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Comparison of phenomenological and supersymmetry-inspired quantum-defect methods in their relativistic and quasirelativistic formulations

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The comparison of phenomenological and supersymmetry-inspired quantum-defect methods in their relativistic and quasirelativistic formulations is undertaken through a systematic study. Derivations, which emphasize similarities and differences between these approaches, are applied to evaluate oscillator strengths for low-lying and Rydberg states for lithiumlike, sodiumlike, and copperlike ions. Relativistic transition matrix elements calculated with the Dirac wave functions are gauge invariant. For the quasirelativistic formalism, an effective transition operator in the velocity gauge is proposed for the calculations. The detailed numerical results we obtained enable us to draw inferences as to the improvements and also to the limitations of these models. [S1050-2947(97)05009-9]

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I. INTRODUCTION

Over the past three decades a great deal of work has been devoted to the calculation of properties related to atomic transition probabilities of highly ionized atoms, i.e., ions with a nuclear charge Z that greatly exceeds the charge of the remaining electrons by about 20 [1]. This interest has been stimulated by everincreasing computing power and by a number of experimental developments in solar, stellar, and laboratory plasmas in the 1970s and 1980s. Under the best circumstances, theory and experiment agree to within 0.1%, making it possible to provide highly reliable data for numerous applications such as plasma modeling, astrophysics, laser design, and high-temperature fusion devices [2]. For example, a detailed knowledge of the structure of highly ionized atoms, such as those with 10 (neonlike ions) or 28 (nickel-like ions) remaining electrons, is essential for the construction of lasers that operate in extreme ultraviolet or soft-x-ray regions [3].

There is general agreement that for atomic transitions in highly stripped ions, relativistic effects become more and more important as the nuclear charge Z of the species increases. In the past 25 years, several theoretical calculations have been made. Some of the computer codes currently available for calculating energy levels and radiative transition probabilities are listed in a review article by Grant [1] and in an excellent compilation by Pyykko [4]. Among these, the multiconfiguration Dirac-Fock (MCDF) method [5] and the relativistic many-body perturbation theory (RMBPT) [6] are the two most successful codes. However, these codes are extremely laborious and become too time consuming when the number of transitions to be determined is very large [7]. For example, in a joint international collaboration known as the ''U.K.-U.S. Opacity Project'' concerning stellar envelope opacities, it was estimated that about 200–500 bound states per ions or atoms and a total of 10^6-10^7 oscillator strengths would be obtained [8]. Therefore, developing simple, reliable, and rapid computational methods is of fundamental importance for the determinations involved.

For this purpose, a great number of nonrelativistic calculations, using the Coulomb approximation technique originally developed by Bates and Damgaard [9], have been performed. Among these, the quantum-defect-orbital (QDO) method, the semiempirical effective orbital quantum number (EOQN) method, and the supersymmetry (SUSY) -inspired quantum-defect (SQDT) model or the exact quantum-defect method proposed for alkali-metal-like elements by Martin and Simons [10] Gruzdev and Sherstyuk [11] and Kostelecky and Nieto [12], respectively, can be pointed out. These methods, compared to the others, offer the advantage that, as with the eigen wave functions, the radial integrals are conveniently solved analytically. This leads to closed-form expressions for the transition probabilities and oscillator strengths [13]. These three quantum-defect models, referred to as phenomenological SUSY (PHSY) approaches, are related to the quantum-defect theory (QDT), developed and applied to the calculations of atomic characteristics by Burgess and Seaton [14] and Greene, Fano, and Strinati [15]. However, they essentially differ from QDT because the ap-

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proximate eigenfunctions of an asymptotically correct Hamiltonian provided by QDT behave correctly only in the large-r limit. The PHSY calculations rather generate exact eigenfunctions of an approximate Hamiltonian that includes an electronic screening term. The resulting orbitals are valid also in the core region.

Although the PHSY calculations are mathematically similar, they are not equivalent, as already mentioned in Ref. [16]. This crucial point appears clearly in the detailed numerical part of this work. Indeed, they interpret nonhydrogenic contributions to the effective potential by incorporating notions of quantum-defect theory by phenomenological (QDO and EOQN) [10,11] and symmetry (SQDT) [12] considerations. The symmetry in question, called SUSY-based quantum-defect symmetry, is broken by nonhydrogenic interactions, whereas in the limit that the central potential is hydrogenic, the symmetry is unbroken.

The fact that the comparison, within the nonrelativistic framework, of the PHSY approaches predicted transition probabilities and f values with accepted values shows good agreement for the low stage of ionization leads us to reformulate the above PHSY approaches in order to include a major part of the relativistic effects of multicharged ions. By using Dirac wave functions, Gruzdev and Sherstyuk [17] and Kwato Njock *et al.* [18] have performed the relativistic generalization of the effective orbital quantum number of (DEOQN) method and the relativistic generalization of the SUSY-based quantum-defect theory (DSQDT), respectively. Alternatively, the quasirelativistic formulation of quantum-defect-orbital (RQDO) method has been worked out by Martin and Karwowski [19]. It should be noted that there are two types of quasirelativistic approaches [20]. The first approach presented by Cowan and Griffin [21] is based on the scalar equation obtained from the Dirac one by a direct elimination of the small component. This approach has been successfully used to study atomic structure by many authors, including Wood and Boring [22], Karwowski and Szulkin [23], and Heully [24]. In the second approach, resulting from an application of Martin and Glauber's transformation [25] to a Dirac radial equation and formulated by Barthelat, Pelissier, and Durand [26], the scalar wave function is derived from the second-order equation obtained by transforming the first-order Dirac equation. This approach, named here the scalar second-order Dirac approach, was adopted and developed by Karwowski and Kobus [20] and Mohanty and Sampson [27] and used to formulate the RQDO method. This latter approach has the main advantage of retaining the simplicity of the nonrelativistic derivation.

Owing to the above-mentioned observations, it is of obvious interest to undertake a systematic study of the three PHSY approaches, where necessary, from the fully relativistic (DQDO, DEOQN, and DSQDT) and quasirelativistic (RQDO, REOQN, and RSQDT) viewpoints. This is a study, for the sake of better appreciation, not only of the effectiveness of each PHSY derivation, but also of the difference between quasirelativistic results and Dirac ones. The motivation of this work stems from that point. In Sec. II we present the theoretical background of the most relevant relativistic PHSY features, with emphasis, when necessary, on the difference between the above PHSY approaches. That difference lies in the determination of their effective parameters. This constitutes the key element in the PHSY derivations involved. In Sec. II C we provide analytically PHSY matrix elements in the dipole length and velocity gauges and give the corresponding oscillator strength closed-form expressions. Results of the numerical application of these calculations to the one-electron alkali-metal-like ions of the Li, Na, and Cu isoelectronic sequences are described and discussed in Sec. III. Such an investigation is of considerable interest since the behavior of the oscillator strength of a particular transition through an isoelectronic sequence is an important feature in evaluating the reliability of various theoretical predictions. In addition, the homologous comparison between isoelectronic sequences can provide a useful indication of the magnitudes of oscillator strengths [28,29]. On the other hand, highly excited states, always present in highly ionized atoms of hot plasma [30,31], have also been studied for Δn transitions variations up to 18. Our conclusion is presented in Sec. IV.

II. THEORETICAL BACKGROUND

A. Dirac effective wave functions

Let us consider radial wave functions $u(r)$ and $v(r)$, related to the well-known Dirac large- and small-component radial wave functions $\varphi(r)$ and $\phi(r)$ by [18,20]

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

where

$$\begin{gathered} \gamma = \frac{z}{\kappa - s}, \quad z = Z'\alpha, \quad \kappa = \epsilon(j + \tfrac{1}{2}), \\ j = l - \epsilon/2, \quad \epsilon = \pm 1, \quad s = \sqrt{\kappa^2 - z^2}, \quad \rho = \text{const.} \end{gathered} \tag{2}$$

In Eqs. (1) and (2) and what follows, relativistic atomic units are used [18]. The quantities α, Z', and j are, respectively, the fine-structure constant, the charge of the ionic core, and the value of the total angular-momentum quantum number of the valence electron. $u(r)$ and $v(r)$ are solutions of the system of first-order differential equations

$$\left[\frac{d}{dr} \mp \left(\frac{s}{r} - \frac{zE}{s}\right)\right] \begin{pmatrix} u(r) \\ v(r) \end{pmatrix} = \left[1 \mp \frac{\kappa E}{s}\right] \begin{pmatrix} v(r) \\ u(r) \end{pmatrix}. \tag{3}$$

E is the total energy. In Eq. (3) the upper (lower) sign refers to the upper (lower) components. The Dirac second-order radial equations deduced from Eq. (3) are

$$\left[\frac{d^2}{dr^2} + 2e + \frac{2\sigma}{r} - \frac{s(s-1)}{r^2}\right] u(r) = 0, \tag{4a}$$

$$\left[\frac{d^2}{dr^2} + 2e + \frac{2\sigma}{r} - \frac{s(s+1)}{r^2}\right] v(r) = 0, \tag{4b}$$

where $\sigma = zE$, $e = -a^2/2$, and $a = \sqrt{1 - E^2}$.

Detailed information about hydrogenic derivation of eigenvectors $u(r)$ and $v(r)$ can be found in Refs. [19,32–34]. In Ref. [18] we have studied the SUSY structure of Eqs. (3) and (4).

The eigenvectors and energy eigenvalues are then

$$u(r)=A_{\overline{n}}x^{S}\exp(-x/2)\mathcal{L}_{\overline{n}}^{(2S-1)}(x). \tag{5a}$$

$$v(r)=B_{\overline{n}}x^{S+1}\exp(-x/2)\mathcal{L}_{\overline{n}}^{(2S+1)}(x), \tag{5b}$$

$$E=[1+z^{2}/\tilde{n}^{2}]^{-1/2},\quad x=2ar,\quad \overline{n}=n-|\kappa|,$$

$$A_{\overline{n}}=\frac{a}{\kappa E-s}\,B_{\overline{n}}.$$

$\overline{n}$ and $\tilde{n}=\overline{n}+s$ are, respectively, the Dirac radial quantum number and the Dirac principal quantum number. The normalization constants $A_{\overline{n}}$ and $B_{\overline{n}}$, chosen to fulfill the condition

$$\int_{0}^{\infty}r^{2}(\phi^{2}+\varphi^{2})dr=1,$$

give rise, after a minor rearrangement, to the generalized Dirac radial wave functions

$$\begin{pmatrix}\varphi(r)\\ \phi(r)\end{pmatrix}=\frac{a^{2}}{s}\sqrt{\frac{(\kappa E-s)\Gamma(\overline{n}+1)}{z(\kappa-s)\Gamma(\overline{n}-s)}}\,x^{S-1}e^{-x/2}\begin{pmatrix}g_{1} & g_{2}\\ f_{1} & f_{2}\end{pmatrix}\times\begin{pmatrix}x\mathcal{L}_{\overline{n}-1}^{(2S+1)}(x)\\ \mathcal{L}_{\overline{n}}^{(2S-1)}(x)\end{pmatrix}, \tag{6}$$

where

$$g_{1}=\frac{az}{\kappa E-s},\quad g_{2}=\kappa-s,\quad f_{1}=\frac{a(\kappa-s)}{\kappa E-s},\quad f_{2}=z. \tag{7}$$

The associated Laguerre polynomials are defined by

$$\mathcal{L}_{N}^{(q)}(x)=\begin{cases}0, & N<0\\ \displaystyle\sum_{t=0}^{N}\frac{(-x)^{t}\Gamma(N+q+1)}{\Gamma(t+1)\Gamma(t+q+1)\Gamma(N-t+1)}, & N\geqslant 0.\end{cases} \tag{8}$$

However, in alkali-metal-like ions, the above treatment is not physically realized. For example, the interactions between the valence electron and the core yield a change in energy eigenvalues relative to the hydrogenic case. To incorporate nonhydrogenic contributions in the derivation in question, several approaches have been worked out. In the present paper, we focus attention on three of them, i.e., the previously mentioned PHSY approaches, in which we use the notion of quantum defect. The common procedure of derivation of relativistic eigensolutions involves the incorporation of nonhydrogenic contributions by simply replacing the hydrogenic radial solutions with ones of a similar form, but involving effective parameters s^{*}, κ^{*}, and $\overline{n^{*}}$ rather than s, κ, and $\overline{n}$. Then Eqs. (6) and (7) become [8]

$$\begin{pmatrix}\varphi^{*}(r)\\ \phi^{*}(r)\end{pmatrix}=\frac{a^{2}}{s^{*}}\sqrt{\frac{(\kappa^{*}E-s^{*})\Gamma(\overline{n^{*}}+1)}{z(\kappa^{*}-s^{*})\Gamma(\overline{n^{*}}-s^{*})}}\,x^{s^{*}-1}\times e^{-x/2}\begin{pmatrix}g_{1}^{*} & g_{2}^{*}\\ f_{1}^{*} & f_{2}^{*}\end{pmatrix}\begin{pmatrix}x\mathcal{L}_{\overline{n^{*}}-1}^{(2S^{*}+1)}(x)\\ \mathcal{L}_{\overline{n^{*}}}^{(2S^{*}-1)}(x)\end{pmatrix}, \tag{9}$$

where

$$g_{1}^{*}=\frac{az}{\kappa^{*}E-s^{*}},\quad g_{2}^{*}=\kappa^{*}-s^{*},\quad f_{1}^{*}=\frac{a(\kappa^{*}-s^{*})}{\kappa^{*}E-s^{*}},$$

$$f_{2}^{*}=z,\quad E=[1+z^{2}/\tilde{n}^{*2}]^{-1/2}. \tag{10}$$

The key element in each of the three approaches involved is the determination of those effective parameters.

1. Quantum-defect orbital approach

DQDO procedure [19] ensures phenomenological modifications in nonhydrogenic systems through the two transformations

$$\overline{n}\rightarrow\overline{n^{*}}=\overline{n}-c, \tag{11a}$$

$$s\rightarrow s^{*}=s-\delta'+c, \tag{11b}$$

where the relativistic quantum defect δ' is determined empirically. The introduction, on the grounds of expediency, of the quantity δ'' defined by

$$\delta''=n-\tilde{n}^{*}=|\kappa|-s+\delta' \tag{12}$$

leads to the sequential determination of DQDO effective parameters

$$\tilde{n}^{*}=\frac{Z'(1+\alpha^{2}\varepsilon)}{\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}},\quad \delta''=n-\tilde{n}^{*},\quad \delta'=\delta''+s-|\kappa|, \tag{13a}$$

$$c=\langle\delta'\rangle, \tag{13b}$$

i.e., the nearest integer value of the quantum defect δ' [10],

$$\overline{n^{*}}=\overline{n}-c,\quad s^{*}=|\kappa|-\delta''+c, \tag{13c}$$

$$\kappa^{*}=\epsilon\sqrt{s^{*2}+z^{2}},\quad a=\alpha\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}. \tag{13d}$$

ε, the binding energies in a.u., are taken from experiments or from others calculations.

It should be noted here that as $\varepsilon=\varepsilon(n,l,j)$, then $\delta'=\delta'(n,l,j)$ and $c=c(n,l,j)$. It is then obvious that δ' phenomenogically models the effective charge Z' generated by $Z-1$ core electrons and nucleus of charge Z by shifting the energy eigenvalues from the hydrogenic values [35]. However, the phenomenological quantum defect $\delta'(n,l,j)$ that varies slightly with n for a given (l,j) yields eigenvectors that are not orthogonal [16].

2. Effective orbital quantum number approach

In the same way as previously shown, DEOQN procedure [17] ensures phenomenological modifications in nonhydrogenic systems through the effective parameters

$$\tilde{n}^{*}=\frac{Z(1+\alpha^{2}\varepsilon)}{\sqrt{-\varepsilon(2+\alpha^{2}\varepsilon)}},\quad \overline{n^{*}}=\overline{n}, \tag{14a}$$

$$s^{*}=\tilde{n}^{*}-\overline{n},\quad \kappa^{*}=\epsilon\sqrt{s^{*2}+z^{2}}. \tag{14b}$$

It clearly appears in the above equations that DEOQN parameters are identical to those of DQDO [Eqs. (13)] with $c=0$, i.e., DEOQN orbitals retain the hydrogenic nodal structure.

3. Supersymmetry-based quantum-defect approach

The search for symmetry is a crucial part of this procedure [18], which combines supersymmetry ideas [12,36] with the notion of quantum defect. It differs from the two others by the sequential determination of effective parameters

$$l^* = l - \delta(l,j) - I, \quad j^* = l^* - \epsilon/2 = j - \delta(l,j) + I, \tag{15a}$$

$$\kappa^* = \epsilon(j^* + \tfrac{1}{2}), \quad s^* = \sqrt{\kappa^{*2} - z^2}, \quad n^* = n - \delta(l,j), \tag{15b}$$

$$\overline{n^*} = n^* - |\kappa^*|, \quad \tilde{n}^* = \overline{n} + s^*. \tag{15c}$$

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

From the above effective parameter derivations, a few features become apparent, of which the following may be relevant.

(i) As its nonrelativistic equivalent [12] the Dirac effective radial quantum number $\overline{n^*}$ is an integer. This explains why solutions still involve the associated Laguerre polynomials.

(ii) The DSQDT method, unlike the two others, can serve to make phenomenological predictions for certain unknown atomic characteristics such as transition probabilities and oscillator strengths.

The implications of numerical studies of the above features will be discussed in Sec. III.

B. Quasirelativistic effective radial wave functions

It has been shown that in the limit of $z \ll 1$ [34] for $\epsilon = -1$, $\kappa = -(l+1)$, with $s \simeq |\kappa| = l+1$,

$$\begin{pmatrix} g_1 & g_2 \\ f_1 & f_2 \end{pmatrix} \sim \begin{pmatrix} z^2 & 1 \\ z & z \end{pmatrix}, \tag{16}$$

so that the equation to consider is (4a), whereas for $\epsilon = 1$, $\kappa = l$, with $s \simeq |\kappa| = l$,

$$\begin{pmatrix} g_1 & g_2 \\ f_1 & f_2 \end{pmatrix} \sim \begin{pmatrix} 1 & z^2 \\ z & z \end{pmatrix}, \tag{17}$$

i.e., the equation to consider now is (4b). The quasirelativistic formulation in question here is based on the relativistic scalar equation obtained from what precedes. Then, taking into account nonhydrogenic effects as defined through the effective parameters, Eqs. (4) can be rewritten in the unified form

$$\left[\frac{d^2}{dr^2} + 2e^* + \frac{2\sigma}{r} - \frac{\Lambda(\Lambda+1)}{r^2}\right]\Psi(r) = 0, \tag{18}$$

where

$$\Lambda = s^* + \frac{\epsilon - 1}{2}, \quad e^* = -\frac{\sigma^2}{2\tilde{n}^{*2}}. \tag{19}$$

This quasirelativistic or Dirac scalar effective radial equation is quite similar to that of Schrödinger [10–12]. It differs from the latter only by numerical constants. Therefore, quasirelativistic generalized eigenvectors can be simply inferred, without any complication, from their nonrelativistic corresponding wave functions, i.e.,

$$\Psi(r) = \sqrt{\frac{a\Gamma(N+1)}{\tilde{n}^*\Gamma(\tilde{n}^* + \Lambda + 1)}}\, x^{\Lambda} e^{-x/2} \mathcal{L}_N^{(q)}(x), \tag{20}$$

where

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

The effective parameters defined in Sec. II A yield various quasirelativistic PHSY approaches.

C. Oscillator strengths

The most convenient way to describe the results of relativistic PHSY calculations is not through the transition probability, but rather through the concept of oscillator strength of a transition [37]. It is a useful tool to test the quality of an atomic model since it is related to observable magnitudes [13]. Among several equivalent formulas for calculating the f value for an electric-dipole transition, the most important ones are the dipole length form

$$f_L = \tfrac{2}{3}(2j_f + 1)\omega \mathcal{G}_j |M_L|^2 \tag{22a}$$

and the dipole velocity form

$$f_V = \frac{2}{3}\,\frac{2j_f + 1}{\omega}\,\mathcal{G}_j |M_V|^2, \tag{22b}$$

which are used in this paper. $\mathcal{G}_j$ is the angular factor of the electric-dipole matrix whose radial part is $M_{L,V}$, and $\omega = \alpha^2(\varepsilon_f - \varepsilon_i)$ is the transition energy. In the following, we carry out $M_{L,V}$ calculations in the fully relativistic and the quasirelativistic expression approaches.

1. Fully relativistic approach

Let us start with the fully relativistic (DPHSY) expressions [37,38]

$$M_L = -\frac{3}{2\omega}\left[-2J_1 + \Delta\kappa^* I_2^+ + 2I_2^-\right], \tag{23}$$

$$M_V = -\tfrac{1}{2}\left[\Delta\kappa^*(I_2^+ - 2I_0^+) + 2(I_2^- + I_0^-)\right], \tag{24}$$

where

$$J_1=\int_0^\infty(\varphi_f^*\varphi_i^*+\phi_f^*\phi_i^*)r^2 j_1(\omega r)dr,$$

$$I_L^{\pm}=\int_0^\infty(\varphi_f^*\phi_i^*\pm\phi_f^*\varphi_i^*)r^2 j_L(\omega r)dr. \tag{25}$$

$j_L(\omega r)$ $(L=0{,}2)$ is the spherical Bessel function $\Delta\kappa^*=\kappa_f^*-\kappa_i^*$.

The angular factor

$$\mathcal{G}_j=\begin{pmatrix} j_i & j_f & 1\\ -\frac{1}{2} & \frac{1}{2} & 0\end{pmatrix}^2=\begin{cases}[4j_f(j_f+1)(2j_f+1)]^{-1}, & j_f=j_i\\ [4j_f]^{-1}, & j_f=j_i+1.\end{cases} \tag{26}$$

After few operations, one finds the radial matrix element closed-form expressions [18]

$$M_L=C_{fi}\sum_{\tau=1}^{2}\sum_{\nu=1}^{2}\left[B_{\tau\nu}K_1(x)-\frac{x}{10}U_{\tau\nu}K_2(x)\right], \tag{27}$$

$$M_V=\frac{C_{fi}}{2F}\sum_{\tau=1}^{2}\sum_{\nu=1}^{2}\left[V_{\tau\nu}K_0(x)+\frac{x^2}{15}U_{\tau\nu}K_2(x)\right], \tag{28}$$

where

$$U_{\tau\nu}=\Delta\kappa^*A_{\tau\nu}^{+}+2A_{\tau\nu}^{-},\quad V_{\tau\nu}=-2\Delta\kappa^*A_{\tau\nu}^{+}+2A_{\tau\nu}^{-};$$

$$A_{\tau\nu}^{\pm}=g_{\tau f}^*f_{\nu i}^*\pm f_{\tau f}^*g_{\nu i}^*,\quad B_{\tau\nu}=g_{\tau f}^*g_{\nu i}^*+f_{\tau f}^*f_{\nu i}^*; \tag{29}$$

$$C_{fi}=\frac{1}{16zs_f^*s_i^*}\times\left[\frac{(\kappa_f^*E_f-s_f^*)(\kappa_i^*E_i-s_i^*)\Gamma(\overline{n_f^*}+1)\Gamma(\overline{n_i^*}+1)}{(\kappa_f^*-s_f^*)(\kappa_i^*-s_i^*)\Gamma(\overline{n_f^*}+2s_f^*)\Gamma(\overline{n_i^*}+2s_i^*)}\right]^{1/2}; \tag{30}$$

$$\begin{aligned}K_L(x)&=K_L(N_f,N_i,\beta_f,\beta_i,b)\\&=Y_f^{s_f^*-\tau+3}Y_i^{s_i^*-\nu+3}\Gamma(N_f+\beta_f+1)\Gamma(N_i+\beta_i+1)\\&\quad\times\sum_{p=0}^{N}\frac{(-Y_f)^p}{\Gamma(p+1)\Gamma(p+\beta_f+1)\Gamma(N_f-p+1)}\\&\quad\times\sum_{t=0}^{N_i}\frac{(-Y_i)^t\Gamma(b)\;{}_2F_1(\frac{1}{2}b,\frac{1}{2}(b+1);L+\frac{3}{2},-x^2)}{\Gamma(t+1)\Gamma(t+\beta_i+1)\Gamma(N_i-t+1)};\end{aligned} \tag{31}$$

$$F=(a_f+a_i)^{-1},\quad x=\omega F,\quad Y_f=2a_fF,\quad Y_i=2a_iF,$$

$$N_f=\overline{n_f^*}+\tau-2,\quad N_i=\overline{n_i^*}+\nu-2,\quad \beta_f=2s_f^*-2\tau+3, \tag{32}$$

$$\beta_i=2s_i^*-2\nu+3,\quad b=s_f^*+s_i^*-\tau-\nu+p+t+L+5.$$

It is noteworthy that M_L and M_V are gauge invariant [38]. Indeed, since all pairs of generalized wave functions $\binom{\varphi_i^*(r)}{\phi_i^*(r)}$ and $\binom{\varphi_f^*(r)}{\phi_f^*(r)}$ given by Eq. (9) are eigensolutions of the same Dirac-like radial equation, the longitudinal matrix element vanishes identically. Therefore, DPHSY f values may be calculated indifferently with Eq. (22a) or (22b). It should also be noted that there are some misprints in the formulas of the oscillator strengths in Ref. [18].

In order to better evaluate the influence in the matrix elements of relativistic changes due only to the DPHSY wave functions, we let only the leading term of the spherical Bessel expansion act on the wave functions in question. In this approximate relativistic approach

$$M_L=\int_0^\infty(\varphi_f^*\varphi_i^*+\phi_f^*\phi_i^*)r^3dr, \tag{33}$$

$$M_V=\int_0^\infty[(\Delta\kappa^*-1)\varphi_f^*\varphi_i^*+(\Delta\kappa^*+1)\phi_f^*\phi_i^*]r^2dr. \tag{34}$$

Taking into account the fact that ${}_2F_1(a,b;c;0)=1$, one finds

$$M_L=\lim_{x\to 0}M_L=C_{fi}\sum_{\tau=1}^{2}\sum_{\nu=1}^{2}B_{\tau\nu}K_1(0), \tag{35}$$

$$M_V=\lim_{x\to 0}M_V=\frac{C_{fi}}{2F}\sum_{\tau=1}^{2}\sum_{\nu=1}^{2}V_{\tau\nu}K_0(0). \tag{36}$$

In this case, the angular factor is given by $\mathcal{G}_j=l_>\begin{Bmatrix} l_i & j_i & \frac{1}{2}\\ j_f & l_f & 1\end{Bmatrix}^2$, $l_>=\frac{1}{2}(l_f+l_i+1)$.

2. *Quasirelativistic approach*

Finally, for the quasirelativistic (RPHSY) approach, we have employed the usual nonrelativistic dipole length operator acting on the quasirelativistic (QR) wave functions. From the formal analogy between the QR equation (18) and the hydrogenic Schrödinger radial equation, the velocity operator has been modified in order to take into account QR effective effects. Therefore, instead of the usual well-known hydrogenic operator $d/dr-l_>\Delta_0/r$, $\Delta_0=l_f-l_i$, we have used $d/dr-\Lambda_>\Delta/r$. The effectiveness of this choice will be discussed in the next section. Here we have

$$M_L=\int_0^\infty\Psi_f r\Psi_i dr=\overline{C_{fi}}Y_fY_i\overline{K(}N_f,N_i,\beta_f,\beta_i,b), \tag{37}$$

$$\begin{aligned}M_V&=\int_0^\infty\Psi_f\left(\frac{d}{dr}-\frac{\Lambda_>\Delta}{r}\right)\Psi_i dr\\&=4\overline{C_{fi}}a_fa_i[(\Lambda_i-\Lambda_>\Delta+1)\overline{K(}N_f,N_i,\beta_f,\beta_i,b)\\&\quad-\tfrac{1}{2}Y_i\overline{K(}N_f,N_i,\beta_f,\beta_i,b+1)\\&\quad-Y_i\overline{K(}N_f,N_{i-1},\beta_f,\beta_{i+1},b+1)],\end{aligned} \tag{38}$$

where

$$\Lambda_{>}=\tfrac{1}{2}(\Lambda_f+\Lambda_i+1), \quad \Delta=\Lambda_f-\Lambda_i,$$

$$\overline{C_{fi}}=\frac{1}{4}\,Y_f^{\Lambda_f+1}Y_i^{\Lambda_i+1}\times\left[\frac{\Gamma(N_f+1)\Gamma(N_i+1)\Gamma(N_f+\beta_f+1)\Gamma(N_i+\beta_i+1)}{a_f a_i(N_f+\Lambda_f+1)(N_i+\Lambda_i+1)}\right]^{1/2}, \tag{39}$$

$$\overline{K}(N_f,N_i,\beta_f,\beta_i,b)=\sum_{p=0}^{N_f}\frac{(-Y_f)^p}{\Gamma(p+1)\Gamma(p+\beta_f+1)\Gamma(N_f-p+1)}\times\sum_{t=0}^{N_i}\frac{(-Y_i)^t\Gamma(b)}{\Gamma(t+1)\Gamma(t+\beta_i+1)\Gamma(N_i-t+1)}.$$

The angular factor is given by

$$\mathcal{G}_j=l_{>}\begin{Bmatrix} l_i & j_i & \frac{1}{2}\\ j_f & l_f & 1\end{Bmatrix}^2, \quad l_{>}=\max(l_f,l_i)=\tfrac{1}{2}(l_f+l_i+1). \tag{40}$$

It appears from Eqs. (27)–(32) and (37)–(40) that fully relativistic calculations will be much more time consuming than quasirelativistic ones.

III. NUMERICAL RESULTS AND DISCUSSION

For the sake of assessing the effectiveness of the various relativistic PHSY approaches, we apply in this section the corresponding formulas derived above to the one-electron alkali-metal-like ions of the lithium, sodium, and copper isoelectronic sequences. Before presenting below the main numerical results of our methods and a comparison with more refined computations as well as experimental results, a few introductory statements concerning our database are in order.

A. Energy database

The basic empirical parameters required by the relativistic QDO and EOQN procedures as inputs are precise energy-level values of electronic states of the ion, as well as the ionization potential. Those employed here are presented in the following.

1. Lithium sequence

The transitions considered in the lithium isoelectronic sequence are the lines of $2s$-$2p$-$3p$ from Li to U^{89+} for low-lying states and $2s$-np ($n=4-20$) of Ca^{17+}, Zr^{37+}, and Yb^{67+} for Rydberg states. The input values for the excitation energies of decaying levels and the ionization potentials of the ground states were taken in the case of $2s$-$2p$ from reliable and comprehensive data of Theodosiou, Curtis, and El-Mekki [39]. These data were obtained through the combined use of available measured data [40] and *ab initio* RMBPT calculations including a semiempirical screening parametrization of the Lamb shift [41]. For U^{89+}, the excitation energies and ionization potential used are those of Ynnerman *et al.* [42] calculated with the above-mentioned RMBPT. The excitation energies employed for $2s$-$3p$ transitions are, for $Z=3-10$, the compilation of measurements given by Lindgård and Nielsen [28]. For ions ranging from $Z=20$ to 25, data are the MCDF values including the transverse Breit and QED corrections [43]. The others are the Dirac-Hartree-Fock data, which include the Breit interaction as a first-order correction to the energy, calculated by Armstrong, Fielder, and Lin [37]. The Rydberg energies of the discrete spectrum under consideration are deduced from the interpolation formula of relativistic quantum defects given by Zilitis [44]. The f results obtained are summarized in Tables I–III.

2. Sodium sequence

In this isoelectronic sequence, the transitions considered are $3s$-$3p$-$4p$ from Na to U^{81+}. The ionization potentials and the excitation energies employed for $3s$-$3p$ transitions are the compilation of observed values given by Lindgård and Nielsen [28] for ions in the range $Z=11-14$ and data given by Edlén in Ref. [40] for $Z=16-29$. For $Z=30-54$, ionization potentials used are deduced by Theodosiou and Curtis [45] from measured and fitted $3s$-$3p$-$3d$-$4f$ intervals in Ref. [46] and polarization parameters from Ref. [47]. The excitation energies are fitted values obtained by Reader *et al.* [46] by parametrizing the differences between the observed values and the corresponding MCDF values. The other data ($Z\geqslant 54$) are extrapolated values given by Theodosiou and Curtis. For the $3s$-$4p$ transitions, we have employed the excitation energies of Lindgård and Nielsen values ($Z=11-20$), MCDF values ($Z=38-45$) [48], and Dirac-Fock-Slater values ($Z\geqslant 48$) [49] fitted to MCDF ones, including both Breit and QED corrections. The f results obtained are summarized in Tables IV and V.

3. Copper sequence

Here we have considered the transitions $4s$-$4p$-$5p$ from Cu to U^{63+}. The input ionization potentials and the $4p$ excitation energies are taken from the excellent compilation of measurements [50–52] proposed by Curtis and Theodosiou [53] and those they obtained through a combined use of *ab initio* MCDF calculations [5], quantum-defect reductions, and screening parameter systematizations [54]. For $5p$ excitation energies, a compilation of measurements given by Lindgård *et al.* [55] are used for ions ranging from $Z=29-42$. The other values ($Z=44-92$), given by Seely, Brown, Feldman [56], are based on the semiempirically corrected wavelengths made by comparing the observed wavelengths [52] and the MCDF (including QED, Breit, and finite nuclear size effects) calculated wavelengths. The f results obtained are summarized in Tables VI and VII.

B. Exact quantum-defect database

The exact quantum defects of s and p states are the input parameters required by relativistic SQDT. It appears that for a given (l,j) and increasing n, the phenomenological $\delta(n,l,j)$ rapidly approach asymptotic values $\delta(l,j)$. In the tables given below, values of $\delta(l,j)$ are listed that yield the best match to experimental and theoretical accepted f values with their corresponding nodal parameters $I(l,j)\equiv I(l)$ for a given $\delta(l,j)$. It is convenient to point out that the search was conducted with the DSQDT approach.

TABLE I. Our oscillator strengths compared with other selected calculations for $2s\ ^2S-^2S-2p\ ^2P$ transitions in the Li isoelectronic sequence, denoted DPHSY gauge-invariant values, RPHSY length form values, and RPHS velocity form values.

		Upper	Relativistic QDO results							Relativistic SQDT results							Others
Z	Ion	level	c_i	δ'_i	c_f	δ'_f	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
3	Li	$2p\ ^2P_{1/2}$	0	0.411 449	0	0.040 593	0.2608	0.2608	0.2608	0	0.419 824	0	0.051 196	0.2584	0.2584	0.2584	0.2472[a]
		$2p\ ^2P_{3/2}$			0	0.040 596	0.5217	0.5217	0.5217			0	0.051 196	0.5167	0.5168	0.5168	0.4943
		$3p\ ^2P_{1/2}$			0	0.044 274	0.0016	0.0016	0.0016			0	0.051 196	0.0014	0.0014	0.0014	0.0014[b]
		$3p\ ^2P_{3/2}$			0	0.044 287	0.0031	0.0031	0.0031			0	0.051 196	0.0028	0.0028	0.0028	0.0028
4	Be^{1+}	$2p\ ^2P_{1/2}$	0	0.271 233	0	0.045 844	0.1728	0.1728	0.1728	0	0.274 018	0	0.050 401	0.1713	0.1713	0.1713	0.1647[a]
		$2p\ ^2P_{3/2}$			0	0.045 842	0.3457	0.3457	0.3457			0	0.050 401	0.3427	0.3427	0.3427	0.3294
		$3p\ ^2P_{1/2}$			0	0.048 344	0.0271	0.0271	0.0271			0	0.050 401	0.0267	0.0267	0.0267	0.0267[b]
		$3p\ ^2P_{3/2}$			0	0.048 397	0.0542	0.0542	0.0542			0	0.050 401	0.0534	0.0534	0.0534	0.0533
5	B^{2+}	$2p\ ^2P_{1/2}$	0	0.203 114	0	0.041 692	0.1253	0.1253	0.1253	0	0.206 081	0	0.047 092	0.1233	0.1233	0.1233	0.1202[a]
		$2p\ ^2P_{3/2}$			0	0.041 682	0.2509	0.2509	0.2509			0	0.047 092	0.2468	0.2468	0.2468	0.2406
		$3p\ ^2P_{1/2}$			0	0.043 078	0.0502	0.0502	0.0502			0	0.047 092	0.0503	0.0503	0.0503	0.0498[b]
		$3p\ ^2P_{3/2}$			0	0.043 198	0.1004	0.1005	0.1005			0	0.047 092	0.1005	0.1005	0.1005	0.1000
6	C^{3+}	$2p\ ^2P_{1/2}$	0	0.162 531	0	0.036 830	0.0976	0.0976	0.0977	0	0.163 040	0	0.040 430	0.0952	0.0952	0.0952	0.0941[a]
		$2p\ ^2P_{3/2}$			0	0.036 813	0.1956	0.1957	0.1957			0	0.040 430	0.1907	0.1907	0.1907	0.1886
		$3p\ ^2P_{1/2}$			0	0.037 463	0.0666	0.0666	0.0666			0	0.040 430	0.0675	0.0675	0.0675	0.0661[b]
		$3p\ ^2P_{3/2}$			0	0.037 676	0.1332	0.1332	0.1332			0	0.040 430	0.1347	0.1348	0.1348	0.1323
7	N^{4+}	$2p\ ^2P_{1/2}$	0	0.135 537	0	0.032 601	0.0798	0.0798	0.0798	0	0.135 031	0	0.035 302	0.0772	0.0773	0.0773	0.0772[a]
		$2p\ ^2P_{3/2}$			0	0.032 575	0.1601	0.1601	0.1602			0	0.035 302	0.1551	0.1551	0.1551	0.1551
		$3p\ ^2P_{1/2}$			0	0.032 744	0.0784	0.0784	0.0783			0	0.035 302	0.0797	0.0796	0.0796	0.0779[b]
		$3p\ ^2P_{3/2}$			0	0.033 077	0.1567	0.1567	0.1567			0	0.035 302	0.1590	0.1590	0.1590	0.1557
8	O^{5+}	$2p\ ^2P_{1/2}$	0	0.116 272	0	0.029 100	0.0674	0.0674	0.0674	0	0.116 947	0	0.031 824	0.0658	0.0658	0.0658	0.0655[a]
		$2p\ ^2P_{3/2}$			0	0.029 065	0.1356	0.1356	0.1356			0	0.031 824	0.1324	0.1324	0.1324	0.1318
		$3p\ ^2P_{1/2}$			0	0.028 873	0.0871	0.0871	0.0871			0	0.031 824	0.0880	0.0879	0.0879	0.0866[b]
		$3p\ ^2P_{3/2}$			0	0.029 353	0.1741	0.1741	0.1741			0	0.031 824	0.1754	0.1754	0.1754	0.1732
9	F^{6+}	$2p\ ^2P_{1/2}$	0	0.101 828	0	0.026 215	0.0583	0.0583	0.0583	0	0.100 097	0	0.026 430	0.0568	0.0568	0.0569	0.0568[a]
		$2p\ ^2P_{3/2}$			0	0.026 171	0.1177	0.1177	0.1177	0		0	0.026 430	0.1147	0.1148	0.1148	0.1147
		$3p\ ^2P_{1/2}$			0	0.025 660	0.0938	0.0937	0.0937			0	0.026 430	0.0950	0.0950	0.0950	0.0933[b]
		$3p\ ^2P_{3/2}$			0	0.026 313	0.1874	0.1875	0.1874			0	0.026 430	0.1893	0.1894	0.1894	0.1865
10	Ne^{7+}	$2p\ ^2P_{1/2}$	0	0.090 592	0	0.023 815	0.0513	0.0514	0.0514	0	0.091 970	0	0.026 704	0.0502	0.0502	0.0503	0.0502[a]
		$2p\ ^2P_{3/2}$			0	0.023 763	0.1041	0.1042	0.1042			0	0.026 704	0.1018	0.1019	0.1019	0.1018
		$3p\ ^2P_{1/2}$			0	0.023 794	0.0994	0.0994	0.0993			0	0.026 704	0.0999	0.0998	0.0998	0.0990[b]
		$3p\ ^2P_{3/2}$			0	0.024 648	0.1986	0.1987	0.1987			0	0.026 704	0.1987	0.1988	0.1988	0.1981
18	Ar^{15+}	$2p\ ^2P_{1/2}$	0	0.048 329	0	0.013 591	0.0263	0.0264	0.0264	0	0.047 609	0	0.013 507	0.0260	0.0261	0.0261	0.0260[a]
		$2p\ ^2P_{3/2}$			0	0.013 461	0.0582	0.0583	0.0584			0	0.013 507	0.0575	0.0576	0.0577	0.0575
		$3p\ ^2P_{1/2}$			0	0.008 261	0.1176	0.1174	0.1173			0	0.013 507	0.1205	0.1203	0.1202	0.1200[c]
		$3p\ ^2P_{3/2}$			0	0.011 689	0.2342	0.2348	0.2346			0	0.013 507	0.2365	0.2371	0.2369	0.2360
20	Ca^{17+}	$2p\ ^2P_{1/2}$	0	0.043 336		0.012 254	0.0235	0.0236	0.0236	0	0.042 756	0	0.012 242	0.0232	0.0233	0.0234	0.0232
		$2p\ ^2P_{3/2}$			0	0.012 102	0.0540	0.0541	0.0542			0	0.012 242	0.0534	0.0535	0.0536	0.0534
		$3p\ ^2P_{1/2}$			0	0.012 389	0.1228	0.1225	0.1224			0	0.012 242	0.1229	0.1226	0.1225	0.1223[d]
		$3p\ ^2P_{3/2}$			0	0.012 255	0.2399	0.2406	0.2404			0	0.012 242	0.2401	0.2409	0.2406	0.2386
21	Sc^{18+}	$2p\ ^2P_{1/2}$	0	0.041 218	0	0.011 679	0.0223	0.0224	0.0224	0	0.040 658	0	0.011 619	0.0221	0.0222	0.0222	0.0221[a]
		$2p\ ^2P_{3/2}$			0	0.011 517	0.0523	0.0525	0.0526			0	0.011 619	0.0519	0.0520	0.0521	0.0519
		$3p\ ^2P_{1/2}$			0	0.011 772	0.1238	0.1235	0.1234			0	0.011 619	0.1239	0.1236	0.1235	0.1234[d]
		$3p\ ^2P_{3/2}$			0	0.011 652	0.2413	0.2421	0.2419			0	0.011 619	0.2415	0.2423	0.2420	0.2401
22	Ti^{19+}	$2p\ ^2P_{1/2}$	0	0.039 302	0	0.011 150	0.0212	0.0213	0.0213	0	0.038 722	0	0.011 078	0.0210	0.0211	0.0212	0.0210[a]
		$2p\ ^2P_{3/2}$			0	0.010 982	0.0510	0.0511	0.0512			0	0.011 078	0.0506	0.0507	0.0508	0.0506
		$3p\ ^2P_{1/2}$			0	0.011 324	0.1248	0.1245	0.1244			0	0.011 078	0.1248	0.1245	0.1244	0.1244[d]

TABLE I. (Continued).

		Upper	Relativistic QDO results							Relativistic SQDT results							Others
Z	Ion	level	c_i	δ'_i	c_f	δ'_f	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
		$3p\ ^2P_{3/2}$			0	0.011 090	0.2424	0.2434	0.2431			0	0.011 078	0.2426	0.2436	0.2433	0.2413
23	V^{20+}	$2p\ ^2P_{1/2}$	0	0.037 563	0	0.010 673	0.0202	0.0203	0.0204	0	0.036 983	0	0.010 613	0.0201	0.0202	0.0202	0.0200[a]
		$2p\ ^2P_{3/2}$			0	0.010 491	0.0499	0.0501	0.0502			0	0.010 613	0.0495	0.0496	0.0497	0.0495
		$3p\ ^2P_{1/2}$			0	0.010 807	0.1257	0.1253	0.1251			0	0.010 613	0.1257	0.1254	0.1252	0.1252[d]
		$3p\ ^2P_{3/2}$			0	0.010 578	0.2434	0.2445	0.2441			0	0.010 613	0.2436	0.2447	0.2444	0.2423
24	Cr^{21+}	$2p\ ^2P_{1/2}$	0	0.035 976	0	0.010 230	0.0193	0.0194	0.0195	0	0.035 396	0	0.010 134	0.0192	0.0193	0.0194	0.0192[a]
		$2p\ ^23_{/2}$			0	0.010 036	0.0490	0.0492	0.0493			0	0.010 134	0.0487	0.0489	0.0490	0.0487
		$3p\ ^2P_{1/2}$			0	0.010 598	0.1266	0.1262	0.1260			0	0.010 134	0.1265	0.1261	0.1259	0.1261[d]
		$3p\ ^2P_{3/2}$			0	0.010 063	0.2441	0.2453	0.2449			0	0.010 134	0.2444	0.2455	0.2452	0.2430
25	Mn^{22+}	$2p\ ^2P_{1/2}$	0	0.034 524	0	0.009 820	0.0185	0.0186	0.0187	0	0.034 064	0	0.009 808	0.0184	0.0186	0.0186	0.0184[a]
		$2p\ ^2P_{3/2}$			0	0.009 613	0.0484	0.0485	0.0487			0	0.009 808	0.0481	0.0483	0.0484	0.0481
		$3p\ ^2P_{1/2}$			0	0.009 901	0.1271	0.1267	0.1265			0	0.009 808	0.1271	0.1267	0.1265	0.1268[d]
		$3p\ ^2P_{3/2}$			0	0.009 685	0.2448	0.2461	0.2457			0	0.009 808	0.2449	0.2462	0.2458	0.2437
26	Fe^{22+}	$2p\ ^2P_{1/2}$	0	0.033 189	0	0.009 446	0.0177	0.0179	0.0179	0	0.032 944	0	0.009 646	0.0177	0.0178	0.0179	0.0177[a]
		$2p\ ^2P_{3/2}$			0	0.009 228	0.0479	0.0481	0.0482			0	0.009 646	0.0476	0.0478	0.0479	0.0476
		$3p\ ^2P_{1/2}$			0	0.010 684	0.1284	0.1279	0.1277			0	0.009 646	0.1277	0.1273	0.1271	0.1280[c]
		$3p\ ^2P_{3/2}$			0	0.018 457	0.2544	0.2559	0.2554			0	0.009 646	0.2453	0.2467	0.2462	0.2450
36	Kr^{33+}	$2p\ ^2P_{1/2}$	0	0.024 124	0	0.006 838	0.0127	0.0129	0.0130	0	0.022 558	0	0.005 815	0.0127	0.0129	0.0130	0.0127[a]
		$2p\ ^2P_{3/2}$			0	0.006 499	0.0501	0.0504	0.0507			0	0.005 815	0.0498	0.0502	0.0504	0.0501
		$3p\ ^2P_{1/2}$			0	0.006 102	0.1318	0.1308	0.1304			0	0.005 815	0.1322	0.1313	0.1309	0.1350[e]
		$3p\ ^2P_{3/2}$			0	0.005 880	0.2428	0.2456	0.2447			0	0.005 815	0.2438	0.2466	0.2457	0.2490
40	Zr^{37+}	$2p\ ^2P_{1/2}$	0	0.022 610	0	0.006 900	0.0114	0.0117	0.0117	0	0.021 509	0	0.006 395	0.0115	0.0117	0.0118	0.0115[a]
		$2p\ P^2P_{3/2}$			0	0.006 100	0.0543	0.0548	0.0552			0	0.006 395	0.0535	0.0540	0.0543	0.0538
		$3p\ ^2P_{1/2}$			0	0.006 900	0.1331	0.1319	0.1314			0	0.006 395	0.1331	0.1319	0.1314	0.1330[f]
		$3p\ ^2P_{3/2}$			0	0.006 100	0.2396	0.2431	0.2420			0	0.006 395	0.2402	0.2437	0.2426	0.2400
42	Mo^{39}	$2p\ ^2P_{1/2}$	0	0.020 900	0	0.005 899	0.0109	0.0111	0.0112	0	0.020 233	0	0.005 873	0.0109	0.0111	0.0112	0.0109[a]
		$2p\ ^2P_{3/2}$			0	0.005 482	0.0559	0.0565	0.0569			0	0.005 873	0.0556	0.0562	0.0567	0.0561
		$3p\ ^2P_{1/2}$			0	0.004 952	0.1331	0.1318	0.1312			0	0.005 873	0.1336	0.1323	0.1317	0.1330[c]
		$3p\ ^2P_{3/2}$			0	0.003 992	0.2368	0.2406	0.2394			0	0.005 873	0.2384	0.2422	0.2410	0.2380
70	Yb^{67+}	$2p\ ^2P_{1/2}$	0	0.015 350	0	0.005 500	0.0065	0.0070	0.0072	0	0.014 851	0	0.005 944	0.0068	0.0073	0.0075	0.0068[a]
		$2p\ ^2P_{3/2}$			0	0.003 500	0.1166	0.1201	0.1231			0	0.004 094	0.1181	0.1216	0.1247	0.1181
		$3p\ ^2P_{1/2}$			0	0.005 500	0.1359	0.1317	0.1300			0	0.005 944	0.1354	0.1313	0.1295	0.1350[f]
		$3p\ ^2P_{3/2}$			0	0.003 500	0.1866	0.1965	0.1924			0	0.004 094	0.1852	0.1951	0.1911	0.1820
74	W^{71+}	$2p\ ^2P_{1/2}$	0	0.014 284	0	0.004 655	0.0063	0.0068	0.0070	0	0.013 044	0	0.004 592	0.0065	0.0070	0.0072	0.0065[a]
		$2p\ ^2P_{3/2}$			0	0.003 670	0.1277	0.1319	0.1357			0	0.002 079	0.1315	0.1359	0.1398	0.1315
		$3p\ ^2P_{1/2}$			0	0.003 621	0.1353	0.1306	0.1287			0	0.004 592	0.1356	0.1308	0.1288	0.1360[c]
		$3p\ ^2P_{3/2}$			0	0.002 093	0.1760	0.1868	0.1822			0	0.002 079	0.1749	0.1857	0.1811	0.1760
92	U^{89+}	$2p\ ^2P_{1/2}$	0	0.012 979	0	0.003 489	0.0056	0.0064	0.0067	0	0.010 251	0	0.003 627	0.0052	0.0059	0.0062	0.0052[a]
		$2p\ ^2P_{3/2}$			0	0.001 727	0.1993	0.2092	0.2197			0	0.000 424	0.2020	0.2120	0.2227	0.2076
		$3p\ ^2P_{1/2}$			0	0.000 409	0.1331	0.1251	0.1217			0	0.003 627	0.1349	0.1267	0.1234	0.1350[c]
		$3p\ ^2P_{3/2}$			0	0.002 689	0.1200	0.1341	0.1263			0	0.000 424	0.1216	0.1358	0.1280	0.1210

[a] Theodosiou, Curtis, and El-Mekki, Ref. [39].

[b] Lindgård and Nielsen, Ref. [28].

[c] Armstrong, Fielder and Lin, Ref. [37].

[d] Zhu, Pan, and Zeng, Ref. [43].

[e] Martin and Wiese, Ref. [66].

[f] Anderson *et al.*, Ref. [64].

C. Oscillator strength database

In all tables given below, we have included, for comparative purposes, together with the relativistic PHSY values, some experimental or theoretical data that we find relevant to our analysis. The cited data have been selected according to the following criteria.

(i) For available experimental data deduced from lifetimes, the choice has been restricted, as much as possible, to studies reported recently. It is well established that beam-foil

TABLE II. Experimental and our theoretical oscillator strengths for $2s\ ^2S-2p\ ^2P$ transitions in the Li isoelectronic sequence. The numbers in parentheses denote errors.

Z	Ion	Upper level	Experiment	DQDO	DSQDT
3	Li	$2p\ ^2P_{1/2}$	0.2472(4)[a]	0.2608	0.2584
		$2p\ ^2P_{3/2}$	0.4944(8)	0.5217	0.5167
6	C^{3+}	$2p\ ^2P_{1/2}$	0.0980(23)[b]	0.0976	0.0952
		$2p\ ^2P_{3/2}$	0.1948(52)	0.1956	0.1907
7	Ni^{4+}	$2p\ ^2P_{1/2}$	0.0752(37)[c]	0.0798	0.0772
		$2p\ ^2P_{3/2}$	0.1475(71)	0.1601	0.1551
8	O^{5+}	$2p\ ^2P_{1/2}$	0.0643(26)[d]	0.0674	0.0658
		$2p\ ^2P_{3/2}$	0.1293(52)	0.1356	0.1324
9	F^{6+}	$2p\ ^2P_{1/2}$	0.0583(26)[e]	0.0583	0.0568
		$2p\ ^2P_{3/2}$	0.1146(51)	0.1177	0.1147
10	Ne^{7+}	$2p\ ^2P_{1/2}$	0.0486(23)[b]	0.0513	0.0502
		$2p\ ^2P_{3/2}$	0.0957(46)	0.1041	0.1018
26	Fe^{23+}	$2p\ ^2P_{1/2}$	0.0177(6)[f]	0.0177	0.0177
		$2p\ ^2P_{3/2}$	0.0470(20)	0.0479	0.0476
36	Kr^{33+}	$2p\ ^2P_{1/2}$	0.0142(13)[g]	0.0127	0.0127
		$2p\ ^2P_{3/2}$	0.0478(28)	0.0501	0.0498

[a] Gaupp, Kuske, and Andrä, Ref. [59].
[b] Knystautas *et al.*, Ref. [67].
[c] Kernahan, Livingston, and Pinnington, Ref. [69].
[d] Pinnington *et al.*, Ref. [69].
[e] Barrette *et al.*, Ref. [70].
[f] Dietrich *et al.*, Ref. [71].
[g] Dietrich *et al.*, Ref. [72].

spectroscopy (BFS) is a general way to perform measurements of atomic lifetimes. However, there seems to exist the tendency to overestimate the ns-np BFS lifetimes, which can be attributed to the heavy repopulation of the np levels by cascades from higher-lying levels [57]. Although this problem may be handled with the beam-foil technique itself, a much more accurate way to analyze heavy cascade decays is provided by the so-called arbitrary normalized decay curve or method. This method suggested by Curtis, Berry, and Bromander [58] exploits dynamical correlations among cascade-related decay curves to reliably extract lifetimes [41]. Precision measurements are also made by laser excitation methods such as the fast-beam laser [59] and time-resolved laser spectroscopy [60] that either exclude or properly account for cascading repopulation.

(ii) Theoretical data have been restricted, as much as possible, to studies that consider rather long isoelectronic sequences and give separate f values for the different fine-structure transitions. In addition, we have distinguished two types of theoretical calculations.

(a) *Ab initio* calculations are very elaborate theoretical calculations that include leading terms of correlation, relativistic, and QED corrections. Many of these calculations have been made for the sequences considered here using Dirac-Fock calculations [43,48,49,61–64]. These methods treat the fine structure of np in a fully relativistic manner, which is very important at high stages of ionization. However, they do not adequately describe correlation effects and show some discrepancies with experiment [2,45]. There is a tendency for *ab initio* calculations to systematically slightly overestimate f values. These discrepancies have been removed by RMBPT and MCDF calculations of Guet, Blundell, and Johnson [65] and Baik *et al.* [62], respectively, in the case of Na-like ions.

(b) *Semiempirical methods* provide the means for investigating the accuracy and consistency of theoretical and experimental results. They also provide a data set with higher accuracy than that of any single point. A recent reliable semiempirical prediction of f values using the Coulomb approximation with a Hartree-Slater core (CAHS) has been made by Theodosiou and Curtis. Their calculations cover most of the Li-like [39], Na-like [45], and Cu-like [53] transitions studied by us. This method involves the integration of the Schrödinger equation with a realistic model potential, i.e., a potential that has parameters adjusted to fit the observed energy. CAHS results agree more closely with experimental values, in general, than do results using *ab initio* methods. Another reliable semiempirical f values are numerical Coulomb approximation (NCA) results of Lindgård and co-workers [28,55]. NCA wave functions were computed by *inward* integration of the radial Schrödinger equation from the asymptotic region to a distance determined by

TABLE III. Our oscillator strengths compared with Dirack-Fock calculations for $2s\ ^2S-n'p\ ^2P_{1/2}$ (first entry) and $2s\ ^2S-n'p\ ^2P_{3/2}$ (second entry) transitions of Ca^{17+}, Zr^{37+}, and Yb^{67+} of the Li isoelectronic sequence, with the same meaning as in Table I.

			Relativistic QDO results			Relativistic SQDT results			EXT^{a}	DF
Z	Ion	n'	f	f_L	f_V	f	f_L	f_V	f	f
20	Ca^{17+}	4	0.030 762	0.030 661	0.030 667	0.030 806	0.030 705	0.030 711	0.031 325	
		4	0.060 609	0.060 697	0.060 706	0.060 740	0.060 826	0.060 837	0.061 979	
		6	0.006 658	0.006 630	0.006 637	0.006 664	0.006 636	0.006 643	0.006 681	
		6	0.013 184	0.013 187	0.013 200	0.013 203	0.013 205	0.013 218	0.013 249	
		8	0.002 537	0.002 525	0.002 529	0.002 539	0.002 528	0.002 531	0.002 540	0.002 533^{b}
		8	0.005 032	0.005 031	0.005 037	0.005 038	0.005 037	0.005 043	0.005 041	
		9	0.001 734	0.001 726	0.001 729	0.001 736	0.001 728	0.001 730	0.001 736	0.001 73^{c}
		9	0.003 442	0.003 441	0.003 445	0.003 446	0.003 444	0.003 449	0.003 446	
		10	0.001 240	0.001 235	0.001 237	0.001 241	0.001 236	0.001 238	0.001 241	0.001 238^{c}
		10	0.002 462	0.002 461	0.002 465	0.002 465	0.002 464	0.002 467	0.002 464	
		11	0.000 919	0.000 915	0.000 916	0.000 920	0.000 915	0.000 917	0.000 919	0.000 916^{c}
		11	0.001 825	0.001 824	0.001 826	0.001 826	0.001 825	0.001 828	0.001 825	
		12	0.000 700	0.000 697	0.000 698	0.000 701	0.000 697	0.000 699	0.000 700	0.000 698^{c}
		12	0.001 391	0.001 390	0.001 392	0.001 392	0.001 391	0.001 393	0.001 391	
		13	0.000 546	0.000 544	0.000 544	0.000 547	0.000 544	0.000 545	0.000 546	0.000 544^{c}
		13	0.001 085	0.001 084	0.001 086	0.001 086	0.001 085	0.001 087	0.001 085	
		16	0.000 288	0.000 287	0.000 287	0.000 288	0.000 287	0.000 287	0.000 288	0.000 288^{b}
		16	0.000 573	0.000 572	0.000 573	0.000 573	0.000 573	0.000 574	0.000 573	
		18	0.000 201	0.000 200	0.000 200	0.000 201	0.000 200	0.000 201	0.000 201	
		18	0.000 400	0.000 399	0.000 400	0.000 400	0.000 400	0.000 400	0.000 399	
		20	0.000 146	0.000 145	0.000 145	0.000 146	0.000 145	0.000 146	0.000 146	
		20	0.000 290	0.000 290	0.000 290	0.000 290	0.000 290	0.000 290	0.000 290	
40	Zr^{37+}	4	0.032 184	0.031 723	0.031 775	0.032 188	0.031 727	0.031 779	0.032 122	0.0322^{c}
		4	0.060 502	0.060 882	0.060 936	0.060 589	0.060 968	0.061 023	0.061 457	
		6	0.006 824	0.006 700	0.006 738	0.006 825	0.006 701	0.006 739	0.006 793	0.006 81^{c}
		6	0.013 122	0.013 128	0.013 191	0.013 133	0.013 139	0.013 203	0.013 130	
		8	0.002 582	0.002 532	0.002 550	0.002 583	0.002 532	0.002 550	0.002 574	0.002 569^{a}
		8	0.005 002	0.004 994	0.005 025	0.005 005	0.004 997	0.005 028	0.004 993	
		9	0.001 762	0.001 727	0.001 740	0.001 762	0.001 727	0.001 740	0.001 757	
		9	0.003 420	0.003 413	0.003 435	0.003 422	0.003 415	0.003 437	0.003 412	
		10	0.001 258	0.001 233	0.001 242	0.001 258	0.001 233	0.001 243	0.001 255	0.001 251^{c}
		10	0.002 446	0.002 440	0.002 456	0.002 447	0.002 441	0.002 458	0.002 440	
		11	0.000 931	0.000 912	0.000 919	0.000 931	0.000 912	0.000 919	0.000 929	
		11	0.001 812	0.001 807	0.001 819	0.001 813	0.001 808	0.001 820	0.001 807	
		12	0.000 709	0.000 694	0.000 700	0.000 709	0.000 694	0.000 700	0.000 708	
		12	0.001 381	0.001 376	0.001 386	0.001 381	0.001 377	0.001 387	0.001 377	
		13	0.000 552	0.000 541	0.000 545	0.000 552	0.000 541	0.000 546	0.000 552	
		13	0.001 077	0.001 073	0.001 081	0.001 077	0.001 074	0.001 082	0.001 074	
		16	0.000 291	0.000 285	0.000 287	0.000 291	0.000 285	0.000 287	0.000 291	0.000 289^{b}
		16	0.000 568	0.000 566	0.000 570	0.000 568	0.000 566	0.000 571	0.000 567	
		18	0.000 203	0.000 199	0.000 200	0.000 203	0.000 199	0.000 200	0.000 203	
		18	0.000 396	0.000 395	0.000 398	0.000 397	0.000 395	0.000 398	0.000 395	
		20	0.000 147	0.000 144	0.000 145	0.000 147	0.000 144	0.000 145	0.000 147	0.000 143^{c}
		20	0.000 288	0.000 286	0.000 289	0.000 288	0.000 287	0.000 289	0.000 287	
70	Yb^{67+}	4	0.031 842	0.030 299	0.030 479	0.031 765	0.030 220	0.030 396	0.031 079	
		4	0.050 768	0.052 083	0.051 916	0.050 511	0.051 829	0.051 651	0.053 262	
		6	0.006 592	0.006 192	0.006 313	0.006 579	0.006 178	0.006 298	0.006 504	
		6	0.011 375	0.011 455	0.011 561	0.011 328	0.011 410	0.011 514	0.011 539	
		8	0.002 468	0.002 308	0.002 364	0.002 463	0.002 303	0.002 359	0.002 449	
		8	0.004 370	0.004 372	0.004 432	0.004 353	0.004 356	0.004 415	0.004 399	
		9	0.001 678	0.001 567	0.001 608	0.001 675	0.001 564	0.001 604	0.001 668	
		9	0.002 992	0.002 989	0.003 033	0.002 981	0.002 978	0.003 022	0.003 007	

TABLE III. (continued).

			Relativistic QDO results			Relativistic SQDT results			EXT[a]	DF
Z	Ion	n'	f	f_L	f_V	f	f_L	f_V	f	f
		10	0.001 195	0.001 115	0.001 145	0.001 193	0.001 113	0.001 142	0.001 189	
		10	0.002 142	0.002 137	0.002 171	0.002 134	0.002 130	0.002 163	0.002 150	
		11	0.000 882	0.000 823	0.000 845	0.000 880	0.000 821	0.000 843	0.000 879	
		11	0.001 588	0.001 583	0.001 609	0.001 582	0.001 577	0.001 603	0.001 593	
		12	0.000 670	0.000 625	0.000 642	0.000 669	0.000 624	0.000 641	0.000 668	
		12	0.001 211	0.001 206	0.001 226	0.001 206	0.001 201	0.001 221	0.001 213	
		13	0.000 522	0.000 486	0.000 500	0.000 521	0.000 485	0.000 499	0.000 520	
		13	0.000 944	0.000 940	0.000 956	0.000 941	0.000 937	0.000 953	0.000 946	
		16	0.000 274	0.000 255	0.000 262	0.000 273	0.000 254	0.000 262	0.000 273	
		16	0.000 498	0.000 496	0.000 505	0.000 497	0.000 494	0.000 503	0.000 499	
		18	0.000 191	0.000 177	0.000 183	0.000 190	0.000 177	0.000 182	0.000 190	
		18	0.000 348	0.000 346	0.000 352	0.000 346	0.000 344	0.000 351	0.000 348	
		20	0.000 138	0.000 128	0.000 132	0.000 138	0.000 128	0.000 132	0.000 138	
		20	0.000 252	0.000 251	0.000 255	0.000 251	0.000 250	0.000 254	0.000 252	

[a] Zilitis, Ref. [44].

[b] Guet, Ref. [63].

[c] Anderson *et al.*, Ref. [64].

the strength of the divergence at the origin. For Rydberg state of Li-like ions, Zilitis [44] used a simple analytical formula, obtained by extrapolating the cross section (EXT) into the region of discrete spectra, to calculate easily and quite accurately f values. Our results will mainly be compared with those of the CAHS ($\Delta n=0$), NCA ($\Delta n=1$), and EXT ($\Delta n\geqslant 2$), not only because of the above observations, but also because we used the same input energies.

D. Results and discussion

It is worth pointing out, on the one hand, that the RQDO calculations derived in this paper yield for $c=0$ exactly the same f values obtained by Martin *et al.* [19] using Edlén's energy data for sodiumlike ions. However, for $Z=11,12$, despite the use of the same energy inputs, the identity of our RQDO values with those of Martin *et al.* is curiously obtained rather for $c=1$. The differences are, respectively, about 37% ($Z=11$) and 7% ($Z=12$) for $c=0$. On the other hand, the reader should keep in mind that the comparison of our results with other theoretical calculations and/or experiments refers to the input energies used by us and succinctly presented above.

All f results displayed in Tables I and II have been obtained with $c=0$. As a consequence, the relativistic EOQN f results have not been reported because they are identical to the relativistic QDO ones. Therefore, all the results to be reported in the following concerning the QDO procedure for $c=0$ will also be valid for EOQN whatever the sequence.

The DPHSY f results given in all tables are, as already mentioned in Sec. II, gauge invariant, whereas the RPHSY f results are given in the length and velocity form. Let

$$d(n,n')=\frac{|f_{\mathrm{PHSY}}-f_{\mathrm{RD}}|}{f_{\mathrm{RD}}}\times 100$$

be a measure of the difference between our results (PHSY) with the reference data (RD) for ns-$n'p$ transitions. ($n'=n,\ n+1$). Plots of $d(n,n)$ against Z are displayed in Figs. 1–9. Reference data considered are CAHS values.

When cross examining these figures together with Tables I, II, and IV–VII, a few relevant features become apparent, including the following.

(a) The DSQDT f values, with the exception of a few, agree with reference data within 1% in the three sequences (see Figs. 1–3). The magnitude of $d(n,n+1)$ seems to be larger than that of $d(n,n)$. One also sees that the accuracy of DSQDT f results decreases from lithium-like ions to copper-like ions, i.e., with the growth of the number of remaining electrons. However, the discrepancies remained within a few percent.

(b) Figures 4–6 clearly show that the same tendencies are observed for the DEOQN and the DQDO results with, however, more marked divergences. Indeed, if the DEOQN f values are close to reference data (within 8%; see Fig. 7) for Li-like ions, $d(n,n')$ increases as the number of remaining electrons increases, with drastic discrepancies occurring in $\Delta n=1$ transitions. For this type of transition, the DEOQN and the DQDO approaches are in error for neutral end elements. As Z increases, the divergence decreases such that the agreement becomes reasonable for high-Z elements. For transitions with $c=\langle\delta'\rangle\neq 0$, one observes, comparing DQDO f results with their DEOQN equivalents, a substantial improvement in DQDO values that reduced until it got to half the magnitude of $d(n,n')$ (see Figs. 8 and 9). It then clearly appears that the DQDO procedure is more effective than the DEOQN one.

(c) If in Tables II, V, and VII, for resonance lines, the DQDO and the DEOQN calculations seem in general to agree well with experimental values; the DSQDT f values, do so best with agreement within experimental error limits.

(d) Switching our attention to the RPHSY results, one sees that each of them is in general less accurate than its corresponding DPHSY, whatever the sequence considered. In fact, in the Li sequence, the high-Z elements, the RPHSY

TABLE IV. Our oscillator strengths compared with other selected calculations for $3s\ ^2S-3p\ ^2P$ transitions in the Na isoelectronic sequence, with the same meaning as in Table I.

		Upper	Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	level	c_i	δ_i'	c_f	δ_f'	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
11	Na	$3p\ ^2P_{1/2}$	1	1.372 82	1	0.882 566	0.3317	0.3317	0.3317	0.2705	0.2097	0.2097	1	1.1512 339	1	0.978 340	0.3188	0.3188	0.3188	0.3180[a]
		$3p\ ^2P_{3/2}$			1	0.882 579	0.6633	0.6633	0.6633	0.5411	0.4194	0.4194			1	0.978 340	0.6376	0.6376	0.6376	0.6365
		$4p\ ^2P_{1/2}$			1	0.866 569	0.0019	0.0019	0.0019	0.0145	0.0130	0.0130			1	0.978 340	0.0051	0.0051	0.0051	0.0051[b]
		$4p\ ^2P_{3/2}$			1	0.866 583	0.0037	0.0037	0.0037	0.0289	0.0260	0.0260			1	0.978 340	0.0102	0.0102	0.0102	0.0102
12	Mg^{1+}	$3p\ ^2P_{4/2}$	1	1.097 391	1	0.734 205	0.2931	0.2931	0.2931	0.2847	0.2728	0.2728	1	1.346 564	1	0.914 289	0.3063	0.3063	0.3063	0.3043[a]
		$3p\ ^2P_{3/2}$			1	0.734 258	0.5862	0.5862	0.5863	0.5694	0.5456	0.5456			1	0.914 289	0.6127	0.6127	0.6127	0.6103
		$4p\ ^2P_{1/2}$			1	0.712 536	0.0056	0.0056	0.0056	0.0039	0.0043	0.0043			1	0.914 289	0.0000	0.0000	0.0000	0.0000[b]
		$4p\ ^2P_{3/2}$			1	0.712 590	0.0111	0.0111	0.0111	0.0078	0.0085	0.0085			1	0.914 289	0.0001	0.0001	0.0001	0.0001
14	Si^{3+}	$3p\ ^2P_{1/2}$	1	0.740 804	0	0.460 611	0.2729	0.2729	0.2729	0.2930	0.2929	0.2930	0	0.623 451	0	0.401 708	0.2539	0.2539	0.2539	0.2552[a]
		$3p\ ^2P_{3/2}$				0.460 824	0.5457	0.5458	0.5458	0.5860	0.5859	0.5859			0	0.401 708	0.5088	0.5088	0.5088	0.5142
		$4p\ ^2P_{1/2}$			0	0.261 731	0.0121	0.0121	0.0121	0.0109	0.0109	0.0109			0	0.401 708	0.0093	0.0092	0.0092	0.0093[b]
		$4p\ ^2P_{3/2}$			0	0.261 944	0.0241	0.0241	0.0241	0.0219	0.0219	0.0219			0	0.401 708	0.0183	0.0183	0.0183	0.0185
16	S^{5+}	$3p\ ^2P_{1/2}$	1	0.640 839	0	0.442 549	0.2108	0.2108	0.2108	0.2273	0.2273	0.2273	0	0.498 357	0	0.319 414	0.2183	0.2183	0.2183	0.2163[a]
		$3p\ ^2P_{3/2}$			0	0.440 352	0.4266	0.4266	0.4267	0.4602	0.4602	0.4602			0	0.319 414	0.4385	0.4385	0.4385	0.4384
		$4p\ ^2P_{1/2}$			0	0.421 304	0.0043	0.0043	0.0043	0.0093	0.0093	0.0093			0	0.319 414	0.0231	0.0230	0.0230	0.0227[b]
		$4p\ ^2P_{3/2}$			0	0.421 784	0.0086	0.0086	0.0086	0.0185	0.0185	0.0185			0	0.319 414	0.0456	0.0456	0.0455	0.0455
17	Cl^{6+}	$3p\ ^2P_{1/2}$	1	0.582 971	0	0.403 416	0.1957	0.1958	0.1958	0.2118	0.2118	0.2119	0	0.470 759	0	0.308 075	0.2010	0.2011	0.2011	0.2010[a]
		$3p\ ^2P_{3/2}$			0	0.400 985	0.3796	0.3977	0.3977	0.4306	0.4306	0.4306			0	0.308 075	0.4048	0.4048	0.4049	0.4090
		$4p\ ^2P_{1/2}$			0	0.382 635	0.0069	0.0069	0.0069	0.0147	0.0146	0.0146			0	0.308 075	0.0292	0.0291	0.0291	0.0292[b]
		$4p\ ^2P_{3/2}$			0	0.383 288	0.0138	0.0139	0.0139	0.0293	0.0293	0.0292			0	0.308 075	0.0576	0.0576	0.0575	0.0584
18	Ar^{7+}	$3p\ ^2P_{1/2}$	1	0.535 133	0	0.370 882	0.1825	0.1826	0.1826	0.1979	0.1979	0.1979	0	0.437 006	0	0.287 371	0.1873	0.1874	0.1874	0.1865[a]
		$3p\ ^2P_{3/2}$			0	0.368 221	0.3724	0.3724	0.3725	0.4039	0.4040	0.4040			0	0.287 371	0.3782	0.3782	0.3783	0.3813
		$4p\ ^2P_{1/2}$			0	0.350 692	0.0096	0.0096	0.0096	0.0202	0.0202	0.0201			0	0.287 371	0.0354	0.0353	0.0353	0.0353[b]
		$4p\ ^2P_{3/2}$			0	0.351 545	0.0192	0.0193	0.0192	0.0403	0.0403	0.0403			0	0.287 371	0.0696	0.0696	0.0696	0.0706
20	Ca^{9+}	$3p\ ^2P_{1/2}$	0	0.460 463	0	0.319 826	0.1742	0.1742	0.1743	0.1742	0.1742	0.1743	0	0.343 733	0	0.216 603	0.1638	0.1639	0.1639	0.1640[a]
		$3p\ ^2P_{3/2}$			0	0.316 705	0.3593	0.3594	0.3595	0.3593	0.3594	0.3595			0	0.217 103	0.3313	0.3314	0.3315	0.3388
		$4p\ ^2P_{1/2}$			0	0.301 527	0.0312	0.0311	0.0311	0.0312	0.0311	0.0311			0	0.216 603	0.0500	0.0499	0.0499	0.0500[c]
		$4p\ ^2P_{3/2}$			0	0.302 861	0.0622	0.0622	0.0622	0.0622	0.0622	0.0622			0	0.217 103	0.0986	0.0986	0.0985	0.0960
22	Ti^{11+}	$3p\ ^2P_{1/2}$	0	0.404 744	0	0.281 553	0.1552	0.1553	0.1553	0.1552	0.1553	0.1553	0	0.259 250	0	0.147 992	0.1465	0.1466	0.1467	0.1465[a]
		$3p\ ^2P_{3/2}$			0	0.277 973	0.3243	0.3244	0.3245	0.3243	0.3244	0.3245			0	0.145 336	0.3066	0.3067	0.3068	0.3065
		$4p\ ^2P_{1/2}$			0	0.270 620	0.0435	0.0433	0.0433	0.0435	0.0433	0.0433			0	0.147 992	0.0635	0.0634	0.0633	0.0639[d]
		$4p\ ^2P_{3/2}$			0	0.267 250	0.0825	0.0825	0.0824	0.0825	0.0825	0.0824			0	0.145 336	0.1217	0.1218	0.1217	0.1213
24	Cr^{13+}	$3p\ ^2P_{1/2}$	0	0.361 535	0	0.251 803	0.1397	0.1399	0.1399	0.1397	0.1399	0.1399	0	0.236 571	0	0.136 823	0.1320	0.1322	0.1322	0.1321[a]
		$3p\ ^2P_{3/2}$			0	0.247 760	0.2967	0.2968	0.2970	0.2967	0.2968	0.2970			0	0.133 833	0.2809	0.2810	0.2811	0.2808

TABLE IV. (Continued).

			Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	Upper level	c_i	δ_i'	c_f	δ_f'	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
		$4p\ ^2P_{1/2}$			0	0.241 091	0.0521	0.0519	0.0518	0.0521	0.0519	0.0518			0	0.136 823	0.0711	0.0709	0.0708	0.0723[d]
		$4p\ ^2P_{3/2}$			0	0.236 744	0.0978	0.0978	0.0977	0.0978	0.0978	0.0977			0	0.133 833	0.1353	0.1354	0.1352	0.1360
26	Fe^{15+}	$3p\ ^2P_{1/2}$	0	0.327 050	0	0.228 034	0.1270	0.1272	0.1272	0.1270	0.1272	0.1272	0	0.246 889	0	0.156 099	0.1199	0.1201	0.1202	0.1204[a]
		$3p\ ^2P_{3/2}$			0	0.223 525	0.2748	0.2749	0.2751	0.2748	0.2749	0.2751			0	0.152 577	0.2611	0.2613	0.2614	0.2610
		$4p\ ^2P_{1/2}$			0	0.217 902	0.0598	0.0595	0.0594	0.0598	0.0595	0.0594			0	0.156 099	0.0748	0.0745	0.0744	0.0756[d]
		$4p\ ^2P_{3/2}$			0	0.212 793	0.1111	0.1111	0.1110	0.1111	0.1111	0.1110			0	0.152 677	0.1406	0.1407	0.1405	0.1410
28	Ni^{17+}	$3p\ ^2P_{1/2}$	0	0.298 902	0	0.208 630	0.1164	0.1166	0.1167	0.1164	0.1166	0.1167	0	0.191 850	0	0.109 011	0.1107	0.1109	0.1110	0.1107[a]
		$3p\ ^2P_{3/2}$			0	0.203 649	0.2573	0.2575	0.2577	0.2573	0.2575	0.2577			0	0.105 511	0.2449	0.2452	0.2453	0.2453
		$4p\ ^2P_{1/2}$			0	0.198 863	0.0665	0.0661	0.0660	0.0665	0.0661	0.0660			0	0.109 011	0.0841	0.0837	0.0836	0.0854[d]
		$4p\ ^2P_{3/2}$			0	0.193 878	0.1229	0.1231	0.1228	0.1229	0.1231	0.1228			0	0.105 511	0.1575	0.1578	0.1575	0.1581
29	Co^{18+}	$3p\ ^2P_{1/2}$	0	0.286 688	0	0.200 212	0.1117	0.1119	0.1120	0.1117	0.1119	0.1120	0	0.187 646	0	0.108 881	0.1053	0.1055	0.1056	0.1063[a]
		$3p\ ^2P_{3/2}$			0	0.194 993	0.2500	0.2502	0.2504	0.2500	0.2502	0.2504			0	0.104 458	0.2383	0.2386	0.2388	0.2384
		$4p\ ^2P_{1/2}$			0	0.190 943	0.0697	0.0692	0.0691	0.0697	0.0692	0.0691			0	0.108 881	0.0868	0.0863	0.0862	0.0881[d]
		$4p\ ^2P_{3/2}$			0	0.185 680	0.1282	0.1283	0.1281	0.1282	0.1283	0.1281			0	0.104 458	0.1609	0.1612	0.1609	0.1623
30	Zn^{19+}	$3p\ ^2P_{1/2}$	0	0.275 505	0	0.192 516	0.1073	0.1076	0.1077	0.1073	0.1076	0.1077	0.	0.162 965	0	0.086 783	0.1024	0.1026	0.1027	0.1024[a]
		$3p\ ^2P_{3/2}$			0	0.187 056	0.2434	0.2437	0.2439	0.2434	0.2437	0.2439			0	0.082 468	0.2334	0.2337	0.2339	0.2333
		$4p\ ^2P_{1/2}$			0	0.183 733	0.0727	0.0722	0.0720	0.0727	0.0722	0.0720			0	0.086 783	0.0906	0.0901	0.0900	0.0907[d]
		$4p\ ^2P_{3/2}$			0	0.177 895	0.1327	0.1329	0.1326	0.1327	0.1329	0.1326			0	0.082 468	0.1678	0.1681	0.1678	0.1662
34	Se^{23+}	$3p\ ^2P_{1/2}$	0	0.238 944	0	0.167 364	0.0929	0.0932	0.0933	0.0929	0.0932	0.0933	0	0.139 805	0	0.073 790	0.0892	0.0895	0.0896	0.0892[a]
		$3p\ ^2P_{3/2}$			0	0.160 929	0.2237	0.2241	0.2244	0.2237	0.2241	0.2244			0	0.069 034	0.2153	0.2156	0.2159	0.2152
		$4p\ ^2P_{1/2}$			0	0.159 313	0.0825	0.0818	0.0815	0.0825	0.0818	0.0815			0	0.073 790	0.0988	0.0981	0.0979	0.0992[d]
		$4p\ ^2P_{3/2}$			0	0.152 676	0.1476	0.1479	0.1475	0.1476	0.1479	0.1475			0	0.069 034	0.1796	0.1800	0.1796	0.1779
38	St^{27+}	$3p\ ^2P_{1/2}$	0	0.211 561	0	0.148 497	0.0819	0.0823	0.0824	0.0819	0.0823	0.0824	0	0.158 604	0	0.100 170	0.0789	0.0792	0.0794	0.0790[a]
		$3p\ ^2P_{3/2}$			0	0.141 053	0.2122	0.2127	0.2131	0.2122	0.2127	0.2131			0	0.095 156	0.2052	0.2056	0.2060	0.2051
		$4p\ ^2P_{1/2}$			0	0.140 613	0.0901	0.0890	0.0887	0.0901	0.0890	0.0887			0	0.100 170	0.1013	0.1002	0.1000	0.1022[e]
		$4p\ ^2P_{3/2}$			0	0.133 016	0.1571	0.1575	0.1570	0.1571	0.1575	0.1570			0	0.095 156	0.1789	0.1795	0.1789	0.1786
42	Mo^{31+}	$3p\ ^2P_{1/2}$	0	0.190 659	0	0.134 206	0.0733	0.0737	0.0739	0.0733	0.0737	0.0739	0	0.131 612	0	0.079 386	0.0710	0.0714	0.0716	0.0710[a]
		$3p\ ^2P_{3/2}$			0	0.125 721	0.2067	0.2073	0.2077	0.2067	0.2073	0.2077			0	0.073 590	0.2008	0.2014	0.2019	0.2008
		$4p\ ^2P_{1/2}$			0	0.126 924	0.0964	0.0950	0.0946	0.0964	0.0950	0.0946			0	0.079 386	0.1078	0.1065	0.1061	0.1077[e]
		$4p\ ^2P_{3/2}$			0	0.118 119	0.1631	0.1638	0.1630	0.1631	0.1638	0.1630			0	0.073 590	0.1855	0.1863	0.1855	0.1828
45	Rh^{34+}	$3p\ ^2P_{1/2}$	0	0.177 249	0	0.124 808	0.0680	0.0684	0.0686	0.0680	0.0684	0.0686	0	0.128 340	0	0.079 907	0.0661	0.0665	0.0667	0.0661[a]
		$3p\ ^2P_{3/2}$			0	0.115 492	0.2058	0.2065	0.2071	0.2058	0.2065	0.2071			0	0.073 630	0.2009	0.2016	0.2021	0.2008
		$4p\ ^2P_{1/2}$			0	0.116 286	0.0995	0.0978	0.0973	0.0995	0.0978	0.0973			0	0.079 907	0.1104	0.1087	0.1083	0.0111[e]

TABLE IV. (Continued).

			Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	Upper level	c_i	δ_i'	c_f	δ_f'	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
		$4p\ ^2P_{3/2}$			0	0.106 954	0.1643	0.1652	0.1643	0.1643	0.1652	0.1643			0	0.073 630	0.1852	0.1862	0.1853	0.1841
48	Cd^{+37}	$3p\ ^2P_{1/2}$	0	0.167 066	0	0.118 117	0.0633	0.0638	0.0640	0.0633	0.0638	0.0640	0	0.105 066	0	0.060 138	0.0617	0.0622	0.0624	0.0617[a]
		$3p\ ^2P_{3/2}$			0	0.107 980	0.2069	0.2077	0.2084	0.2069	0.2077	0.2084			0	0.053 033	0.2021	0.2029	0.2036	0.2023
		$4p\ ^2P_{1/2}$			0	0.111 452	0.1038	0.1018	0.1013	0.1038	0.1018	0.1013			0	0.060 138	0.1151	0.1131	0.1126	0.1173[d]
		$4p\ ^2P_{3/2}$			0	0.100 260	0.1660	0.1670	0.1660	0.1660	0.1670	0.1660			0	0.053 033	0.1887	0.1899	0.1889	0.1894
51	Sb^{40+}	$3p\ ^2P_{1/2}$	0	0.157 848	0	0.111 881	0.0593	0.0599	0.0601	0.0593	0.0599	0.0601	0	0.099 760	0	0.057 802	0.0578	0.0584	0.0586	0.0581[a]
		$3p\ ^2P_{3/2}$			0	0.100 874	0.2102	0.2112	0.2120	0.2102	0.2112	0.2120			0	0.049 881	0.2064	0.2074	0.2082	0.2065
		$4p\ ^2P_{1/2}$			0	0.105 384	0.1068	0.1044	0.1038	0.1068	0.1044	0.1038			0	0.057 802	0.1174	0.1152	0.1145	0.1198[d]
		$4p\ ^2P_{3/2}$			0	0.092 982	0.1654	0.1666	0.1654	0.1654	0.1666	0.1654			0	0.049 881	0.1868	0.1882	0.1870	0.1880
54	Xe^{43+}	$3p\ ^2P_{1/2}$	0	0.149 930	0	0.106 560	0.0558	0.0564	0.0566	0.0558	0.0564	0.0566	0	0.085 333	0	0.045 796	0.0548	0.0554	0.0556	0.0548[a]
		$3p\ ^2P_{3/2}$			0	0.094 646	0.2153	0.2164	0.2174	0.2153	0.2164	0.2174			0	0.040 154	0.2036	0.2047	0.2056	0.2023
		$4p\ ^2P_{1/2}$			0	0.100 253	0.1094	0.1067	0.1060	0.1094	0.1067	0.1060			0	0.045 796	0.1205	0.1179	0.1172	0.1220[d]
		$4p\ ^2P_{3/2}$			0	0.087 345	0.1645	0.1660	0.1645	0.1645	0.1660	0.1645			0	0.040 154	0.1901	0.1917	0.1903	0.1855
74	W^{63+}	$3p\ ^2P_{1/2}$	0	0.118 253	0	0.086 361	0.0397	0.0407	0.0411	0.0397	0.0407	0.0411	0	0.068 580	0	0.041 193	0.0396	0.0406	0.0410	0.0396[a]
		$3p\ ^2P_{3/2}$			0	0.065 143	0.2928	0.2959	0.2988	0.2928	0.2959	0.2988			0	0.027 860	0.2867	0.2898	0.2925	0.2868
		$4p\ ^2P_{1/2}$			0	0.078 623	0.1194	0.1134	0.1119	0.1194	0.1134	0.1119			0	0.041 193	0.1289	0.1230	0.1215	0.1314[d]
		$4p\ ^2P_{3/2}$			0	0.058 771	0.1321	0.1349	0.1320	0.1321	0.1349	0.1320			0	0.027 860	0.1483	0.1514	0.1485	0.1484
90	Th^{79+}	$3p\ ^2P_{1/2}$	0	0.108 786	0	0.081 518	0.0326	0.0340	0.0345	0.0326	0.0340	0.0345	0	0.059 619	0	0.038 341	0.0325	0.0339	0.0344	0.0325[a]
		$3p\ ^2P_{3/2}$			0	0.050 502	0.3995	0.4055	0.4120	0.3995	0.4055	0.4120			0	0.019 042	0.3944	0.4005	0.4067	0.3948
		$4p\ ^2P_{1/2}$			0	0.071 288	0.1220	0.1121	0.1096	0.1220	0.1121	0.1096			0	0.038 341	0.1323	0.1225	0.1200	0.1342[d]
		$4p\ ^2P_{3/2}$			0	0.041 561	0.0853	0.0888	0.0846	0.0853	0.0888	0.0846			0	0.019 042	0.0995	0.1034	0.0992	0.1001
92	U^{81+}	$3p\ ^2P_{1/2}$	0	0.109 571	0	0.082 877	0.0317	0.0331	0.0337	0.0317	0.0331	0.0337	0	0.061 083	0	0.040 475	0.0318	0.0332	0.0337	0.0318[a]
		$3p\ ^2P_{3/2}$			0	0.059 539	0.3923	0.3986	0.4053	0.3923	0.3986	0.4053			0	0.021 551	0.4085	0.4151	0.4219	0.4115
		$4p\ ^2P_{1/2}$			0	0.074 322	0.1234	0.1129	0.1102	0.1234	0.1129	0.1102			0	0.040 475	0.1323	0.1218	0.1192	0.1352[d]
		$4p\ ^2P_{3/2}$			0	0.043 251	0.0805	0.0840	0.0798	0.0805	0.0840	0.0798			0	0.021 551	0.0929	0.0969	0.0925	0.0933

[a] Theodosiou and Curtis, Ref. [45].

[b] Lindgård and Nielsen, Ref. [28].

[c] Karwowski and Szulkin, Ref. [23].

[d] Sampson *et al.*, Ref. [49].

[e] Zhang *et al.*, Ref. [48].

TABLE V. Experimental and our theoretical oscillator strengths for $3s\ ^2S-3p\ ^2P$ transitions in the Na isoelectronic sequence. The numbers in parentheses denote errors.

Z	Ion	Upper level	Experiment	DQDO	DEOQN	DSQDT
11	Na	$3p\ ^2P_{1/2}$	0.318(2)[a]	0.3317	0.2705	0.3188
		$3p\ ^2P_{3/2}$	0.636(4)	0.6633	0.5411	0.6376
12	Mg^{1+}	$3p\ ^2P_{1/2}$	0.306(2)[b]	0.2931	0.2847	0.3063
		$3p\ ^2P_{3/2}$	0.615(6)	0.5862	0.5694	0.6127
14	Si^{3+}	$3p\ ^2P_{1/2}$	0.254(11)[c]	0.2729	0.2930	0.2539
		$3p\ ^2P_{3/2}$	0.511(22)	0.5457	0.5860	0.5088
16	S^{5+}	$3p\ ^2P_{1/2}$	0.227(8)[d]	0.2108	0.2273	0.2183
		$3p\ ^2P_{3/2}$	0.435(15)	0.4266	0.4602	0.4385
17	Cl^{6+}	$3p\ ^2P_{1/2}$	0.194(8)[e]	0.1957	0.2118	0.2010
		$3p\ ^2P_{3/2}$	0.409(9)	0.3976	0.4306	0.4048
18	Ar^{7+}	$3p\ ^2P_{1/2}$	0.183(4)[f]	0.1825	0.1979	0.1873
		$3p\ ^2P_{3/2}$	0.398(10)	0.3724	0.4039	0.3782
22	Ti^{11+}	$3p\ ^2P_{1/2}$	0.143(9)[g]	0.1552	0.1552	0.1465
		$3p\ ^2P_{3/2}$	0.312(19)	0.3243	0.3243	0.3066
26	Fe^{15+}	$3p\ ^2P_{1/2}$	0.115(7)[g]	0.1270	0.1270	0.1199
		$3p\ ^2P_{3/2}$	0.244(15)	0.2748	0.2748	0.2611
28	Ni^{17+}	$3p\ ^2P_{1/2}$	0.109(7)[g]	0.1164	0.1164	0.1107
		$3p\ ^2P_{3/2}$	0.226(14)	0.2573	0.2573	0.2449
29	Co^{18+}	$3p\ ^2P_{1/2}$	0.112(7)[g]	0.1117	0.1117	0.1053
		$3p\ ^2P_{3/2}$		0.2500	0.2500	0.2383
54	Xe^{43+}	$3p\ ^2P_{1/2}$	0.055(4)[h]	0.0558	0.0558	0.0548
		$3p\ ^2P_{3/2}$	0.195(17)	0.2153	0.2153	0.2036

[a] Carlsson, Ref. [60].
[b] Ansbacher, Li, and Pinnington, Ref. [73].
[c] Maniak, Träbert, and Curtis, Ref. [74].
[d] Ekberg *et al.*, Ref. [75].
[e] Jupén *et al.*, Ref. [76].
[f] Reistad, Engström, and Berry, Ref. [77].
[g] Hutton, Engström, and Träbert, Ref. [78].
[h] Träbert *et al.*, Ref. [79].

f values experience a 7% divergence with a slight improvement for RSQDT. In general, one observes a better accuracy of RPHSY values for the resonance lines. For Na-like ions, Fig. 2 shows that the RSQDT values remain essentially identical (within a few percent) to CAHS values, except again for the high-Z elements, whereas for the REOQN f values, the magnitude of $d(n,n')$, which is about 34 for neutral sodium, rapidly decreases and stabilizes at around 4 as Z increases. For $\Delta n=1$ transitions, the REOQN values are completely in error for neutral end elements. In the same way, the REOQN approach collapses for neutral copper. This explains why the corresponding values are not given in Table VI. With the increase of Z, the discrepancies decrease but remain important. It can be observed in Table IV that, with $c\neq 0$ for ions in the range $Z=11-18$, the RQDO f values with respect to corresponding REOQN are significantly improved; nevertheless, they are only reliable for $\Delta n=0$ transitions. Regarding the Cu sequence, it appears that as in the two previous sequences, the RSQDT f values agree well with reference data with, however, here and there, some large divergence points (within 12%) for $4s$-$5p_{3/2}$ transitions. For RDQO and REOQN, Figs. 5 and 6 show similar tendencies to what one observes in the case of Na-like ions with a large discrepancy. For the ions in the range $Z=29-70$, the RQDO values are found to be significantly modified by $c\neq 0$.

(e) Comparing dipole length and velocity results, it clearly appears in Figs. 1–6 that, whatever the sequence, discrepancies between f_L and f_V are fairly small along the entire sequence. However, one never observes, as expected [90] better agreement between the two forms with increasing Z, but rather poor agreement. The velocity values seem to be, in most cases, a little too large.

In Table III we present oscillator strengths for the $2s\ ^2S$-$np\ ^2P$ transitions ($n=4-20$) of Ca^{17+}, Zr^{37+}, and Yb^{67+} of the Li isoelectronic sequence. All relativistic QDO and SQDT results have been obtained with zero nodal pa-

TABLE VI. Our oscillator strengths compared with other selected calculations for $4s\ ^2S-4p\ ^2P$ transitions in the Cu isoelectronic sequence, with the same meaning as in Table I.

			Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	Upper level	c_i	δ_i'	c_f	δ_f'	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
29	Cu	$4p\ ^2P_{1/2}$	3	2.672 975	2	2.141 789	0.2235	0.2235	0.2235	0.2144			3	2.655 832	2	2.140 893	0.2227	0.2227	0.2227	0.2218[a]
		$4p\ ^2P_{3/2}$			2	2.134 498	0.4493	0.4493	0.4493	0.2035					2	2.140 893	0.4454	0.4454	0.4454	0.4476
		$5p\ ^2P_{1/2}$			2	2.087 105	0.0116	0.0116	0.0116	0.0106					2	2.140 893	0.0066	0.0066	0.0066	0.0066[b]
		$5p\ ^2P_{3/2}$			2	2.087 154	0.0232	0.0232	0.0232	0.0186					2	2.140 893	0.0133	0.0133	0.0133	0.0133
30	Zn^{1+}	$4p\ ^2P_{1/2}$	2	2.259 399	2	1.866 186	0.2953	0.2953	0.2953	0.2694	0.0712	0.0712	3	2.003 143	2	1.605 305	0.2521	0.2521	0.2521	0.2527[a]
		$4p\ ^2P_{3/2}$			2	1.856 501	0.6032	0.6032	0.6032	0.4643	0.1414	0.1414			2	1.590 268	0.5187	0.5187	0.5187	0.5160
		$5p\ ^2P_{1/2}$			2	1.824 293	0.0002	0.0002	0.0002	0.0033	0.0042	0.0042			2	1.605 305	0.0002	0.0002	0.0002	0.0002[b]
		$5p\ ^2P_{3/2}$			2	1.815 353	0.0002	0.0002	0.0002	0.0207	0.0086	0.0086			2	1.590 268	0.0010	0.0010	0.0010	0.0010
31	Ga^{2+}	$4p\ ^2P_{1/2}$	2	2.003 671	2	1.674 712	0.2747	0.2748	0.2748	0.2871	0.1522	0.1522	3	1.984 497	2	1.570 741	0.2614	0.2615	0.2615	0.2614[a]
		$4p\ ^2P_{3/2}$			2	1.663 822	0.5675	0.5675	0.5676	0.5424	0.3065	0.3065			2	1.585 942	0.5082	0.5082	0.5083	0.5386
		$5p\ ^2P_{1/2}$			2	1.632 308	0.0099	0.0099	0.0099	0.0011	0.0058	0.0058			2	1.570 741	0.0005	0.0005	0.0005	0.0005[b]
		$5p\ ^2P_{3/2}$			2	1.622 068	0.0168	0.0168	0.0168	0.0126	0.0126	0.0126			2	1.585 942	0.0004	0.0004	0.0004	0.0004
32	Ge^{3+}	$4p\ ^2P_{1/2}$	2	1.817 493	2	1.527 954	0.2537	0.2537	0.2537	0.2890	0.1968	0.1968	2	1.509 341	1	1.264 591	0.2615	0.2615	0.2615	0.2625[a]
		$4p\ ^2P_{3/2}$			2	1.516 089	0.5292	0.5293	0.5293	0.5691	0.4009	0.4009			1	1.250 833	0.5475	0.5475	0.5475	0.5453
		$5p\ ^2P_{1/2}$			1	1.486 300	0.0005	0.0005	0.0005	0.0002	0.0044	0.0044			1	1.264 591	0.0026	0.0026	0.0026	0.0026[b]
		$5p\ ^2P_{3/2}$			1	1.474 871	0.0018	0.0018	0.0018	0.0064	0.0102	0.0102			1	1.250 833	0.0032	0.0032	0.0032	0.0032
33	As^{4+}	$4p\ ^2P_{1/2}$	2	1.669 081	1	1.406 443	0.2651	0.2651	0.2652	0.2863	0.2220	0.2220	2	1.303 667	1	1.077 819	0.2571	0.2571	0.2571	0.2616[a]
		$4p\ ^2P_{3/2}$			1	1.393 615	0.5508	0.5509	0.5509	0.5780	0.4568	0.4568			1	1.062 077	0.5453	0.5454	0.5454	0.5480
		$5p\ ^2P_{1/2}$			1	1.367 079	0.0000	0.0000	0.0000	0.0000	0.0025	0.0025			1	1.077 819	0.0054	0.0054	0.0054	0.0054[b]
		$5p\ ^2P_{3/2}$			1	1.355 209	0.0001	0.0001	0.0001	0.0026	0.0063	0.0063			1	1.062 077	0.0073	0.0073	0.0073	0.0073
34	Se_{5+}	$4p\ ^2P_{1/2}$	2	1.552 735	1	1.312 407	0.2548	0.2548	0.2548	0.2790	0.2335	0.2336	2	1.074 738	1	0.862 634	0.2562	0.2562	0.2562	0.2560[a]
		$4p\ ^2P_{3/2}$			1	1.298 785	0.5340	0.5340	0.5341	0.5737	0.4853	0.4853			1	0.846 923	0.5465	0.5465	0.5466	0.5409
		$5p\ ^2P_{1/2}$			1	1.273 556	0.0005	0.0005	0.0005	0.0002	0.0010	0.0010			1	0.862 634	0.0086	0.0086	0.0086	0.0086[b]
		$5p\ ^2P_{3/2}$			1	1.259 894	0.0002	0.0002	0.0002	0.0000	0.0016	0.0016			1	0.846 923	0.0126	0.0126	0.0126	0.0126
36	Kr^{7+}	$4p\ ^2P_{1/2}$	1	1.368 435	1	1.159 795	0.2630	0.2631	0.2631	0.2641	0.2408	0.2409	2	0.656 400	1	0.472 027	0.2452	0.2452	0.2542	0.2448[a]
		$4p\ ^2P_{3/2}$			1	1.144 583	0.5639	0.5640	0.5641	0.5581	0.5102	0.5103			1	0.454 290	0.5346	0.5347	0.5348	0.5265
		$5p\ ^2P_{1/2}$			1	1.130 214	0.0131	0.0130	0.0130	0.0017	0.0001	0.0001			1	0.472 027	0.0169	0.0169	0.0169	0.0169[b]
		$5p\ ^2P_{3/2}$			1	1.115 559	0.0200	0.0200	0.0200	0.0006	0.0000	0.0000			1	0.454 290	0.0262	0.0262	0.0262	0.0260
40	Zr^{11+}	$4p\ ^2P_{1/2}$	1	1.117 413		0.948 534	0.2294	0.2295	0.2296	0.2364	0.2310	0.2311	1	0.292 067	0	0.160 075	0.2221	0.2222	0.2222	0.2222[a]
		$4p\ ^2P_{3/2}$			1	0.930 146	0.5135	0.5137	0.5138	0.5226	0.5103	0.5104			0	0.142 270	0.5097	0.5098	0.5099	0.4976
		$5p\ ^2P_{1/2}$			1	0.919 473	0.0357	0.0356	0.0356	0.0061	0.0045	0.0045			0	0.160 075	0.0297	0.0296	0.0296	0.0299[b]
		$5p\ ^2P_{3/2}$			1	0.901 581	0.0572	0.0573	0.0572	0.0067	0.0048	0.0048			0	0.142 270	0.0456	0.0456	0.0456	0.0451
42	Mo^{13+}	$4p\ ^2P_{1/2}$	1	1.027 451	1	0.872 469	0.2148	0.2150	0.2150	0.2245	0.2223	0.2224	0	0.613 816	0	0.490 088	0.2122	0.2122	0.2122	0.2114[a]
		$4p\ ^2P_{3/2}$			1	0.852 490	0.4925	0.4928	0.4930	0.5081	0.5028	0.5029			0	0.478 231	0.4846	0.4846	0.4847	0.4846

TABLE VI. (*Continued*).

			Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	Upper level	c_i	δ'_i	c_f	δ'_f	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
		$5p\ ^2P_{1/2}$			1	0.845 217	0.0473	0.0472	0.0472	0.0095	0.0083	0.0083			0	0.490 088	0.0389	0.0386	0.0385	0.0361[b]
		$5p\ ^2P_{3/2}$			1	0.825 687	0.0761	0.0762	0.0761	0.0112	0.0098	0.0098			0	0.478 231	0.0622	0.0620	0.0619	0.0622
48	Cd^{19+}	$4p\ ^2P_{1/2}$	1	0.835 224	1	0.709 741	0.1796	0.1799	0.1801	0.1959	0.1956	0.1957	0	0.554 292	0	0.450 719	0.1838	0.1839	0.1840	0.1838[a]
		$4p\ ^2P_{3/2}$			1	0.684 879	0.4482	0.4487	0.4490	0.4810	0.4799	0.4802			0	0.436 556	0.4573	0.4573	0.4576	0.4573
		$5p\ ^2P_{1/2}$			1	0.687 265	0.0787	0.0785	0.0783	0.0228	0.0217	0.0216			0	0.450 719	0.0508	0.0501	0.0500	0.0528[b]
		$5p\ ^2P_{3/2}$			1	0.662 900	0.1244	0.1247	0.1245	0.0281	0.0274	0.0272			0	0.436 556	0.0755	0.0753	0.0751	0.0753
53	I^{24+}	$4p\ ^2P_{1/2}$	1	0.728 322	1	0.619 281	0.1580	0.1584	0.1585	0.1763	0.1763	0.1765	0	0.489 530	0	0.398 619	0.1656	0.1658	0.1660	0.1657[a]
		$4p\ ^2P_{3/2}$			1	0.590 100	0.4290	0.4297	0.4301	0.4698	0.4692	0.4697			0	0.382 603	0.4468	0.4469	0.4473	0.4469
		$5p\ ^2P_{1/2}$			1	0.599 628	0.0998	0.0995	0.0993	0.0341	0.0326	0.0325			0	0.398 619	0.0612	0.0601	0.0599	0.0641[b]
		$5p\ ^2P_{3/2}$			1	0.570 974	0.1531	0.1537	0.1534	0.0408	0.0401	0.0398			0	0.382 603	0.0862	0.0859	0.0856	0.0863
54	Xe^{25+}	$4p\ ^2P_{1/2}$	1	0.710 017	1	0.603 651	0.1544	0.1548	0.1550	0.1729	0.1729	0.1731	0	0.484 164	0	0.395 393	0.1625	0.1627	0.1629	0.1625[a]
		$4p\ ^2P_{3/2}$			1	0.573 619	0.4268	0.4275	0.4280	0.4688	0.4683	0.4688			0	0.379 053	0.4464	0.4466	0.4470	0.4466
		$5p\ ^2P_{1/2}$			1	0.583 504	0.1030	0.1026	0.1024	0.0358	0.0343	0.0342			0	0.395 393	0.0626	0.0613	0.0612	0.0652[b]
		$5p\ ^2P_{3/2}$			1	0.553 840	0.1565	0.1572	0.1568	0.0423	0.0416	0.0413			0	0.379 053	0.0868	0.0865	0.0861	0.0867
60	Nd^{31+}	$4p\ ^2P_{1/2}$	1	0.624 345	1	0.531 637	0.1353	0.1358	0.1360	0.1540	0.1543	0.1545	0	0.418 888	0	0.341 920	0.1447	0.1451	0.1453	0.1453[a]
		$4p\ ^2P_{3/2}$			0	0.496 183	0.4499	0.4507	0.4514	0.4686	0.4683	0.4691			0	0.322 398	0.4487	0.4490	0.4497	0.4485
		$5p\ ^2P_{1/2}$			1	0.515 212	0.1232	0.1227	0.1224	0.0483	0.0461	0.0458			0	0.341 920	0.0737	0.0719	0.0716	0.0768[b]
		$5p\ ^2P_{3/2}$			0	0.480 119	0.0343	0.0350	0.0346	0.0530	0.0523	0.0518			0	0.322 398	0.0940	0.0937	0.0932	0.0936
70	Yb^{31+}	$4p\ ^2P_{1/2}$	1	0.526 100	0	0.449 111	0.1258	0.1264	0.1268	0.1301	0.1307	0.1310	0	0.380 406	0	0.317 657	0.1236	0.1241	0.1245	0.1236[a]
		$4p\ ^2P_{3/2}$			0	0.403 237	0.4719	0.4732	0.4745	0.4950	0.4952	0.4965			0	0.295 791	0.4783	0.4789	0.4801	0.4775
		$5p\ ^2P_{1/2}$			0	0.432 335	0.0424	0.0410	0.0405	0.0628	0.0592	0.0587			0	0.317 657	0.0840	0.0806	0.0800	0.0868[b]
		$5p\ ^2P_{3/2}$			0	0.386 772	0.0331	0.0342	0.0335	0.0562	0.0556	0.0548			0	0.295 791	0.0877	0.0874	0.0865	0.0870
74	W^{45+}	$4p\ ^2P_{1/2}$	0	0.499 893	0	0.427 591	0.1225	0.1231	0.1235	0.1225	0.1231	0.1235	0	0.360 466	0	0.302 394	0.1166	0.1173	0.1176	0.1166[a]
		$4p\ ^2P_{3/2}$			0	0.377 326	0.5125	0.5128	0.5144	0.5125	0.5128	0.5144			0	0.279 399	0.4962	0.4970	0.4984	0.4961
		$5p\ ^2P_{1/2}$			0	0.412 964	0.0687	0.0644	0.0638	0.0687	0.0644	0.0638			0	0.302 394	0.0881	0.0840	0.0833	0.0916[b]
		$5p\ ^2P_{3/2}$			0	0.362 879	0.0559	0.0553	0.0544	0.0559	0.0553	0.0544			0	0.279 399	0.0841	0.0838	0.0827	0.0838
79	Au^{51+}	$4p\ ^2P_{1/2}$	0	0.472 618	0	0.405 345	0.1140	0.1148	0.1153	0.1140	0.1148	0.1153	0	0.340 466	0	0.287 625	0.1089	0.1097	0.1101	0.1089[a]
		$4p\ ^2P_{3/2}$			0	0.348 764	0.5412	0.5417	0.5437	0.5412	0.5417	0.5437			0	0.262 578	0.5270	0.5280	0.5299	0.5263
		$5p\ ^2P_{1/2}$			0	0.391 959	0.0747	0.0695	0.0687	0.0747	0.0695	0.0687			0	0.287 625	0.0924	0.0873	0.0865	0.0958[b]
		$5p\ ^2P_{3/2}$			0	0.335 794	0.0526	0.0520	0.0510	0.0526	0.0520	0.0510			0	0.262 578	0.0765	0.0762	0.0750	0.0764
82	Pb^{53+}	$4p\ ^2P_{1/2}$	0	0.459 074	0	0.394 449	0.1094	0.1103	0.1108	0.1094	0.1103	0.1108	0	0.332 466	0	0.282 791	0.1042	0.1051	0.1056	0.1047[a]
		$4p\ ^2P_{3/2}$			0	0.333 739	0.5615	0.5621	0.5644	0.5615	0.5621	0.5644			0	0.256 834	0.5477	0.5488	0.5511	0.5474
		$5p\ ^2P_{1/2}$			0	0.381 838	0.0781	0.0722	0.0713	0.0781	0.0722	0.0713			0	0.282 791	0.0947	0.0889	0.0880	0.0981[b]

TABLE VI. (*Continued*).

		Upper	Relativistic QDO results							Relativistic EOQN results			Relativistic SQDT results							Others
Z	Ion	level	c_i	δ_i'	c_f	δ_f'	f	f_L	f_V	f	f_L	f_V	I_i	δ_i	I_f	δ_f	f	f_L	f_V	f
		$5p\ ^2P_{3/2}$			0	0.321 417	0.0495	0.0489	0.0478	0.0495	0.0489	0.0478			0	0.256 834	0.0708	0.0706	0.0692	0.0708
83	Bi^{59+}	$4p\ ^2P_{1/2}$	0	0.454 978	0	0.391 155	0.1080	0.1090	0.1095	0.1080	0.1090	0.1095	0	0.326 466	0	0.277 426	0.1034	0.1043	0.1048	0.1034[a]
		$4p\ ^2P_{3/2}$			0	0.329 154	0.5683	0.5690	0.5715	0.5683	0.5690	0.5715			0	0.250 976	0.5552	0.5564	0.5587	0.5545
		$5p\ ^2P_{1/2}$			0	0.378 647	0.0790	0.0729	0.0720	0.0790	0.0729	0.0720			0	0.277 426	0.0955	0.0895	0.0886	0.1002[b]
		$5p\ ^2P_{3/2}$			0	0.316 989	0.0483	0.0478	0.0466	0.0483	0.0478	0.0466			0	0.250 976	0.0693	0.0691	0.0677	0.0689
88	Ra^{69+}	$4p\ ^2P_{1/2}$	0	0.437 766	0	0.377 305	0.1020	0.1031	0.1036	0.1020	0.1031	0.1036	0	0.289 194	0	0.243 712	0.0979	0.0989	0.0994	0.0980[a]
		$4p\ ^2P_{3/2}$			0	0.307 980	0.6084	0.6092	0.6123	0.6084	0.6092	0.6123			0	0.213 100	0.5932	0.5948	0.5978	0.5964
		$5p\ ^2P_{1/2}$			0	0.366 947	0.0843	0.0769	0.0758	0.0843	0.0769	0.0758			0	0.243 712	0.1009	0.0939	0.0928	0.1009[b]
		$5p\ ^2P_{3/2}$			0	0.245 298	0.0236	0.0207	0.0201	0.0236	0.0207	0.0201			0	0.213 100	0.0629	0.0628	0.0612	0.0632
90	Th^{61+}	$4p\ ^2P_{1/2}$	0	0.431 415	0	0.372 647	0.0990	0.1001	0.1007	0.0990	0.1001	0.1007	0	0.305 669	0	0.262 582	0.0951	0.0962	0.0968	0.0952[a]
		$4p\ ^2P_{3/2}$			0	0.299 957	0.6252	0.6260	0.6295	0.6252	0.6260	0.6295			0	0.232 895	0.6167	0.6181	0.6215	0.6140
		$5p\ ^2P_{1/2}$			0	0.361 449	0.0855	0.0776	0.0765	0.0855	0.0776	0.0765			0	0.262 582	0.0999	0.0922	0.0910	0.1025[b]
		$5p\ ^2P_{3/2}$			0	0.288 974	0.0383	0.0379	0.0365	0.0383	0.0379	0.0365			0	0.232 895	0.0539	0.0537	0.0521	0.0535
92	U^{63+}	$4p\ ^2P_{1/2}$	0	0.426 243	0	0.369 010	0.0962	0.0674	0.0980	0.0962	0.0974	0.0980	0	0.310 588	0	0.269 560	0.0926	0.0938	0.0944	0.0926[a]
		$4p\ ^2P_{3/2}$			0	0.292 760	0.6432	0.6440	0.6478	0.6432	0.6440	0.6478			0	0.242 119	0.6322	0.6335	0.6372	0.6331
		$5p\ ^2P_{1/2}$			0	0.358 004	0.0872	0.0788	0.0776	0.0872	0.0788	0.0776			0	0.269 560	0.1001	0.0916	0.0903	0.1035[b]
		$5p\ ^2P_{3/2}$			0	0.282 392	0.0352	0.0348	0.0334	0.0352	0.0348	0.0334			0	0.242 119	0.0486	0.0483	0.0468	0.0491

[a] Curstis and Theodosiou, Ref. [53].

[b] Nana *et al.*, Ref. [80].

TABLE VII. Experimental and our theoretical oscillator strengths for $4s\ ^2S-4p\ ^2P$ transitions in the CU isoelectronic sequence. The numbers in parentheses denote errors.

Z	Ion	Upper level	Experiment	DQDO	DEOQN	DSQDT
29	Cu	$4p\ ^2P_{1/2}$	0.2210(18)[a]	0.2235	0.2144	0.2227
		$4p\ ^2P_{3/2}$	0.4410(37)	0.4493	0.2035	0.4454
30	Zn^{1+}	$4p\ ^2P_{1/2}$		0.2953	0.2694	0.2521
		$4p\ ^2P_{3/2}$	0.513(60)[b]	0.6032	0.4643	0.5187
31	Ga^{2+}	$4p\ ^2P_{1/2}$		0.2747	0.2871	0.2614
		$4p\ ^2P_{3/2}$	0.549(45)[c]	0.5675	0.5424	0.5082
32	Ge^{3+}	$4p\ ^2P_{1/2}$	0.249(14)[d]	0.2537	0.2890	0.2615
		$4p\ ^2P_{3/2}$	0.517(32)	0.5292	0.5691	0.5475
33	As^{4+}	$4p\ ^2P_{1/2}$	0.233(20)[e]	0.2651	0.2863	0.2571
		$4p\ ^2P_{3/2}$	0.542(40)	0.5508	0.5780	0.5453
34	Se^{5+}	$4p\ ^2P_{1/2}$	0.262(30)[f]	0.2548	0.2790	0.2562
		$4p\ ^2P_{3/2}$	0.548(60)	0.5340	0.5737	0.5465
36	Kr^{7+}	$4p\ ^2P_{1/2}$	0.25(1)[g]	0.2630	0.2641	0.2452
		$4p\ ^2P_{3/2}$	0.53(2)	0.5639	0.5581	0.5346
42	Mb^{13+}	$4p\ ^2P_{1/2}$	0.23(2)[h]	0.2148	0.2245	0.2122
		$4p\ ^2P_{3/2}$	0.53(4)	0.4925	0.5081	0.4846
53	I^{24+}	$4p\ ^2P_{1/2}$	0.190(8)[i]	0.1580	0.1763	0.1656
		$4p\ ^2P_{3/2}$	0.439(19)	0.4290	0.4698	0.4468

[a] Carlsson, Sturesson, and Svanberg, Ref. [8].
[b] Martinson *et al.*, Ref. [82].
[c] Ansbacher *et al.*, Ref. [83].
[d] Pinnington, Bahr, and Irwin, Ref. [84].
[e] Pinnington, Bahr, and Irwin, Ref. [85].
[f] Bahr *et al.*, Ref. [86].
[g] Pinnington *et al.*, Ref. [87].
[h] Denne and Poulsen, Ref. [88].
[i] Johnson *et al.*, Ref. [89].

rameter. The following main points can be drawn out.

For a given ion, the increase of the principal quantum number of the final state in the transition reduces the disagreement between (a) the DPHSY and the RPHSY calculations for each method, (b) the dipole length and the dipole velocity f values of the RPHSY calculation for each method (this observation is in harmony with the conclusion of Barrientos and Martin [13]), and (c) the relativistic SQDT and

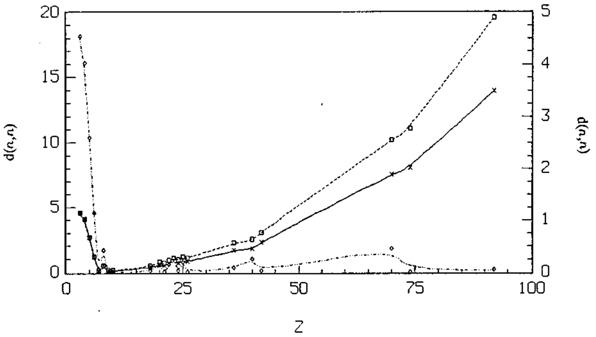

FIG. 1. Plot of the difference $d(n,n)$ between the relativistic SQDT values and CAHS values vs the nuclear charge for the $2s$-$2p$ transitions in the Li isoelectronic sequence. Curves are drawn to guide the eye: —, the RSQDT length form calculations (×) (right-hand scale); -----, the RSQDT velocity form calculations (□) (left-hand scale); ········-, the DSQDT calculations (◇) (left-hand scale).

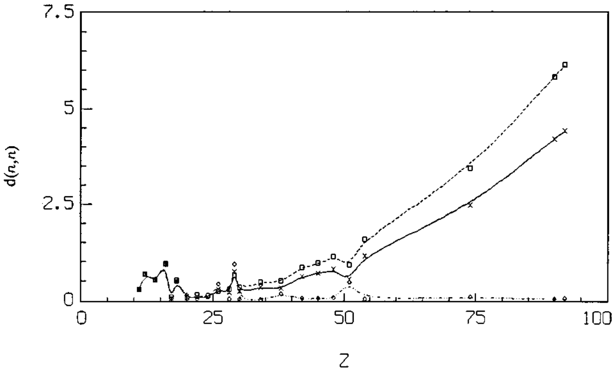

FIG. 2. Plot of the difference $d(n,n)$ between the relativistic SQDT values and CAHS values vs the nuclear charge for the $3s$-$3p$ transitions in the Na isoelectronic sequence. Curves are drawn to guide the eye: —, the RSQDT length form calculations (×); -----, the RSQDT velocity form calculations (□); ········-, the DSQDT calculations (◇).

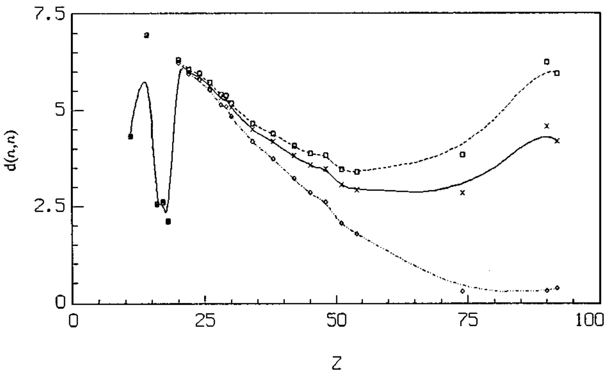

FIG. 3. Plot of the difference $d(n,n)$ between the relativistic SQDT values and CAHS values vs the nuclear charge for the $4s$-$4p$ transitions in the Cu isoelectronic sequence. Curves are drawn to guide the eye: —, the RSQDT length form calculations (×); -----, the RSQDT velocity form calculations (□); ·-·-·-·-·-, the DSQDT length form calculations (◇).

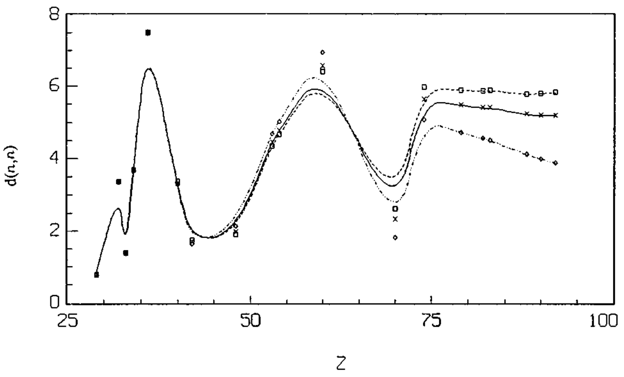

FIG. 5. Plot of the difference $d(n,n)$ between the relativistic QDO values and CAHS values vs the nuclear charge for the $4s$-$4p_{1/2}$ transitions in the Cu isoelectronic sequence. Curves are drawn to guide the eye: —, the RQDO length form calculations (×); -----, the RQDO velocity form calculations (□); ·-·-·-·-·-, the DQDO calculations (◇).

QDO (and EOQN) calculations. For this last case, the DSQDT and DQDO results on the one hand and the RSQDT and RQDO f values in dipole length and velocity gauges on the other hand, are identical for high n.

For a given transition, the discrepancies increase with Z between (a) the DPHSY and the RPHSY calculations for each method and (b) the dipole length and the dipole velocity f results of the RPHSY calculations for each method.

The good performance of the DSQDT and the RSQDT calculations for the $2s\ ^2S - np\ ^2P$ transitions, using $\delta(l,j)$ and $I(l,j) \equiv I(l)$ obtained from transitions between low-lying states, points out one of the main advantages of the SQDT procedure in comparison with the two others: it can serve to make phenomenological predictions for certain unknown atomic characteristics as transitions probabilities and oscillator strengths.

It is noteworthy that the approximate relativistic f results are not given in the above tables because their agreement with those of complete relativistic calculations are within a fraction of a percent. This agreement leads us to believe that relativistic changes in the matrix elements are essentially due to the DPHSY wave functions. In other words, as previously pointed out in Ref. [18], replacing the relativistic operator by the nonrelativistic one introduces only a very little error in the calculation of the DPHSY f values. It becomes then evident that Eqs. (33)–(36) are very simple formulas and form the fastest procedure for the computation of the DPHSY f values.

The residual difference between f_L and f_V RPHSY values pointed out along this section is partly due to the approximate nature of the RPHSY calculations. However, it is worth mentioning here that the residual in question ceases to be small and becomes very important if instead of our effective operator $d/dr - \Lambda_> \Delta/r$ one uses the well-known hydrogenic operator $d/dr - l_> \Delta_0/r$. For example for W^{71+}, the RQDO calculations for $2s$-$2p_{1/2}$ and $2s$-$2p_{3/2}$ transitions, respectively, give 0.68 and 0.1319 in the length gauge and 0.1757 and 0.1697 in the velocity gauge with the usual operator. With our operator, one obtains 0.70 and 0.1357. The effec-

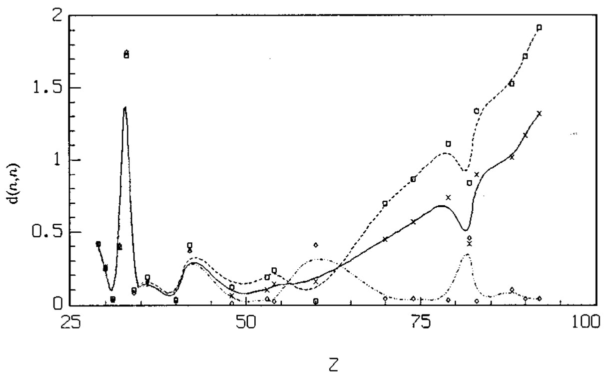

FIG. 4. Plot of the difference $d(n,n)$ between the relativistic QDO values and CAHS values vs the nuclear charge for the $3s$-$3p_{1/2}$ transitions in the Na isoelectronic sequence. Curves are drawn to guide the eye: —, the RQDO length form calculations (×); -----, the RQDO velocity form calculations (□); ·-·-·-·-·-, the DQDO calculations (◇).

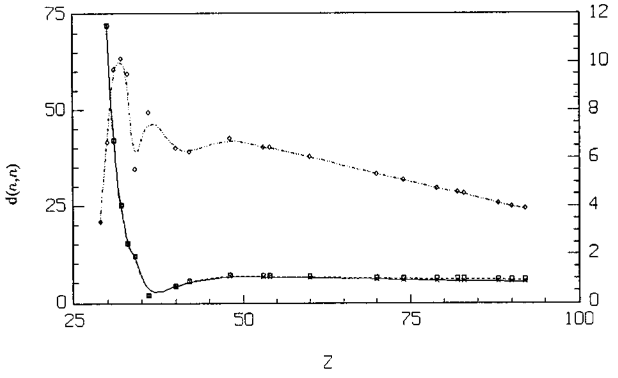

FIG. 6. Plot of the difference $d(n,n)$ between the relativistic EOQN values and CAHS values vs the nuclear charge for the $4s$-$4p_{1/2}$ transitions in the Cu isoelectronic sequence. Curves are drawn to guide the eye: —, the REOQN length form calculations (×) (right-hand scale); -----, the REOQN velocity form calculations (□) (left-hand scale); ·-·-·-·-·-, the DEOQN length form calculations (◇) (left-hand scale).

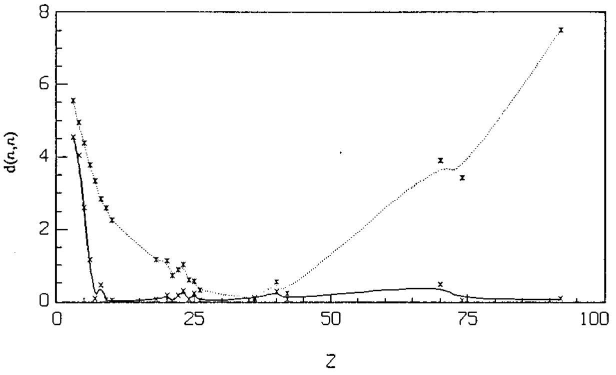

FIG. 7. Plot of the comparison of the difference $d(n,n)$ between the DSQDT and DQDO values and CAHS values vs the nuclear charge for the $2s$-$2p_{1/2}$ transitions in the Li isoelectronic sequence. Curves are drawn to guide the eye: —, the DSQDT calculations (×); ········, the DQDO calculations (*).

tiveness of the effective velocity operator is then evident.

The plots of the $n'p$ phenomenological quantum defects and exact quantum defects presented in Tables I, IV, and VI versus the nuclear charge Z are displayed in Figs. 10–12. The following clearly arises from these figures.

(a) Along an isoelectronic sequence, the quantum defects are nearly identical for the two fine-structure components of the spectra, illustrating that the ionic Coulomb potential is mainly responsible for the fine structure of these lines.

(b) For a given degree of ionization, the growth of the number of remaining electrons leads to the increase of the quantum defect.

(c) Phenomenological quantum defects show a regular and a slow (rapid) isoelectronic variation for elements with a high (low) degree of ionization, with, however, a few irregularities here and there due to the use of different energy data sources along an isoelectronic sequence for a given transition.

(d) The increase of the principal quantum number n leads to the decrease of the phenomenological quantum defect.

(e) In the Li sequence the exact quantum defects δ seem to be slightly larger than the phenomenological ones δ', whereas the first become smaller and smaller than the second as one proceeds from Na to Cu sequences. The ratio δ/δ' are within 1.3–0.85, 1.1–0.4, and 1–0.15 for Li, Na, and Cu sequences, respectively. The closest agreement between δ and δ' for Li-like ions with zero nodal parameters explain the closeness of the corresponding f values.

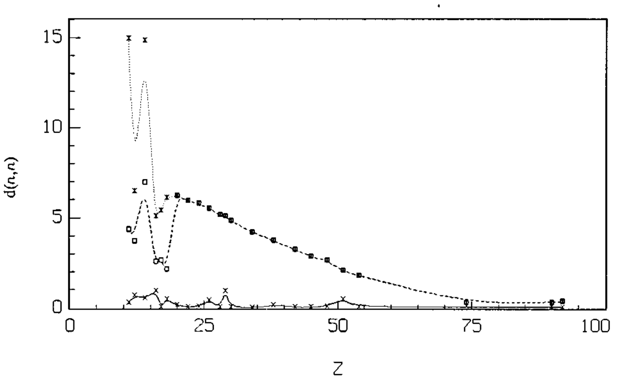

FIG. 8. Plot of the comparison of the difference $d(n,n)$ between the DPHSY values and CAHS values vs the nuclear charge for the $3s$-$3p_{1/2}$ transitions in the Na isoelectronic sequence. Curves are drawn to guide the eye: —, the DSQDT calculations (×); -----, the DQDO calculations (□); ········, the DEOQN calculations (*).

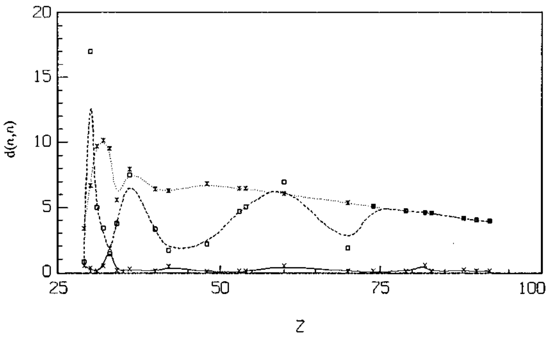

FIG. 9. Plot of the comparison of the difference $d(n,n)$ between the DPHSY values and CAHS values vs the nuclear charge for the $4s$-$4p_{1/2}$ transitions in the Cu isoelectronic sequence. Curves are drawn to guide the eye: —, the DSQDT calculations (×); -----, the DQDO calculations (□); ········, the DEOQN calculations (*).

(f) Except for a few high-Z elements for Li-like ions, the exact quantum defects are spin independent. Furthermore, they are similar to the spectroscopic quantum defects given by Lindgård and Nielsen [28] for high n.

From the preceding, it seems clear that symmetry is better taken into account in the relativistic SQDT approach, with the use of exact quantum defect and the nodal-modifying parameter I, than in the relativistic QDO approach with the use of phenomenological quantum defect and the nodal-modifying parameter $c=\langle\delta'\rangle$ and more in this latter case in the relativistic EOQN approach.

IV. CONCLUSION

In this paper we have undertaken, through a systematic study, a comparison of the phenomenological QDO, EOQN,

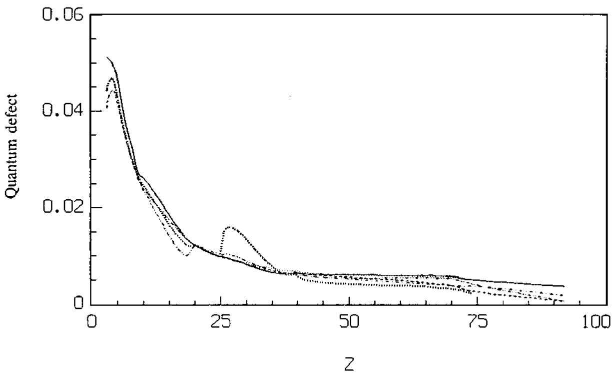

FIG. 10. Plot of the phenomenological and the exact np quantum defects vs the nuclear charge in the Li isoelectronic sequence. — interpolates p exact quantum-defect values, ----- interpolates p exact quantum-defect values, ······· interpolates $2p_{1/2}$ phenomenological quantum-defect values, -·-·-·- interpolates $2p_{3/2}$ phenomenological quantum-defect values, ··-··-··- interpolates $3p_{1/2}$ phenomenological quantum-defect values, and ······ interpolates $3p_{3/2}$ phenomenological quantum-defect values.

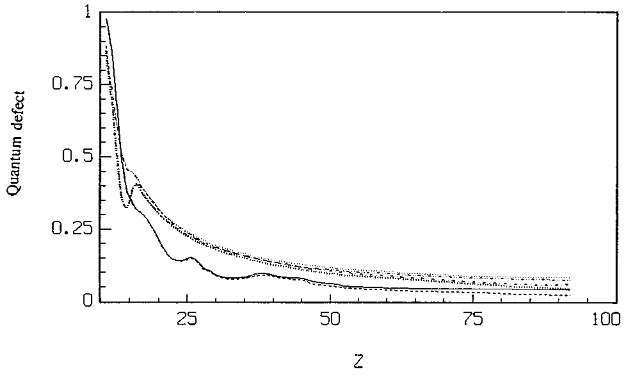

FIG. 11. Plot of the phenomenological and the exact np quantum defects vs the nuclear charge in the Na isoelectronic sequence. — interpolates p exact quantum-defect values, ----- interpolates p exact quantum-defect values, ······· interpolates $2p_{1/2}$ phenomenological quantum-defect values, -·-·-·- interpolates $2p_{3/2}$ phenomenological quantum-defect values, ··-··-··- interpolates $3p_{1/2}$ phenomenological quantum-defect values, and ····· interpolates $3p_{3/2}$ phenomenological quantum-defect values.

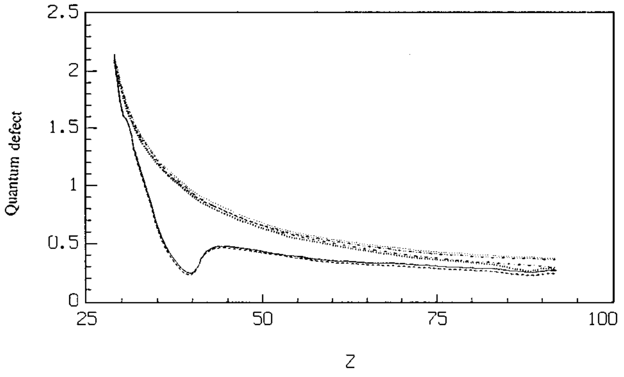

FIG. 12. Plot of the phenomenological and the exact np quantum defects vs the nuclear charge in the Cu isoelectronic sequence. — interpolates p exact quantum-defect values, ----- interpolates p exact quantum-defect values, ······· interpolates $2p_{1/2}$ phenomenological quantum-defect values, -·-·-·- interpolates $2p_{3/2}$ phenomenological quantum-defect values, ··-··-··- interpolates $3p_{1/2}$ phenomenological quantum-defect values, and ····· interpolates $3p_{3/2}$ phenomenological quantum-defect values.

and the supersymmetry-inspired quantum-defect SQDT methods in their relativistic and quasirelativistic formulations. We have done so by emphasizing the similarities and differences between phenomenological and symmetry-based approaches. It arises, for example, that the relativistic QDO and EOQN procedures become identical by setting $c=0$ in the former. Transition matrix elements calculated in the Dirac approach are gauge invariant. The numerical application of our derivations to the calculation of oscillator strengths for lithiumlike, sodiumlike, and copperlike ions clearly points out the highest accuracy of Dirac results and the simplicity of the scalar formulation. Among several conclusions that can be drawn from Sec. III, one can draw out the following most relevant ones.

If the three procedures are mathematically similar, they are not equivalent. The nodal-modifying parameter $c=\langle\delta'\rangle$ not only ensures the main difference between the two phenomenological procedures, i.e., the relativistic QDO and EOQN approaches, but also gives more symmetry to the first approach. In the same way, in the relativistic SQDT approach, the exact quantum defect $\delta(l,j)$ and the nodal-modifying parameter $I(l,j)\equiv I(l)$ not only give rise to a strongly marked symmetry, but also may serve to make phenomenological predictions for certain unknown atomic characteristics such as transitions probabilities and oscillator strengths.

Our modified velocity operator $d/dr-\Lambda_{>}\Delta/r$ yields reasonably accurate f values in comparison with the usual velocity operator, which completely fails. The fairly small discrepancy that appears between the dipole length and the dipole velocity f values in the RPHSY procedures along an isoelectronic sequence never decreases as Z increases, as expected.

The relativistic PHSY calculations agree in general for resonance transitions with the experimental measurements. The comparison with the others theoretical calculations shows a discrepancy as the number of the remaining electrons increases. In order words, the polarization effects must be taken into account.

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