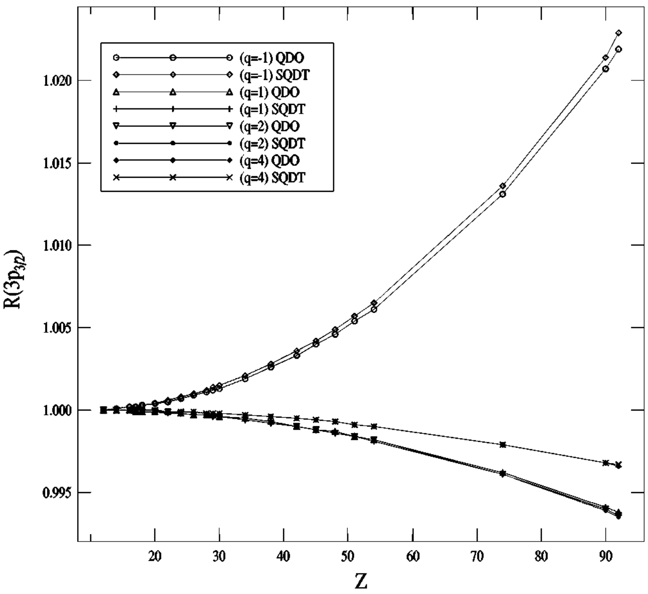

FIG. 8. Plot of the ratio values vs the nuclear charge for $3p_{3/2}$ energy level of the Na isoelectronic sequence. Curves are drawn to guide the eye.

quasirelativistic treatments do not account for relativistic effects at the same scale. The quasirelativistic models give a poor description of these effects at high *Z*. To illustrate this fact, it is relevant to underline that matrix elements of r^q for the same *l* but different *j*, say, for example, $np_{1/2}$ and $np_{3/2}$ levels, may significantly differ with increasing *Z* as it is shown in Ref. [91]. This is not the case with our quasirelativistic results. Instead, our fully relativistic approaches follow this trend and are therefore reliable.

From the above observations, it becomes evident that quasirelativistic approaches are not adequate for the description of relativistic features related to atomic structure calculations. A fully relativistic procedure is still needed if one has to make a correct treatment of highly ionized and Rydberg species where relativistic effects show up strongly. Note, however, that for a moderate manifestation of these effects, the QR technique still hold as a good alternative to the Dirac formalism. We may then see in our complete relativistic derivations given above a useful tool to deal with in analytical treatments in which consistent inclusion of relativistic effects is in order.

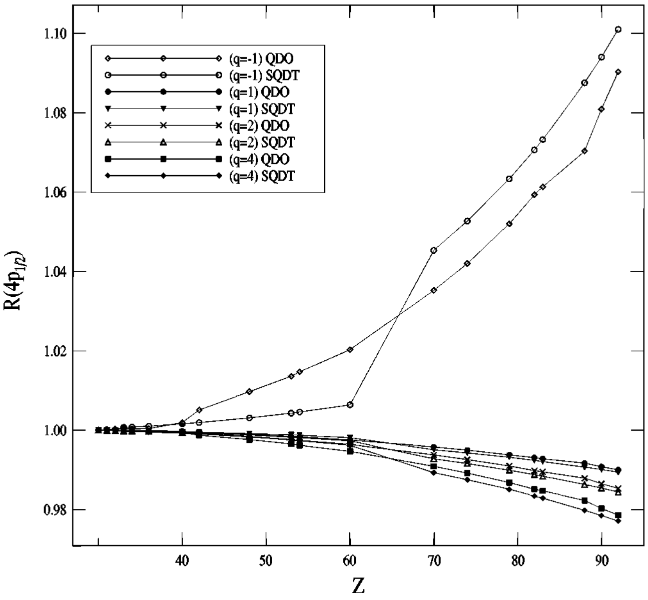

FIG. 9. Plot of the ratio values vs the nuclear charge for $4p_{1/2}$ energy level of the Cu isoelectronic sequence. Curves are drawn to guide the eye.

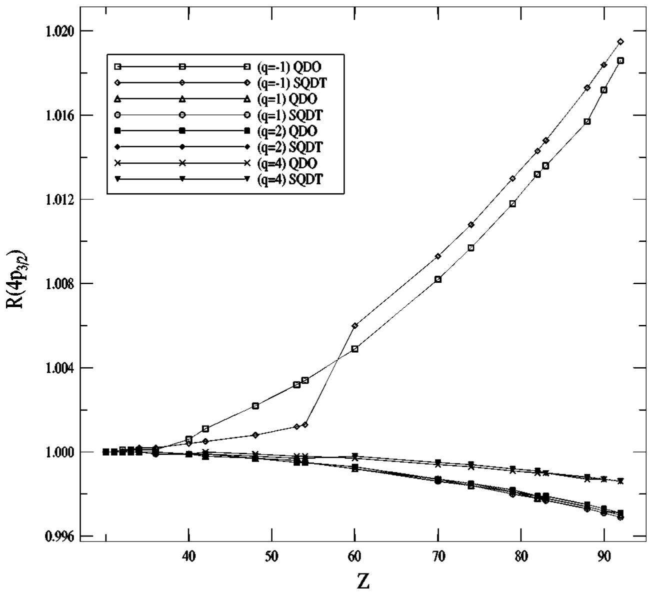

FIG. 10. Plot of the ratio values vs the nuclear charge for $4p_{3/2}$ energy level of the Cu isoelectronic sequence. Curves are drawn to guide the eye.

V. FINAL REMARKS

In the present work, we have used the HVT to obtain recurrence relations between expectation values of powers of *r* in the quantum-defect approximation. Relativistic and quasirelativistic radial wave functions have been employed. The formulas derived have been applied to the one electron alkali-metal-like atoms and ions to test the validity of our formulas. Our results suggest that a complete relativistic treatment may be used for a better account of relativistic effects. Also, SUSY-QD numbers indicate that this formalism is superior to the others.

Referring to what precedes we are inclined to believe in the convenience of combining QDTs and HVT to obtain recurrence relations between $\langle r^q \rangle$, which found practical applications in many interesting derivations in physics.

ACKNOWLEDGMENTS

Two of the authors (L. C. O. O. and B. O.) are grateful to the Center de Physique Atomique Moléculaire et Optique Quantique (CEPAMOQ) of the University of Douala (Cameroon) for warm hospitality during their stay at the center where part of this work was executed. M. G. K. N. acknowledges the financial support from SIDA and ICTP for his visits to The Abdus Salam International Center for Theoretical Physics (ICTP) under the Associate Scheme.

[1] E. A. Hessels, W. G. Sturrus, and S. R. Lundeen, Phys. Rev. A **35**, 4489 (1987).
[2] E. A. Hessels, F. J. Deck, P. W. Arcuni, and S. R. Lundeen, Phys. Rev. A **41**, 3663 (1990).
[3] W. G. Sturrus, E. A. Hessels, P. W. Arcuni, and S. R. Lundeen, Phys. Rev. A **38**, 135 (1988).
[4] P. W. Arcuni, E. A. Hessels, and S. R. Lundeen, Phys. Rev. A **41**, 3648 (1990).
[5] R. M. Sternheimer and H. M. Foley, Phys. Rev. **102**, 731 (1956).
[6] R. M. Sternheimer, Phys. Rev. **146**, 140 (1966).
[7] R. M. Sternheimer, Z. Naturforsch. Teil A **41A**, 24 (1986).
[8] V. A. Kostelecky and M. M. Nieto, Phys. Rev. A **32**, 1293 (1985).
[9] V. A. Kostelecky and M. M. Nieto, Phys. Rev. A **32**, 3243 (1985).
[10] S. G. Nana Engo, M. G. Kwato Njock, L. C. Owono Owono, B. Oumarou, G. Lagmago Kamta, and O. Motapon, Phys. Rev. A **56**, 2624 (1997).
[11] D. R. Bates and A. Damgaard, Philos. Trans. R. Soc. London, Ser. A **242**, 101 (1949).
[12] G. Simons, J. Chem. Phys. **60**, 645 (1974).
[13] I. Martin and G. Simons, J. Chem. Phys. **62**, 4799 (1975).
[14] I. Martin and G. Simons, Mol. Phys. **32**, 1017 (1976).
[15] P. F. Gruzdev and A. I. Sherstyuk, Opt. Spectrosk. **40**, 617 (1978) [Opt. Spectrosc. **40**, 353 (1976)].
[16] P. F. Gruzdev and N. Afanaseva, Opt. Spectrosk. **44**, 1047 (1978) [Opt. Spectrosc. **44**, 614 (1978)].
[17] P. F. Gruzdev and N. Afanaseva, Opt. Spectrosk. **45**, 631 (1978) [Opt. Spectrosc. **45**, 611 (1978)].
[18] V. A. Kostelecky and M. M. Nieto, Phys. Lett. **56**, 96 (1986).
[19] V. A. Kostelecky, M. M. Nieto, and D. R. Truax, Phys. Rev. A **38**, 4413 (1988).
[20] R. Bluhm and V. A. Kostelecky, Phys. Rev. A **47**, 794 (1993).
[21] A. Burgess and M. J. Seaton, Rev. Mod. Phys. **30**, 992 (1958).
[22] A. Burgess and M. J. Seaton, Mon. Not. R. Astron. Soc. **120**, 121 (1960).
[23] M. J. Seaton, Proc. Phys. Soc. London **88**, 801 (1966).
[24] M. J. Seaton, Rep. Prog. Phys. **46**, 167 (1983).
[25] U. Fano, Phys. Rev. A **2**, 353 (1970).
[26] C. H. Greene, U. Fano, and G. Strinati, Phys. Rev. A **19**, 1485 (1979).
[27] C. H. Greene, A. Rau, and G. Strinati, Phys. Rev. A **26**, 2441 (1982).
[28] M. G. Kwato Njock, B. Oumarou, L. C. Owono, J. D. Kenmogne, S. G. Nana, and M. Onana Boyomo, Phys. Lett. A **184**, 352 (1994).
[29] P. F. Gruzdev and A. I. Sherstyuk, Opt. Spectrosk. **46**, 625 (1979) [Opt. Spectrosc. **46**, 4 (1979)].
[30] I. Martin and J. Karwowski, J. Phys. B **24**, 1539 (1991).
[31] J. Karwoski and I. Martin, Phys. Rev. A **43**, 4833 (1991).
[32] I. Martin, J. Karwowski, C. Lavin, and G. H. F. Diercksen, Phys. Scr. **44**, 567 (1991).
[33] I. Martin, J. Karwowski, G. H. F. Diercksen, and C. Barrientos, Astron. Astrophys., Suppl. Ser. **100**, 595 (1993).
[34] C. Lavin, I. Martin, and M. J. Vallejo, Int. J. Quantum Chem., Symp. **26**, 455 (1992).
[35] C. Lavin and I. Martin, J. Quant. Spectrosc. Radiat. Transf. **50**, 611 (1993).
[36] I. Martin, C. Lavin, and C. Barrientos, Int. J. Quantum Chem., Symp. **26**, 465 (1992).
[37] C. Lavin, C. Barrientos, and I. Martin, Int. J. Quantum Chem. **50**, 411 (1994).
[38] C. Lavin and I. Martin, J. Quant. Spectrosc. Radiat. Transf. **52**, 21 (1994).
[39] C. Lavin, P. Martin, I. Martin, and J. Karwowski, Int. J. Quantum Chem., Symp. **27**, 385 (1993).
[40] P. Martin, C. Lavin, and I. Martin, Z. Phys. D: At., Mol. Clusters **30**, 279 (1994).
[41] C. Lavin, M. A. Almaraz, and I. Martin, Z. Phys. D: At., Mol. Clusters **34**, 143 (1995).
[42] I. Martin, M. A. Almaraz, and C. Lavin, Z. Phys. D: At., Mol. Clusters **35**, 228 (1995).
[43] E. Charro, I. Martin, and C. Lavin, J. Quant. Spectrosc. Radiat. Transf. **56**, 241 (1996).
[44] E. Charro, I. Martin, and C. Lavin, Astron. Astrophys., Suppl. Ser. **124**, 1 (1997).
[45] C. Lavin, A. B. Alvarez, and I. Martin, J. Quant. Spectrosc. Radiat. Transf. **57**, 831 (1997).
[46] C. Lavin, A. M. Velasco, and I. Martin, Astron. Astrophys. **328**, 426 (1997).
[47] A. M. Velasco, I. Martin, and C. Lavin, J. Quant. Spectrosc. Radiat. Transf. **57**, 509 (1997).
[48] J. Karwowski and J. Kobus, Int. J. Quantum Chem. **28**, 741 (1985).
[49] J. Karwowski and J. Kobus, Int. J. Quantum Chem. **30**, 809 (1986).
[50] J. Kobus, J. Karwowski, and W. Jaskólski, J. Phys. A **20**, 3347 (1987).
[51] J. Karwowski, W. Jaskólski, and J. Kobus, Phys. Scr. **38**, 554 (1988).
[52] R. D. Cowan and D. C. Griffin, J. Opt. Soc. Am. **66**, 1010 (1976).
[53] P. C. Martin and R. J. Glauber, Phys. Rev. **109**, 1307 (1958).
[54] J. C. Barthelat, M. Pelissier, and Ph. Durand, Phys. Rev. A **21**, 1773 (1980).
[55] P. O. Löwdin, J. Mol. Spectrosc. **3**, 46 (1959).
[56] J. O. Hirschfelder, J. Chem. Phys. **33**, 1462 (1960).
[57] J. H. Epstein and S. T. Epstein, Am. J. Phys. **30**, 266 (1962).
[58] O. L. de Lange and R. E. Raab, *Operator Methods in Quantum Mechanics* (Oxford Science Publications, Oxford, 1991).
[59] F. M. Fernandez and E. A. Castro, *Hypervirial Theorems* (Springer-Verlag, Berlin, 1987), and references cited therein.
[60] J. Killingbeck, Phys. Lett. A **65**, 87 (1978).
[61] M. Grant and C. S. Lai, Phys. Rev. A **20**, 718 (1979).
[62] M. G. Kwato Njock, M. Nsangou, Z. Bona, S. G. Nana Engo, and B. Oumarou, Phys. Rev. A **61**, 042105 (2000).
[63] W. Gordon, Ann. Phys. **2**, 1031 (1929).
[64] H. A. Kramer, *Quantum Mechanics* (North-Holland, Amsterdam, 1957).
[65] J. Morales, J. J. Peña, and J. Lopez-Bonilla, J. Mol. Struct.: THEOCHEM **330**, 63 (1995).
[66] H. Marxer, J. Phys. B **28**, 341 (1995).
[67] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[68] C. Froese Fischer, Comput. Phys. Commun. **4**, 107 (1976).
[69] M. K. F. Wong and H-Y. Yeh, Phys. Rev. A **27**, 2300 (1983).
[70] J. H. Wood and A. M. Boring, Phys. Rev. B **18**, 2701 (1978).

[71] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, 2nd ed. (Oxford University Press, London, 1949).
[72] A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. **184**, 1 (1969).
[73] L. C. Biedenharn, Phys. Rev. **126**, 845 (1962).
[74] Y. I. Salamin, Phys. Scr. **51**, 137 (1994).
[75] Y. I. Salamin, Phys. Scr. **51**, 9 (1995).
[76] D. Andrae, J. Phys. B **30**, 4435 (1997).
[77] R. P. Martinez-y-Romero, H. N. Nú̃ñez-Yépez, and A. L. Salas-Brito, J. Phys. B **35**, L71 (2002).
[78] I. Martin, J. Karwowski, and D. Bielinska-Waz, J. Phys. A **33**, 823 (2000).
[79] K. Bockasten, Phys. Rev. A **9**, 1087 (1974).
[80] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Theory* (McGraw-Hill, New York, 1964), Vol. 1.
[81] M. G. Kwato Njock, S. G. Nana Engo, L. C. Owono Owono, G. Lagmago, and B. Oumarou, Phys. Lett. A **187**, 191 (1994).
[82] J. J. Sakuraï, *Advanced Quantum Mechanics* (Addison Wesley, New York, 1982).
[83] C. Itzykson, and J-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1985).
[84] S. G. Nana Engo, L. C. Owono Owono, J. P. Dada, L. Waha Ndeuna, M. G. Kwato Njock, B. Oumarou, and O. Motapon, J. Phys. B **28**, 2333 (1995).
[85] J-Y. Su, Phys. Rev. A **32**, 3251 (1985).
[86] P. F. Gruzdev and A. I. Sherstyuk, Opt. Spectrosk. **46**, 625 (1979) [Opt. Commun. **46**, 353 (1979)].
[87] H. Nicolai, J. Phys. A **9**, 1497 (1976).
[88] E. Witten, Nucl. Phys. B **188**, 513 (1981).
[89] F. Copper, J. N. Ginocchio, and A. Khare, Phys. Rev. D **36**, 2458 (1987).
[90] A. Nikiforov and V. Ouvarov, *Fonctions Spéciales de la Physique Mathématique* (Mir, Moscow, 1983).
[91] J. P. Desclaux, At. Data Nucl. Data Tables **12**, 311 (1973).
[92] I. P. Grant, J. Phys. B **7**, 1458 (1974).
[93] E. K. Anderson *et al.*, in Abstracts of the Sixth International Conference on Atomic Physics, Riga, 1978 (unpublished), p. 180.
[94] E. J. Baerends, W. H. E. Schawrz, P. Schwerdtfeger, and J. G. Snijders, J. Phys. B **23**, 3225 (1990).
[95] V. Kellö and A. J. Sadlej, Int. J. Quantum Chem. **68**, 159 (1998).
[96] M. Barysz, Pol. J. Chem. **74**, 1329 (2000).