Relativistic many-body calculations for the oscillator strengths of the resonance lines of neon, argon, krypton, and xenon

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The f values for the $np^6 \rightarrow np^5(n+1)s$ dipole transitions of neon, argon, krypton, and xenon are studied using relativistic many-body perturbation theory. The contributions from the correlation corrections of single and pair excitations are calculated to all orders. It is hoped that the present work may help to distinguish among the considerable variety of experimental and theoretical values presently available. [S1050-2947(98)08306-1]

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I. INTRODUCTION

For almost a decade, various theoretical schemes based on relativistic many-body perturbation theory (RMBPT) [1–9] as well as on relativistic coupled cluster method (RCC) [10–12] have been successfully applied to the investigation of atomic transition energies. An important feature of these calculations is that they lead to highly correlated wave functions which can readily be used for the evaluation of other atomic properties such as oscillator strengths and hyperfine constants [1,3,13–16].

Based on this framework, our goal is to evaluate *ab initio* f values for the lowest resonance lines of the heavier noble gases, a challenging subject both from the experimental [17–64] and the theoretical [65–83] standpoint. Of particular interest are the oscillator strengths of krypton where the disagreement among recently performed measurements [18–22] is not uniformly accounted for by an overlapping of the quoted experimental errors while the need of higher-order correlations is reflected to the general disagreement of the previous theoretical approaches [67–71].

Following Ref. [5], our wave functions are created via the the action of the correlation operator on a model space that includes the lowest-order particle-hole states corresponding to the allowed electric-dipole transitions. The hole orbital belongs to the outer shell of the closed core and the valence orbital belongs to the first excited state. All core and valence states are generated in a V^{N-1} Dirac-Hartree-Fock potential where the excited states are evaluated in the absence of an electron from the core outer subshell. The first approximation to the particle-hole wave functions and energies comes from the diagonalization of the lowest-order effective Hamiltonian H^{eff}. The higher-order corrections are calculated in the linear cluster approximation [84], an iterative process complete in second-order many-body perturbation theory and with correlations from single and pair excitations calculated to all orders [3,5,6,84]. In this approach, the correlation operator is decomposed in four sectors: core-core, core-hole, valence-core, and valence-hole. For neon it was found that the use of the V^{N-1} potential constrained the dominant corrections of the transition energies to the core-hole sector alone [5]. However, for the purpose of calculating transition matrix elements, a more computationally demanding iterative solution for all sectors is necessary. The main reason is the change in the relative contributions of the different sectors when we calculate transition matrix elements using the correlated particle-hole wave functions and especially those of the valence-hole sector that correspond to corrections due to the random-phase approximation (RPA) [85,65]. Also, the part corresponding to the core-core sector defines the wave operator of the core wave function. The correlation coefficients obtained from the all-order solution of the pair equations are used to calculate the oscillator strengths of the $np^6 \rightarrow np^5(n+1)s$ dipole transitions of neon, argon, krypton, and xenon. The difference between the length and velocity forms of the calculated absorption oscillator strengths is in almost all cases less than 5%. Our results are in very good agreement with those experiments that support the relatively larger f values.

II. FORMALISM

First, we give an outline of the method presented in detail in Ref. [5] for the calculation of the particle-hole energies and wave functions.

We seek to solve the time independent many-body Dirac-Coulomb equation

$$H|\Psi_{ph}(JM)\rangle = E|\Psi_{ph}(JM)\rangle, \tag{2.1}$$

where H stands for the ''no-pair'' Hamiltonian [86] defined as

$$H = H_0 + V_I \tag{2.2}$$

and J,M are the components of the total angular momentum. In the language of second quantization the unperturbed part H_0 is

$$H_0 = \sum_i \varepsilon_i \alpha_i^\dagger \alpha_i \tag{2.3}$$

while the second term V_I that accounts for the interactions among electrons is written as

$$V_I = \frac{1}{2} \sum_{i,j,k,l} g_{ijkl} \alpha_i^\dagger \alpha_j^\dagger \alpha_l \alpha_k - \sum_{ij} U_{i,j} \alpha_i^\dagger \alpha_j, \tag{2.4}$$

with g_{ijkl} and U_{ij} standing, respectively, for the Coulomb and model potential matrix elements

$$g_{ijkl}=\int\int \frac{d^3r_1 d^3r_2}{r_{12}}\varphi_i^\dagger(\mathbf{r}_1)\varphi_j^\dagger(\mathbf{r}_2)\varphi_k(\mathbf{r}_1)\varphi_l(\mathbf{r}_2), \tag{2.5}$$

$$U_{ij}=\int \varphi_i^\dagger(\mathbf{r})U(r)\varphi_j(\mathbf{r})d^3r, \tag{2.6}$$

and ε_i, $\varphi_i(\mathbf{r})$ are the positive-energy solutions of a single-particle Dirac equation. These are obtained using finite basis set techniques based on the method of B splines [87]. Our pseudospectrum included 40 basis functions for every angular quantum number $k=\pm1,\pm2,\ldots,\pm11$. The particle-hole state $|\Psi_{ph}(JM)\rangle$ is realized via the correlation operator χ_{av} acting on a linear combination of almost degenerate model states $|\Phi_{av}(JM)\rangle$,

$$|\Psi_{ph}(JM)\rangle=\sum_{a,v} C_{av}(1+\chi_{av})|\Phi_{av}(JM)\rangle, \tag{2.7}$$

where

$$|\Phi_{av}(JM)\rangle=\sum_{m_a,m_v}(-1)^{j_a-m_a}\langle j_v m_v, j_a -m_a|JM\rangle a_v^\dagger a_a|0_C\rangle. \tag{2.8}$$

Here, $|0_C\rangle$ denotes the lowest-order wave function of the closed core and the index convention is as follows: a,v denote hole and valence states, respectively; m,n,r,s correspond to virtual and b,c,d to core states while i,j,k,l correspond to all orbitals.

These equations lead to a modification of Eq. (2.1) into an eigenvalue problem that involves the effective Hamiltonian H^{eff},

$$\sum_{a,v} H^{\text{eff}}_{a'v',av}C_{av}=EC_{a'v'}, \tag{2.9}$$

where

$$H^{\text{eff}}_{a'v',av}=\langle\Phi_{a'v'}(JM)|H(1+\chi_{av})|\Phi_{av}(JM)\rangle. \tag{2.10}$$

In the pair approximation the correlation operator χ_{av} is defined as

$$\begin{aligned}\chi_{av}a_v^\dagger a_a|0_C\rangle=\Bigg(&\frac{1}{2}\sum_{r,s,b,c}\chi_{bc}^{rs}a_r^\dagger a_s^\dagger a_c a_b a_v^\dagger a_a\\&+\sum_{s,b,c}\chi_{bc}^{as}a_s^\dagger a_c a_b a_v^\dagger+\sum_{r,b}\chi_b^r a_r^\dagger a_b a_v^\dagger a_a\\&+\sum_{b\neq a}\chi_b^a a_b a_v^\dagger+\sum_{r,s,b}\chi_{vb}^{rs}a_r^\dagger a_s^\dagger a_b a_a\\&+\sum_{s,b\neq v,a}\tilde{\chi}_{vb}^{as}a_s^\dagger a_b+\sum_{r\neq v}\chi_v^r a_r^\dagger a_a+\chi_v^a\Bigg)|0_C\rangle,\end{aligned} \tag{2.11}$$

with tilded objects denoting the inclusion of exchange parts (i.e., $\tilde{\chi}_{vb}^{as}=\chi_{vb}^{as}-\chi_{bv}^{as}$). All the correlation coefficients of the second part of Eq. (2.11) are evaluated from a system of coupled algebraic equations presented in Ref. [5]. In this previous work, only the relatively small class of coefficients associated with the dominant core-hole correlation corrections to the energies were calculated to all orders. The rest, and among them those associated with the random-phase approximation [85,65], were calculated only in second-order perturbation theory since their contribution to transition energies was small due to strong cancellations. However, the contribution of these terms plays a very important role in the computation of transition matrix elements and a complete all-order calculation for all the correlation coefficients is carried out in the present work.

The correlated core wave function $|\Psi_C\rangle$ is obtained from the coefficients of the first and third terms of Eq. (2.11) [84],

$$|\Psi_C\rangle=(1+\chi_C)|0_C\rangle, \tag{2.12}$$

where

$$\chi_C|0_C\rangle=\left(\frac{1}{2}\sum_{r,s,b,c}\chi_{bc}^{rs}a_r^\dagger a_s^\dagger a_c a_b+\sum_{r,b}\chi_b^r a_r^\dagger a_b\right)|0_C\rangle. \tag{2.13}$$

Therefore after solving for the operator χ_{av} we can proceed directly into the evaluation of the dipole matrix element,

$$M_{ph}=\frac{\langle\Psi_{ph}(JM)|d|\Psi_C\rangle}{[\langle\Psi_{ph}(JM)|\Psi_{ph}(JM)\rangle\langle\Psi_C|\Psi_C\rangle]^{1/2}}, \tag{2.14}$$

where

$$d=\sum_{j,k} a_j^\dagger a_i d_{jk}. \tag{2.15}$$

In length form

$$d_{jk}=\langle j|\mathbf{r}|k\rangle \tag{2.16}$$

and in velocity form

$$d_{jk}=i\frac{c}{E_{ph}}\langle j|\boldsymbol{\alpha}|k\rangle, \tag{2.17}$$

where E_{ph} is the particle-hole transition energy and $\boldsymbol{\alpha}$ stands for the Dirac matrices.

To avoid the size inconsistent disconnected terms resulting from a direct calculation of matrix elements via Eq. (2.14), we use instead a formula that includes only connected terms [3],

$$M_{ph}=\frac{\langle\Psi_{ph}(JM)|d|\Psi_C\rangle_{\text{conn}}}{\langle\Psi_{ph}(JM)|\Psi_{ph}(JM)\rangle_{\text{conn}}^{1/2}}, \tag{2.18}$$

where

$$\langle\Psi_{ph}|d|\Psi_C\rangle_{\text{conn}}=\sum_{a,v}C_{av}\langle\Phi_{av}(JM)|(1+\chi_{av}^\dagger)\times d(1+\chi_C)|0_C\rangle_{\text{conn}} \tag{2.19}$$

and the norm term is

$$\langle\Psi_{ph}(JM)|\Psi_{ph}(JM)\rangle_{\rm conn}^{1/2}=\left(1+\sum_{(av),(a'v')}C_{av}C_{a'v'}\langle\Phi_{av}(JM)|\chi_{av}^{\dagger}\chi_{a'v'}|\Phi_{a'v'}(JM)\rangle_{\rm conn}\right)^{1/2}. \tag{2.20}$$

This result holds for exact wave functions and it can be proved essentially in the same way as in the case of the evaluation of matrix elements of systems with one electron outside a closed shell (Appendix of Ref. [3]).

The term (2.20) for the norm can be calculated by making a simple modification to Eq. (2.10) for the $H^{\rm eff}$ while the analytical expressions for Eq. (2.19) are

$$\begin{aligned}\langle\Phi_{av}(JM)|(1+\chi_{av}^{\dagger})d(1+\chi_C)|0_C\rangle_{\rm conn}&=d_{va}^{[T_0]}+\sum_{b,m}^{[T_1]}d_{bm}\tilde{\chi}_{ba}^{mv}\\&+\sum_{b,m}^{[T_2]}d_{mb}\tilde{\chi}_{ma}^{bv}+\sum_{m}^{[T_3]}d_{ma}\chi_m^v+\sum_{m}^{[T_4]}d_{vm}\chi_a^m-\sum_{b}^{[T_5]}d_{ba}\chi_b^v\\&-\sum_{b}^{[T_6]}d_{vb}\chi_a^b+T_{G_{\rm RPA}}+T_{G_{\rm BO}}+T_{G_{\rm SR}},\end{aligned} \tag{2.21}$$

where

$$T_{G_{\rm RPA}}=\sum_{b,c,m,n}\tilde{\chi}_{am}^{vb}d_{cn}\tilde{\chi}_{cb}^{nm}+\sum_{b,c,m,n}\tilde{\chi}_{mn}^{cb}d_{mb}\tilde{\chi}_{ac}^{nv}, \tag{2.22}$$

$$\begin{aligned}T_{G_{\rm BO}}=&\sum_{b,c,m,n}\chi_{mn}^{vc}d_{ba}\tilde{\chi}_{bc}^{nm}+\sum_{b,c,m,n}\chi_{mn}^{cb}d_{vb}\tilde{\chi}_{ac}^{mn}\\&+\sum_{b,c,m,n}\chi_{mn}^{cb}d_{ma}\tilde{\chi}_{cb}^{nv}+\sum_{b,m,n}\tilde{\chi}_{mn}^{vb}d_{ma}\chi_b^n\\&+\sum_{b,m,n}\chi_n^b d_{vm}\tilde{\chi}_{ab}^{mn}+\sum_{b,c,m}\tilde{\chi}_{am}^{bc}d_{vc}\chi_b^m\\&+\sum_{b,c,m,n}\chi_{am}^{cb}d_{vn}\tilde{\chi}_{bc}^{nm}+\sum_{b,c,m}\chi_m^b d_{ca}\tilde{\chi}_{bc}^{vm}\\&-\sum_{b,m}\chi_m^b d_{ma}\chi_b^v-\sum_{b,m}\chi_m^b d_{vb}\chi_a^m-\sum_{b,m}\chi_a^b d_{vm}\chi_b^m\\&-\sum_{b,m}\chi_m^v d_{ba}\chi_b^m+\sum_{m,n}\chi_m^v d_{mn}\chi_a^n+\sum_{b,c}\chi_a^c d_{bc}\chi_b^v,\end{aligned} \tag{2.23}$$

$$\begin{aligned}T_{G_{\rm SR}}=&\sum_{b,c,m}\tilde{\chi}_{am}^{bv}d_{cb}\chi_c^m+\sum_{b,c,d,m}\tilde{\chi}_{am}^{cb}d_{db}\tilde{\chi}_{dc}^{mv}\\&+\sum_{b,c,m,n}\chi_{mn}^{vb}d_{cb}\tilde{\chi}_{ac}^{nm}+\sum_{b,m,n}\tilde{\chi}_{am}^{vb}d_{mn}\chi_b^n\\&+\sum_{b,m,n}\chi_m^v d_{bn}\tilde{\chi}_{ba}^{nm}+\sum_{b,m,n}\tilde{\chi}_{mn}^{vb}d_{nb}\chi_a^m\\&+\sum_{b,m,n,r}\tilde{\chi}_{mn}^{vb}d_{mr}\tilde{\chi}_{ab}^{rn}+\sum_{b,c,m}\tilde{\chi}_{am}^{cb}d_{mc}\chi_b^v\\&+\sum_{b,m,n}\chi_m^b d_{mn}\tilde{\chi}_{ab}^{vn}+\sum_{b,c,m}\chi_m^b d_{cb}\tilde{\chi}_{ca}^{vm}\\&+\sum_{b,c,m,n}\chi_{am}^{cb}d_{mn}\tilde{\chi}_{cb}^{nv}+\sum_{b,c,m}\chi_a^b d_{cm}\tilde{\chi}_{bc}^{mv}.\end{aligned} \tag{2.24}$$

The first seven terms in Eq. (2.21) have been named over the summation symbols in reference to their numerical breakdown for the case of krypton presented in Table V. The remaining terms that correspond to the $\langle\Phi_{av}(JM)|\chi_{av}^{\dagger}d\chi_C|0_C\rangle_{\rm conn}$ part of the left-hand side of Eq. (2.21) are grouped following Ref. [88] as they enter in perturbation theory from the first-order approximation to the correlation operator. They form subsets of the RPA, Brueckner [89], and structural radiation type [90] of corrections and are designated as $T_{G_{\rm RPA}}$, $T_{G_{\rm BO}}$, and $T_{G_{\rm SR}}$, respectively. Each member of these groups had to be calculated independently. The remaining terms of these types that appear in perturbation theory start from the second-order approximation to the correlation operator and are directly incorporated in terms $T_1,\ldots,T_6$ after the first iteration.

The absorption oscillator strength is defined [91]

$$f_{\rm absorption}=\frac{2}{3}E_{ph}|M_{ph}|^2. \tag{2.25}$$

The numerical calculations were performed on the two alpha stations available in our group. Due to the neutral nature of the systems, convergence was a serious concern. For the core-hole correlation corrections, we used the approach of Ref. [5]. In addition, a mixing ratio of 0.7 between the results of successive iterations was necessary to obtain convergence for the pair-core-valence and single-valence correlation coefficients corresponding to the sixth and seventh terms of Eq. (2.11). At least ten iterations were necessary to make the transition energies converge to a level of 10^{-5} a.u. This numerical accuracy was considered sufficient, since the agreement with the experimental values [92] of order 10^{-1} a.u. was at the 1% level. This difference must be attributed to the missing correlations from the triple and quadruple excitations since the corrections from the Breit interaction were found at the level of 10^{-4} a.u.

III. RESULTS

For the cases of neon, argon, and krypton, we started from an almost degenerate two dimensional model space where the unperturbed state vectors designated by relation (2.8) were constructed as linear combinations of particle-hole states having $a=np_{3/2}$ or $np_{1/2}$ and $v=(n+1)s_{1/2}$ coupled to $J=1$ with $n=2$, 3, and 4, respectively. The corresponding ratio of the absolute values of the larger over the smaller mixing coefficients C_{av} resulting from the eigenvalue equation (2.9) was 0.751 for neon, 0.518 for argon, and 0.167 for krypton showing a domination of the jj coupling scheme as we go to heavier systems. In all cases we used experimental energies for the calculation of oscillator strengths. The f values for neon are presented in Table I. This system is strongly nonrelativistic with significant mixing between the members of the model space. We found 8% disagreement between length and velocity forms for the $[2p_{1/2}^{-1}3s_{1/2}]_1$ state and 5%

TABLE I. Comparison of the calculated oscillator strengths of the $[2p_{3/2}^{-1}3s_{1/2}]_1$ and $[2p_{1/2}^{-1}3s_{1/2}]_1$ states of neon with experiment and other theoretical calculations.

Author	$[2p_{3/2}^{-1}3s_{1/2}]_1$	$[2p_{1/2}^{-1}3s_{1/2}]_1$
	Transition energies (a.u.)	
This work	0.6095	0.6160
Experiment [92]	0.6127	0.6192
	Oscillator strengths	
This work		
Length (l)	0.0163	0.161
Velocity (v)	0.0156	0.147
Experiment		
Zhong *et al.* (1997) [17]	0.0124±0.0038	0.156±0.009
Gibson and Risley (1995) [19]	0.01095±0.00032	0.1432±0.0038
Curtis *et al.* (1995) [23]	0.0084±0.0003	0.165±0.011
Suzuki *et al.* (1994) [27]	0.0106±0.0014	0.137±0.018
Ligtenberg *et al.* (1994) [28]	0.01017±0.00030	0.1369±0.0035
Chan *et al.* (1992) [29]	0.0118±0.0006	0.159±0.008
Tsurubuchi *et al.* (1990) [22]	0.0122±0.0006	0.123±0.006
Chornay *et al.* (1984) [33]	0.012±0.004	
Aleksandrov *et al.* (1983) [35]	0.012±0.003	0.144±0.024
Westerveld *et al.* (1979) [39]	0.0109±0.0008	0.147±0.012
Bhaskar and Lurio (1976) [44]	0.0122±0.0009	0.148±0.014
Knystautas and Drouin (1974) [46]	0.0078±0.0008	0.161±0.011
Irwin *et al.* (1973) [49]		0.158±0.006
de Jongh and Van Eck (1971) [48]		0.134±0.010
Kazantsev and Chaika (1971) [53]	0.0138±0.0008	
Kernahan *et al.* (1971) [54]	0.0084±0.0007	0.187±0.014
Geiger (1970) [55]	0.009±0.002	0.131±0.026
Lawrence and Liszt (1969) [56]	0.0078±0.0004	0.130±0.013
Kuhn *et al.* (1967) [60]	0.012±0.002	0.168±0.002
Theory		
Hibbert *et al.* (1993) [66] (Configuration interaction)	0.0123(l)	0.1607(l)
Amusia and Cherepkov (1975) [65] (Random-phase approximation)		0.163 (f_1+f_2)
Aleksandrov *et al.* (1983) [35] (Intermediate coupling)	0.0106	0.141
Stewart (1975) [72] (Time-dependent Hartree-Fock)		0.159
Albat and Gruen (1974) [75] (Configuration interaction)	0.0113	0.149
Gruzdev and Loginov (1973) [78] (Multiconfiguration Hartree-Fock)	0.0106	0.138
Aymar *et al.* (1970) [69] (Parametrized potential)	0.0121(l) 0.0100(v)	0.161(l) 0.130(v)
Gruzdev (1967) [80] (Intermediate coupling)	0.035	0.160
Kelly (1964) [82] (Hartree-Fock-Slater)		0.188 (f_1+f_2)
Cooper (1962) [83] (Hartree-Fock)		0.163 (f_1+f_2)

for the $[2p_{3/2}^{-1}3s_{1/2}]_1$ state. In the first case, the estimated oscillator strength agrees with most of the experimental measurements while in the second, it is overestimated but still close to the estimated error of the experiments that support the larger f value. This discrepancy for the neon intercombination line is attributed to the fact that due to the strong mixing, the components of the numerator of Eq. (2.18) are close in absolute values and with opposite signs leading to a

TABLE II. Comparison of the calculated oscillator strengths of the $[3p_{3/2}^{-1}4s_{1/2}]_1$ and $[3p_{1/2}^{-1}4s_{1/2}]_1$ states of argon with experiment and other theoretical calculations.

Author	$[3p_{3/2}^{-1}4s_{1/2}]_1$	$[3p_{1/2}^{-1}4s_{1/2}]_1$
	Transition energies (a.u.)	
This work	0.4307	0.4385
Experiment [92]	0.4272	0.4347
	Oscillator strengths	
This work		
Length (l)	0.0672	0.248
Velocity (v)	0.0670	0.242
Experiment		
Gibson and Risley (1995) [19]	0.0580 ± 0.0017	0.2214 ± 0.0068
Wu *et al.* (1995) [24]	0.0676 ± 0.0040	0.259 ± 0.015
Ligtenberg *et al.* (1994) [28]	0.0616 ± 0.0021	0.2297 ± 0.0093
Chan *et al.* (1992) [20]	0.0662 ± 0.0033	0.265 ± 0.013
Tsurubuchi *et al.* (1990) [22]	0.057 ± 0.003	0.213 ± 0.011
Li *et al.* (1988) [31]	$0.058^{+0.005}_{-0.008}$	$0.222^{+0.02}_{-0.03}$
Chornay *et al.* (1984) [33]	0.065 ± 0.005	
Hahn and Schwentner (1980) [38]	0.077 ± 0.004	0.361 ± 0.060
Westerveld *et al.* (1979) [39]	0.063 ± 0.005	0.240 ± 0.020
Vallee *et al.* (1977) [41]	0.051 ± 0.007	0.210 ± 0.030
Copley and Camm (1974) [47]	0.076 ± 0.008	0.283 ± 0.024
McConkey and Donaldson (1973) [51]	0.096 ± 0.002	
Irwin *et al.* (1973) [50]	0.083 ± 0.027	0.35 ± 0.13
de Jongh and Van Eck (1971) [48]		0.22 ± 0.02
Geiger (1970) [55]	0.047 ± 0.009	0.186 ± 0.037
Lawrence (1968) [59]	0.059 ± 0.003	0.228 ± 0.021
Lewis (1967) [60]	0.063 ± 0.003	0.278 ± 0.020
Theory		
Amusia and Cherepkov (1975) [65] (Random-phase approximation)		0.298 (f_1+f_2)
Stewart (1975) [72] (Time-dependent Hartree-Fock)		0.270
Albat *et al.* (1975) [73] (Multiconfiguration Hartree-Fock)	0.048	0.188
Gruzdev and Loginov (1975) [74] (Multiconfiguration Hartree-Fock)	0.061	0.231
Lee (1974) [76] (Multichannel quantum defect)	0.059	0.30
Lee and Lu (1973) [77] (Multichannel quantum defect)	0.080	0.21
Aymar *et al.* (1970) [69] (Parametrized potential)	0.071(l) 0.065(v)	0.286(l) 0.252(v)
Gruzdev (1967) [80] (Intermediate coupling)	0.075	0.150
Cooper (1962) [83] (Hartree-Fock)		0.330 (f_1+f_2)

small reduced matrix element which is much more sensitive to correlation corrections than in all the other cases. In Table II, we present our results for the $[3p_{3/2}^{-1}4s_{1/2}]_1$ and $[3p_{1/2}^{-1}4s_{1/2}]_1$ states of argon. In this case, the difference between length and velocity is improved to less than 3% while further improvement to 1% level was found for the $[4p_{3/2}^{-1}5s_{1/2}]_1$ and $[4p_{1/2}^{-1}5s_{1/2}]_1$ states of krypton as shown in Table III. For xenon, we considered only the lowest

TABLE III. Comparison of the calculated oscillator strengths of the $[4p_{3/2}^{-1}5s_{1/2}]_1$ and $[4p_{1/2}^{-1}5s_{1/2}]_1$ states of krypton with experiment and other theoretical calculations.

Author	$[4p_{3/2}^{-1}5s_{1/2}]_1$	$[4p_{1/2}^{-1}5s_{1/2}]_1$
	Transition energies (a.u.)	
This work	0.3716	0.3943
Experiment [92]	0.3687	0.3912
	Oscillator strengths	
This work		
Length (l)	0.200	0.190
Velocity (v)	0.198	0.192
Experiment		
Molino *et al.* (1996) [18]	0.18 ± 0.01	0.17 ± 0.01
Gibson and Risley (1995) [19]	0.1775 ± 0.0050	0.1416 ± 0.0041
Ligtenberg *et al.* (1994) [28]	0.1751 ± 0.0049	0.1496 ± 0.0038
Chan *et al.* (1992) [20]	0.214 ± 0.011	0.193 ± 0.010
Takayanagi *et al.* (1990) [21]	0.143 ± 0.015	0.127 ± 0.015
Tsurubuchi *et al.* (1990) [22]	0.155 ± 0.011	0.139 ± 0.010
Ferrell *et al* (1987) [32]		0.180 ± 0.027
Hahn and Schwentner (1980) [38]	0.235 ± 0.019	0.168 ± 0.027
Geiger (1977) [70]	0.195 ± 0.039	0.173 ± 0.035
Matthias *et al.* (1977) [42]	0.208 ± 0.006	0.197 ± 0.006
Delâge and Carette (1976) [45]	0.170 ± 0.006	0.176 ± 0.006
de Jongh and Van Eck (1971) [48]		0.142 ± 0.015
Geiger (1970) [55]	0.173 ± 0.035	0.173 ± 0.035
Griffin and Hutcherson (1969) [57]	0.187 ± 0.006	0.193 ± 0.009
Vaughan (1968) [58]	0.204 ± 0.020	0.184 ± 0.020
Chashchina and Shreider (1967) [61]	0.21 ± 0.05	0.21 ± 0.05
Lewis (1967) [60]	0.204 ± 0.010	0.184 ± 0.010
Theory		
Kim (1993) [67]	$0.208\pm15\%$	$0.166\pm15\%$
(Multiconfiguration Dirac-Fock)		
Amusia and Cherepkov (1975) [65]		0.353 (f_1+f_2)
(Random-phase approximation)		
Aymar and Coulombe (1978) [68]	0.176(l)	0.177(l)
(Parametrized potential)	0.193(v)	0.172(v)
Geiger (1977) [70]	0.250	0.143
(Quantum defect)		
Gruzdev and Loginov (1975) [71]	0.190	0.177
(Multiconfiguration Hartree-Fock)		
Aymar *et al.* (1970) [69]	0.215(l)	0.215(l)
(Parametrized potential)	0.185(v)	0.164(v)
Gruzdev (1967) [80]	0.20	0.20
(Intermediate coupling)		

$[5p_{3/2}^{-1}6s_{1/2}]_1$ resonance state (Table IV), since it is energetically well separated and can be treated starting from a one dimensional model space. Contrary to the previous cases, where the complete core was considered in the correlation corrections, the active core here starts from the $4s$ shell. This constraint slightly affects the agreement between length and velocity forms which is still at the 3% level. To facilitate the presentation of the experimental status and in relation to our calculations, we display the experimental f values for the cases under consideration in Fig. 1 for neon and argon and Fig. 2 for krypton and xenon in reference to the year of their corresponding publication. The horizontal lines in these figures refer to the average of our calculated values in length and velocity forms. Recent reviews of the experimental situation as well as the relative advantages of the applied methods can be found in Refs. [20,25,26,29]. The main fea-

TABLE IV. Comparison of the calculated oscillator strengths of the $[5p_{3/2}^{-1}6s_{1/2}]_1$ state of xenon with experiment and other theoretical calculations.

Author	$[5p_{3/2}^{-1}6s_{1/2}]_1$
	Transition energy (a.u.)
This work	0.3134
Experiment [92]	0.3100
	Oscillator Strengths
This work	
Length (l)	0.249
Velocity (v)	0.256
Experiment	
Molino *et al.* (1996) [18]	0.260±0.010
Anderson *et al.* (1995) [25]	0.264±0.016
Chan *et al.* (1992) [20]	0.273±0.014
Suzuki *et al.* (1991) [30]	0.222±0.027
Ferrell *et al.* (1987) [32]	0.260±0.050
Salamero *et al.* (1984) [34]	0.226±0.026
Bideau-Mehu *et al.* (1981) [36]	0.268±0.008
Smith *et al.* (1981) [37]	0.244±0.015
Wieme and Vanmarcke (1979) [40]	0.226±0.025
Matthias *et al.* (1977) [42]	0.263±0.007
Delâge and Carette (1976) [43]	0.183±0.073
Wieme and Mortier (1973) [52]	0.214±0.020
Geiger (1970) [55]	0.26±0.05
Wilkinson (1966) [62]	0.26±0.02
Chashchina and Shreider (1966) [63]	0.28±0.05
Anderson (1965) [64]	0.256±0.008
Theory	
Aymar and Coulombe (1978) [68]	0.282(l)
(Parametrized potential)	0.294(l)
Geiger (1977) [70]	0.28
(Quantum defect)	
Aymar *et al.* (1970) [69]	0.273(l)
(Parametrized potential)	0.176(v)
Kim *et al.* (1968) [79]	0.212
(Hartree-Fock)	
Gruzdev (1967) [80]	0.28
(Intermediate coupling)	
Dow and Knox (1966) [81]	0.194
(Hartree-Fock)	

tures of our calculation for the transition matrix elements are displayed in Table V where the norm term from Eq. (2.20) as well as a breakdown of the correlation contributions for the case of krypton in correspondence to Eqs. (2.19) and (2.21) are presented. In the first and third pairs of columns, the contributions are obtained from the lowest-order correlation coefficients as well as the mixing coefficients resulting from the diagonalization of H^{eff} in second-order perturbation theory. The second and fourth pairs of columns include the

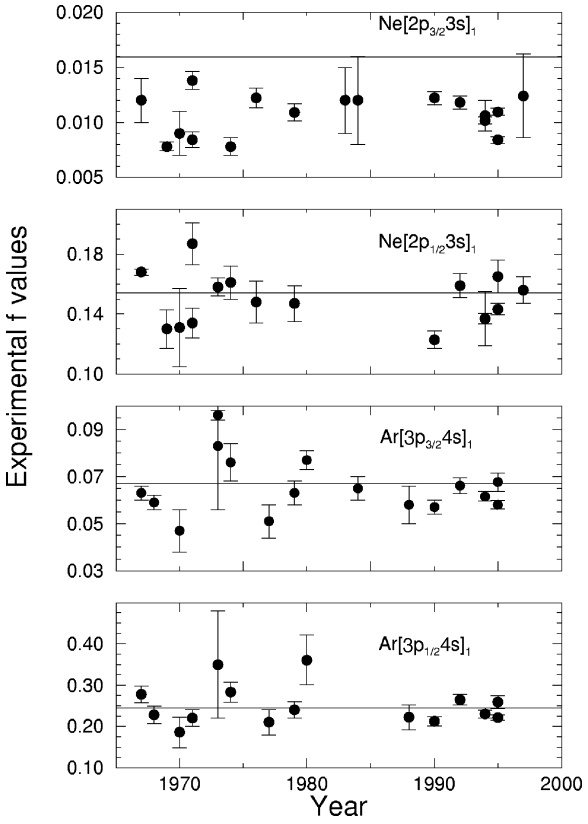

FIG. 1. Experimental f values for the $[2p_{3/2}^{-1}3s_{1/2}]_1$ and $[2p_{1/2}^{-1}3s_{1/2}]_1$ states of neon and the $[3p_{3/2}^{-1}4s_{1/2}]_1$ and $[3p_{1/2}^{-1}4s_{1/2}]_1$ states of argon. The horizontal lines refer to the average of our calculated f values in length and velocity forms.

corrections resulting from the correlation coefficients in the all-order approximation. We see that up to second order, there is poor agreement between the two forms while after the all-order approach, a more than 99% agreement has been

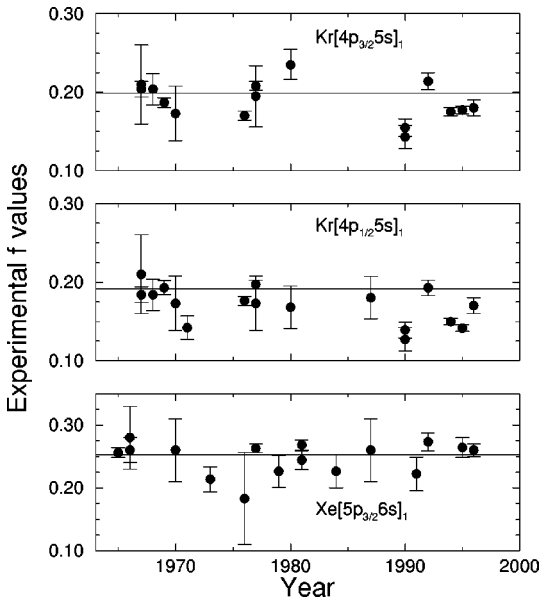

FIG. 2. Experimental f values for the $[4p_{3/2}^{-1}5s_{1/2}]_1$ and $[4p_{1/2}^{-1}5s_{1/2}]_1$ states of krypton and the $[5p_{3/2}^{-1}6s_{1/2}]_1$ state of xenon. The horizontal lines refer to the average of our calculated f values in length and velocity forms.

TABLE V. Breakdown of the contributions to the transition matrix element for the $[4p_{3/2}^{-1}5s_{1/2}]_1$ and $[4p_{1/2}^{-1}5s_{1/2}]_1$ states of krypton.

	$[4p_{3/2}^{-1}5s_{1/2}]_1$				$[4p_{1/2}^{-1}5s_{1/2}]_1$			
	Up to second order		All orders		Up to second order		All orders	
	Length	Velocity	Length	Velocity	Length	Velocity	Length	Velocity
T_0	1.031687	1.042169	0.964641	0.970267	0.798540	0.809619	0.881882	0.888802
T_1	−0.036356	−0.068388	−0.024933	−0.059234	−0.023247	−0.072135	−0.020193	−0.071635
T_2	0.279855	0.534677	0.098824	0.237896	0.274428	0.491167	0.127364	0.264460
T_3	−0.421006	−0.627840	−0.129569	−0.191457	−0.335184	−0.493064	−0.121756	−0.177256
T_4	0.000000	0.000000	−0.025319	0.000563	0.000000	0.000000	−0.022634	−0.000657
T_5	0.000000	0.000000	0.011583	−0.016547	0.000000	0.000000	0.011416	−0.014905
T_6	0.000000	0.000000	0.000078	0.001585	0.000000	0.000000	0.000075	0.001494
$T_{G_{\mathrm{RPA}}}$	0.011977	−0.106839	0.002383	−0.021045	0.000634	−0.068764	−0.001908	−0.013310
$T_{G_{\mathrm{B0}}}$	0.044527	−0.084310	0.016397	−0.029327	0.039744	−0.062961	0.018263	−0.025987
$T_{G_{\mathrm{SR}}}$	0.042027	0.078728	0.006716	0.023165	0.029086	0.094427	0.003887	0.030080
Total	0.952711	0.768199	0.920800	0.915864	0.784000	0.698289	0.876395	0.881087
Norm	1.042183		1.020576		1.049612		1.025879	

established. The terms that do not contribute in the first and third pairs of columns involve the χ_b^m and χ_b^a correlation coefficients from single excitations. These are zero in lowest order because of the choice of the V^{N-1} potential. The term T_0 refers to the lowest-order correction. For this term, there is always good agreement between length and velocity but in second order this agreement is effected mainly because of the sensitivity of the velocity form to the correlation corrections. In the all-order approach, however, this agreement between length and velocity is clearly restored. Terms T_2 and T_3 dominate the correlation corrections. They involve the most singular terms $\tilde{\chi}_{vb}^{am}$ and χ_v^m while in the all-order approach they include the most important type of corrections corresponding to the Tamm-Dancoff approximation [93]. The small overall correction with respect to T_0 reflects the strong cancellations that take place among the correlation corrections as well as the importance of mixing and consequently that of the proper coupling scheme.

With respect to the existing theoretical calculations, formally closer to our method is the nonrelativistic RPA calculation of Amusia and Cherepkov [65]. In comparison to this work, the sums of our calculated f values progressively disagree when we go to the heavier noble gases as expected due to the enhanced significance of relativistic effects and our inclusion of correlation corrections beyond the RPA level. For the case of krypton, we are relatively close to the relativistic multiconfiguration calculation of Kim [67] where 15% difference between length and velocity forms has been quoted. For the case of neon, there is the recent semiempirical calculation of Hibbert *et al.* [66] where the quoted f values in length form are closest to most of the experiments. Of particular importance is also the semiempirical calculation of Aymar *et al.* [69], where the inclusion of second-order corrections led to relatively big disagreement between length and velocity forms.

From the experimental standpoint, even though many measurements have been performed, their values are still rather dispersed. In general, our calculation supports the relatively larger experimental oscillator strengths.

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