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Quantum-defect studies of systematic trends of f values

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The dependence of f values on the reciprocal of the nuclear charge in the sequence is discussed on the basis of quantum-defect computations through three different formulations of the transition dipole moment. Several simple systems are studied.

I. INTRODUCTION

The current interest in astrophysical and controlled thermonuclear fusion calls for accurate theoretical f values, in particular for highly charged ions in the lithium sequence among others.[1,2] In addition, the behavior of f values of a particular transition through an isoelectronic sequence is an important feature in evaluating the reliability of theoretical predictions as well as experimental determinations.

The quantum-defect-orbital (QDO) formalism[3-5] was originally proposed for generating approximate valence and Rydberg orbitals from spectral data. The analytical form of the orbitals allows the analytical determinations of closed-form expressions for various quantities; in the case of transition integrals a simple relationship involving quantum numbers and quantum defects is generated.[4,5] The method has been applied to compute atomic transition probabilities, including resonances and autoionization effects.[3-11]

II. METHOD OF CALCULATION

A complete description of the QDO formalism has been presented in previous papers.[3-11] It may therefore suffice here to summarize its most relevant aspects. It is based on the analytical solution of the one-electron Schrödinger equation containing an effective central-field electron screening potential (in atomic units):

$$V(r)=\frac{\lambda(\lambda+1)-l(l+1)}{2r^2}-\frac{Z_{\rm net}}{r} \tag{1}$$

where $Z_{\rm net}$ is the effective nuclear charge at large radial distances ($Z_{\rm net}=Z-N+1$ for a system with a nuclear charge Z and N electrons), and the parameter λ, which determines the screening aspects of the model potential, is related to the azimuthal quantum number l through the general expression

$$\lambda=l-\delta+c\ . \tag{2}$$

δ is the quantum defect for the electronic state considered obtained from empirical spectral level data and c is an integer whose allowed range of values is determined by imposing the following conditions. (a) The radial orbitals can be normalized. (b) The virial theorem is satisfied.

The quantum defect orbital formalism offers several advantages over other methods, namely, the following.

(i) One can obtain analytic eigen wave functions.

(ii) Transition integrals can be solved in an analytical way leading to closed-form expressions.

(iii) Atomic properties can be studied without prolonged mathematical formalism and computation time.

III. THE OSCILLATOR STRENGTH

The concept of oscillator strength or f value of a transition provides a useful tool to theoreticians to test the quality of a atomic model since it is related to observable magnitudes. The oscillator strength for the $i\rightarrow j$ transition between two states i and j is defined (in atomic units) as

$$f_{i\rightarrow j}=\frac{2\Delta E|M_{ij}|^2}{3} \tag{3}$$

where ΔE is (in atomic units) the energy difference between the final and initial states, and M_{ij} is the dipole matrix element for the valence-electron transition. After performing the relevant angular integration, the calculation of oscillator strength reduces to computing the radial matrix element R_{ij},

$$R_{ij}=\langle R_j(r)|D(r)|R_i(r)\rangle\ , \tag{4}$$

where $D(r)$ is the dipole transition operator and $R_j(r)$ and $R_i(r)$ the valence-electron radial wave functions of the states under consideration.

There are several equivalent formulas for calculating the oscillator strength for an electric dipole transition. Of these the most important ones are the dipole length form

$$f^L_{i\rightarrow j}=\frac{2\Delta E|\langle\Psi_j|r|\Psi_i\rangle|^2}{3} \tag{5}$$

and the dipole velocity form

$$f^V_{i\rightarrow j}=\frac{2\Delta E^{-1}|\langle\Psi_j|\nabla|\Psi_i\rangle|^2}{3} \tag{6}$$

where Ψ_j and Ψ_i are the one-electron wave functions $[\Psi(r,\theta,\varphi)=R(r)Y(\theta,\varphi)]$. The main contributions to the above integrals come from different regions in space. It has been argued that spatial regions relatively distant from the nucleus and unimportant to the energy can contribute significantly to the length f value, whereas contributions to the velocity f values are mainly from energy important regions.

In practice, calculations are frequently made using both length and velocity forms. Seaton[12] suggested that the geometric mean should be taken since it enables the oscillator strength to be expressed independently of the energy, and the Thomas-Reiche-Kuhn sum rule may be applied to calculations with approximate wavefunctions. Hansen[13] also advocate the geometric mean and demonstrate that this is affected by the perturbation only in second order. Roginsky, Clapisch, and Cohen[14] and Laughlin[15] have used a linear combination of length and velocity forms and tested it on heliumlike and $H_2{}^+$ transitions respectively. Since it is rare for the length and velocity results to differ by a factor of more than 2, it follows that usually the geometric mean will differ by only a very few percent from the arithmetic mean.

Core polarization effects are particularly important for orbitals of low angular momenta in the lighter ions for which $l \leq 1$ and $Z \leq 6$.[16] In our formalism we have chosen a treatment leading to the introduction of a correction term in the dipole matrix element. The explicit form of the dipole operator is now[17]

$$D(r)=r\left[1-\frac{\alpha[1-\exp(-r/r_c)^3]}{r^3}\right] \tag{7}$$

where α is the dipole polarizability of the core; the term $[1-\exp(r/r_c)^3]$ is a factor that tends to limit the polarization effect inside the core; and r_c is a cutoff radius whose value is of the same order of magnitude as the mean radius of the core obtained with the QDO wave functions.

Systematic trends for atomic oscillator strengths of a given transition along an isoelectronic sequence were first established by Wiese and Weiss[18] and Wiese.[19,20] Since then, many authors have studied these trends by analyzing the behavior of different transitions in different isoelectronic sequences, e.g., Refs. 21–30. The regular behavior of oscillator strengths along isoelectronic sequences has proven to be a useful tool to facilitate the evaluation of existing data. It has also made possible the determination of additional numerical data by simple interpolation or extrapolation techniques.

The oscillator strength for a fixed transition within an isoelectronic sequence may be written as a series expansion in inverse powers of the nuclear charge Z:

$$f=f_0+f_1Z^{-1}+f_2Z^{-2}+\cdots=\sum_{i=0}^{\infty} f_i Z^{-i} . \tag{8}$$

In the limit of $1/Z \rightarrow 0$, the oscillator strength approaches asymptotically the lead term f_0 which is a hydrogenic quantity.

IV. RESULTS AND DISCUSSION

With the use of empirical energy-level data,[31] we have performed several sets of computations of oscillator strengths involving the principal series ($2s\,{}^2S \rightarrow np\,{}^2P^\circ$ transitions, $n=2-7$) for each of the members of the lithium isoelectronic sequence (Li I–Si XII).

The f values were first computed through the length form Eq. (5) of the dipole transition operator. Secondly, the velocity form Eq. (6) was used. We have also included in the tables the geometric mean of the two types of f values.

In addition, we have calculated oscillator strengths with explicit introduction of core-valence polarization effects in the dipole transition operator Eq. (7). For Li I to C IV the static core dipole polarizabilities were taken from Ref. 32 which correspond to experimental data; for the remaining ions N V–Si XII we only found computed values through a Thomas-Fermi model.[33]

The cutoff radius r_c has been taken as the mean radius of the core obtained with the QDO functions because there is no analytical way of obtaining r_c. Anyway, several calculations were performed with different r_c values and, in this particular isoelectronic sequence, the matrix elements were relatively insensitive to the value of r_c employed.

Since a large amount of comparative theoretical and experimental data is available in the literature for the $2s\,{}^2S \rightarrow np\,{}^2P^\circ$ transitions in Li I, especially for the lower transitions, and, in order to visualize better the accuracy of our f values, we present in Tables I and II oscillator strengths corresponding to $2s\,{}^2S \rightarrow 2p\,{}^2P^\circ$ and $2s\,{}^2S \rightarrow 3p\,{}^2P^\circ$ transitions, respectively for this element.

The f values from different sources are classified, in these tables, in three groups: experimental, semiempirical, and *ab initio* results. Within the experimental set we have included different data running from that of an early work of Filippov[39] to the recent measurement of Gaupp, Kuske, and Andrä,[34] who have reached great accuracy with a fast-beam laser technique. In addition, we have introduced in this group oscillator strengths from a critical compilation by Martin and Wiese.[40] In the second group, we included our present QDO f values together with other semiempirical results of different degrees of complexity, from a numerical Coulomb approximation (CA),[41] to those which explicitly account for core polarization effects.[16,17,41,45] Finally, in the third group, oscillator strengths from *ab initio* calculations are given. As in the preceding group, we have included results computed with different methods, from the simplest, Hartree-Fock (HF),[46] to those which introduce relativistic effects.[47,46,50] A special mention is deserved of the first *ab initio* correlation calculation for the resonance transition by Weiss.[54] As early as 1963, Weiss computed oscillator strengths for the $2s\,{}^2S \rightarrow 2p\,{}^2P^\circ$ transition of some species of the lithium isoelectronic sequence with a high degree of accuracy by employing a 45-term configuration interaction wave function for both states. f values in both the dipole-length and dipole-velocity forms are given along the tables.

When cross examining Tables I and II, a few features become apparent, of which the following may be relevant.

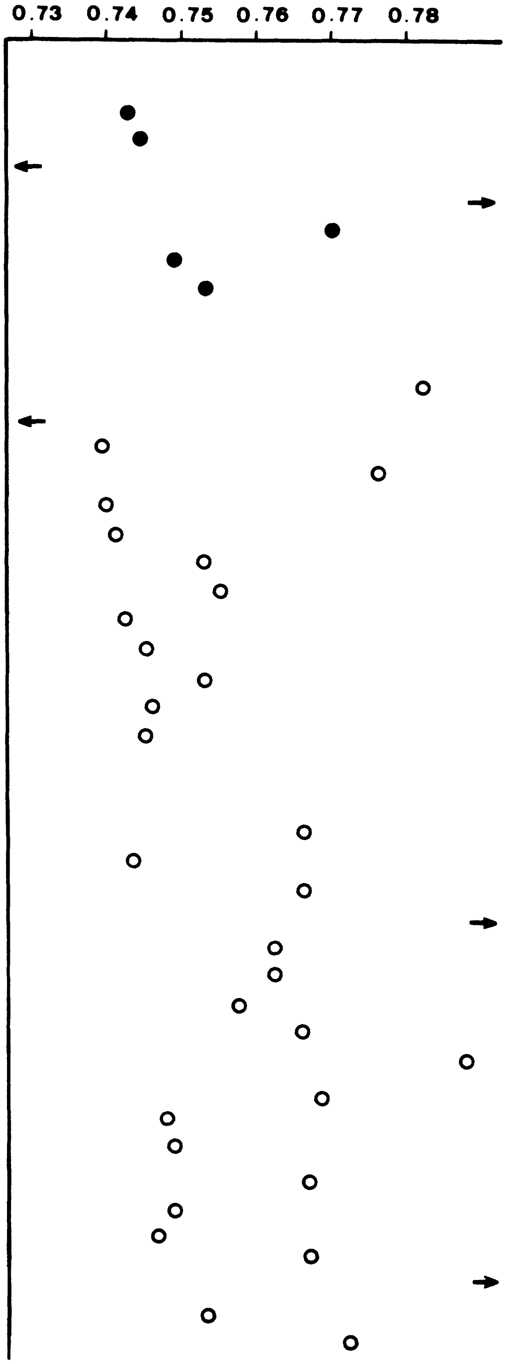
(i) For the resonance transition $2s\,{}^2S \rightarrow 2p\,{}^2P^\circ$ the QDO f value which is the geometric mean of the length and velocity results is the one which best agrees with the most recent, and probably most accurate, experimentally determined f value.[34] For the $2s\,^2S \rightarrow 3p\,^2P^\circ$ transition this QDO value is also the closest one to the critically compiled f value.[40] For this transition not many measures of f values were found in the literature.

(ii) The magnitude of the dipole length value seems to be a little too large in the resonance transition. For the $2s\,^2S \rightarrow 3p\,^2P^\circ$ transition the length result is in good agreement with the early experimental f value[39] whereas the velocity result is much larger.

(iii) The introduction of core polarization effects in the QDO results slightly lowers the magnitude of the resonance transition f value and leads to improvement: the relative difference between both results, with and without polarization, is about 0.72%. For the other transition, the opposite effect is observed, the relative difference being, in this case, about 5.36%. These effects the decrease in f value for the resonance transition and the increase in that corresponding to the $2s\,^2S \rightarrow 3p\,^2P^\circ$ transition are also detected in other results, e.g., the f values computed with model potential[17] and with the core-charge-polarization procedure.[53]

TABLE I. Comparative results of oscillator strengths for Li I, $2s\,^2S \rightarrow 2p\,^2P^\circ$ transition.

Reference	Method	f
	(a) Experiment	
34	Fast beam laser	0.7416±0.0012
35	Level crossing	0.744±0.011
36	Beam gas	0.63±0.03
37	Beam foil	0.81±0.03
38	Beam foil	0.77±0.03
39	Dispersion hook	0.749
40	Critical compilation	0.753
	(b) Semiempirical results	
	QDO, length (present paper)	0.7825
	QDO, velocity (present paper)	0.6990
	QDO, mean value (present paper)	0.7396
	QDO, Pol. (present paper)	0.7768
41	Semiempirical potential + polarization	0.74
42	Coulomb approximation	0.7412
43	Screened potential, length	0.753
43	Screened potential, velocity	0.755
44	Scaled Thomas-Fermi	0.7425
45	Thomas-Fermi + polarization	0.745
17	Model potential	0.753
17	Model potential + polarization	0.746
16	Model potential + polarization	0.7435
	(c) *Ab initio* results	
46	Hartree-Fock	0.766
46	Relativistic HF + polarization	0.743
47	Dirac-Fock, length	0.766
47	Dirac-Fock, velocity	0.796
48	MBPT, length	0.7625
48	MBPT, velocity	0.7626
49	Random phase approximation exchange	0.7575
50	Dirac-HF, length	0.766
50	Dirac-HF, velocity	0.788
51	SCF	0.769
51	SCF + polarization	0.748
52	CI	0.749
53	SCHF	0.767
53	SCHF + polarization	0.749
16	Close coupling	0.7475
54	HF, length	0.7678
54	HF, velocity	0.7905
54	45-term CI, length	0.7531
54	45-term CI, velocity	0.7725



(iv) By comparing the results obtained from a HF approximation[54] and from a multiconfigurational treatment[54] it can be observed that the use of configuration-interaction wave functions not only improves the f values, but also leads to a better agreement between the length and velocity forms. Both forms experienced a 2–3 % change due to the increase in the number of configurations.

(v) In general, for the resonance transition, the theoretical results compare well with the experimentally determined f values, while for the $2s\,{}^2S \rightarrow 3p\,{}^2P^\circ$ transition, large discrepancies between both kinds of results are observed. The QDO results show reasonable agreement with experiment for the resonance transition as well as for the $2s\,{}^2S \rightarrow 3p\,{}^2P^\circ$ transition.

In Tables III and IV we show oscillator strengths for the $2s\,{}^2S \rightarrow np\,{}^2P^\circ$ transitions $n=4$ and 7, in several atomic species of the lithium isoelectronic sequence (Li I–Si XII). In order to reduce the tables to a minimum we have only included our QDO f values, in the first four columns, and those of the other authors who present results for the majority of the transitions and atomic species studied in the present paper.

In order to summarize the results shown in the tables it seems convenient to us to distinguish between two situations we have observed when analyzing our results.

(a) For a given atomic species. The higher the principal quantum number of the final state in the transition the smaller the relative difference between the dipole length and dipole velocity oscillator strengths. Generally, the introduction of core polarization effects in the transition matrix element does improve our QDO results

TABLE II. Comparative results of oscillator strengths for Li I, $2s\,{}^2S \rightarrow 3p\,{}^2P^\circ$ transition.

Reference	Method	f
	(a) Experiment	
39	Dispersion hook	0.00478
40	Critical compilation	0.0055
	(b) Semiempirical results	
	QDO, length (present paper)	0.004720
	QDO, velocity (present paper)	0.006121
	QDO, mean value (present paper)	0.005375
	QDO, polarization (present paper)	0.004973
41	Semiempirical potential + polarization	0.0047
42	Coulomb approximation	0.004225
43	Screened potential, length	0.0043
43	Screened potential, velocity	0.0043
44	Scaled Thomas-Fermi	0.00475
45	Thomas-Fermi + polarization	0.00462
17	Model potential	0.0045
17	Model potential + polarization	0.00477
16	Model potential + polarization	0.00488
	(c) *Ab initio* results	
46	Hartree-Fock	0.0034
46	Relativistic HF + polarization	0.0051
47	Dirac-Fock, length	0.00336
47	Dirac-Fock, velocity	0.00261
48	MBPT, length	0.00369
48	MBPT, velocity	0.00369
49	Random phase approximation exchange	0.00406
50	Dirac-HF, length	0.003
50	Dirac-HF, velocity	0.003
51	SCF	0.0036
51	SCF + polarization	0.0047
52	CI	0.0047
53	SCHF	0.0032
53	SCHF + polarization	0.0044
16	Close coupling	0.00482
54	HF, length	0.0027
54	HF, velocity	0.0026

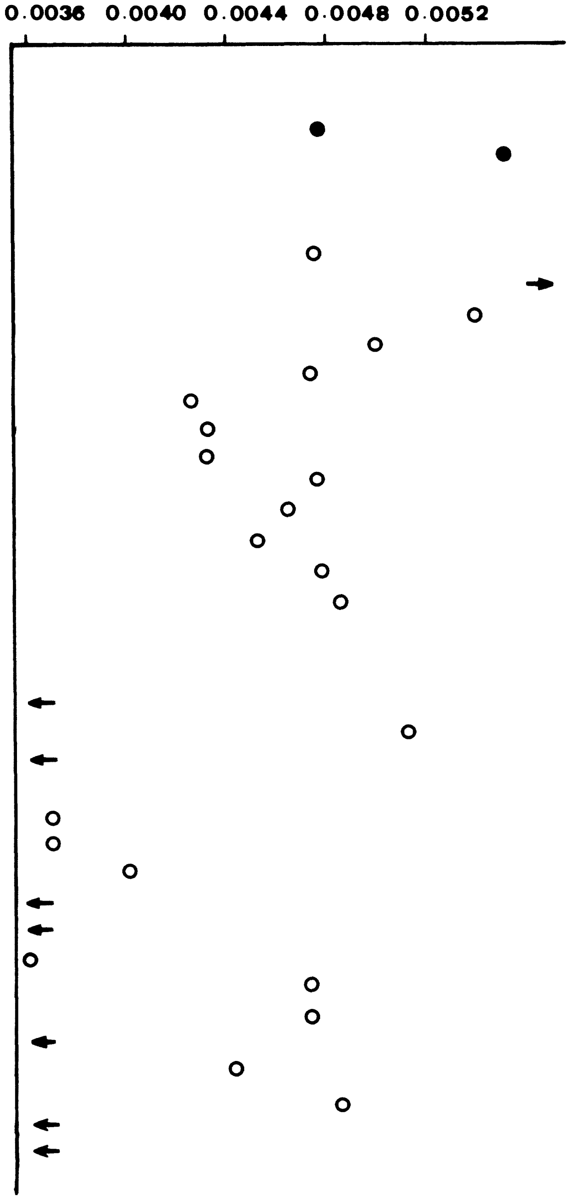


TABLE III. Oscillator strengths for the $2s\,^2S \rightarrow 4p\,^2P^\circ$ transition in the lithium isoelectronic sequence.

Species	f_1[a]	f_2[b]	f_3[c]	f_4[d]	f_5[e]	f_6[f]
Li I	0.004 299	0.004 939	0.004 608	0.004 452	0.0045	0.004 225
Be II	0.030 64	0.031 09	0.030 86	0.031 89	0.0306	0.030 17
B III	0.048 91	0.049 11	0.049 01	0.051 75	0.0486	0.048 51
C IV	0.060 32	0.060 41	0.060 36	0.063 65	0.0610	0.059 94
N V	0.067 89	0.067 93	0.067 91	0.068 77	0.0696	0.067 53
O VI	0.073 21	0.073 22	0.073 21	0.074 04	0.0766	0.072 86
F VII	0.077 15	0.077 14	0.077 14	0.077 88	0.0814	0.076 89
Ne VIII	0.080 29	0.080 28	0.080 28	0.080 99	0.0850	0.080 14
Na IX	0.082 56	0.082 55	0.082 55	0.083 13	0.0830	0.082 41
Mg X	0.084 99	0.084 99	0.084 99	0.085 49	0.0890	0.085 17
Al XI	0.086 20	0.086 20	0.086 20	0.086 66	0.092	0.086 24
Si XII	0.087 62	0.087 63	0.087 62	0.087 99	0.094	0.087 77

[a] QDO, length form (present paper).
[b] QDO, velocity form (present paper).
[c] QDO, mean value (present paper).
[d] QDO, polarization (present paper).
[e] Critical compilation (Reference 40).
[f] Coulomb approximation (Reference 42).

TABLE IV. Oscillator strengths for the $2s\,^2S \rightarrow 7p\,^2P^\circ$ transition in the lithium isoelectronic sequence. f_1 through f_6 have the same meanings as in Table III.

Species	f_1	f_2	f_3	f_4	f_5	f_6
Li I	0.001 030	0.001 136	0.001 082	0.001 061	0.0011	0.009 496
Be II	0.004 957	0.005 012	0.004 984	0.005 155	0.0052	0.004 885
B III	0.0072[a]	0.0072[a]	0.0072[a]	0.0076[a]	0.0078	0.007 217
C IV	0.008 597	0.008 602	0.008 599	0.009 028	0.0092	0.008 55
N V	0.009 429	0.009 428	0.009 428	0.009 535	0.0102	0.009 389
O VI	0.010 04	0.010 04	0.010 04	0.010 20	0.0107	0.010 05
F VII	0.010 50	0.010 50	0.010 50	0.010 57	0.0112	0.010 55
Ne VIII	0.009 028	0.009 076	0.009 052	0.009 191	0.0114	0.007 702
Na IX	0.010 99	0.011 00	0.010 99	0.011 04	0.0116	0.011 04
Mg X	0..011 26	0.011 28	0.011 27	0.011 29	0.0118	0.011 40
Al XI	0.011 42	0.011 45	0.011 43	0.011 44	0.0119	0.011 59
Si XII	0.011 41	0.011 41	0.011 41	0.011 43	0.0120	0.011 45

[a] Interpolated from the graphs.

TABLE V. Dependence of the oscillator strengths of Mg X on the ionization potential.

Transition	f_1[a]	f_2[b]	f_3[c]
$2s\,^2S \rightarrow 2p\,^2P^\circ$	0.1267±0.0000	0.1224±0.0001	0.1240±0.0001
$2s\,^2S \rightarrow 3p\,^2P^\circ$	0.3211±0.0003	0.3211±0.0003	0.3234±0.0003
$2s\,^2S \rightarrow 4p\,^2P^\circ$	0.084 99±0.000 13	0.084 99±0.00 13	0.085 49±0.000 12
$2s\,^2S \rightarrow 5p\,^2P^\circ$	0.035 94±0.000 09	0.035 95±0.000 09	0.036 11±0.000 08
$2s\,^2S \rightarrow 6p\,^2P^\circ$	0.018 93±0.000 06	0.018 96±0.000 07	0.019 00±0.000 06
$2s\,^2S \rightarrow 7p\,^2P^\circ$	0.011 26±0.000 05	0.011 28±0.000 06	0.011 29±0.000 05

[a] QDO, length form (present paper).
[b] QDO, velocity form (present paper).
[c] QDO, polarization (present paper).

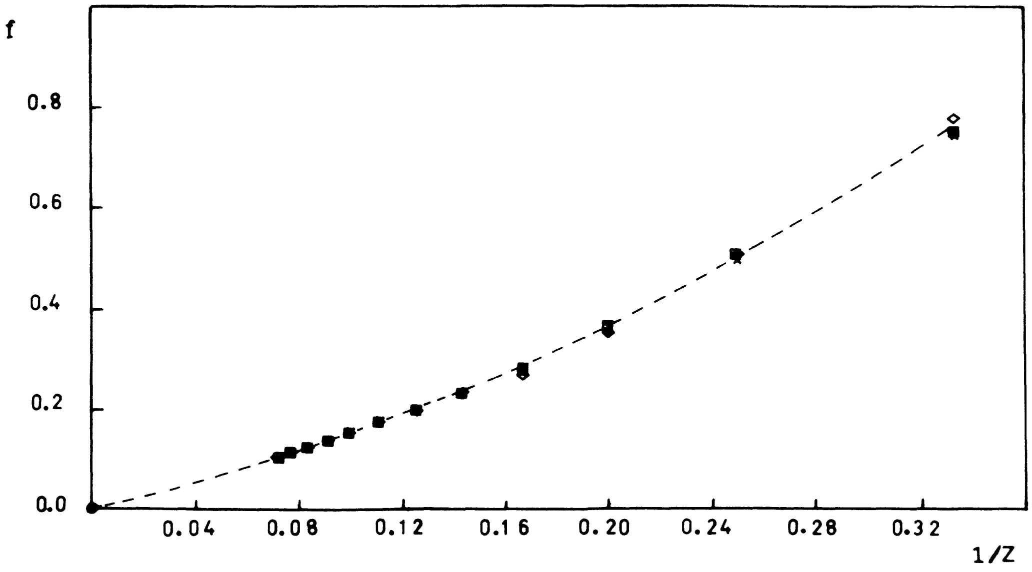


FIG. 1. Oscillator strengths versus the reciprocal of the nuclear charge for the $2s\,^2S \rightarrow 2p\,^2P^\circ$ transition in the lithium isoelectronic sequence. ◇, QDO, polarization (present paper); +, QDO, mean value (present paper); □, critical compilation (Reference 40); ×, Coulomb approximation (Reference 41).

by slightly lowering the resonance transition f value and by raising those corresponding to transitions to higher excited states.

(b) For a given transition. The dipole length and dipole velocity QDO results come closer together as the nuclear charge Z increases. The core polarization effect is important for the first few atomic species, Li I–C IV; in the remaining ions this effect gradually decreases in going from N V to Si XII. This feature very probably arises from the relative magnitudes of the core polarizabilities running from 0.20 for Li I to 0.081 for C IV and 0.013 for N V to 0.0082 for Si XII.[32]

In order to give an idea of how sensitive the QDO f values are to the variation of the ionization potential (IP) we have analyzed in detail the oscillator strengths of one of the atomic species of the lithium isoelectronic sequence, the Mg X atomic system. There has been found in the literature[55] an uncertainty for the IP of Mg X of about ±250 cm^{-1}. This uncertainty in the IP give uncertainties in the quantum defect of ±0.0001 for the $2s$ state

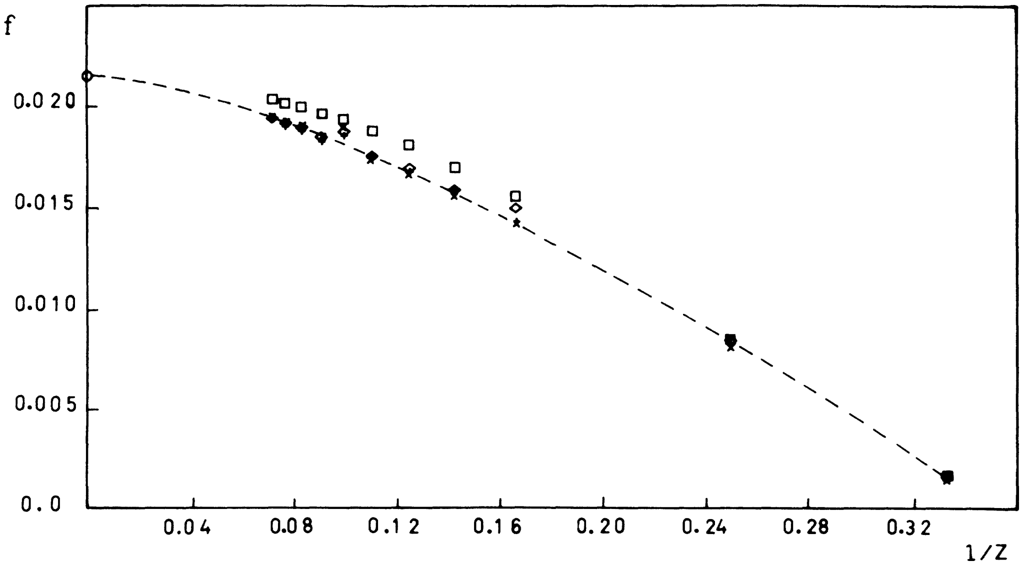


FIG. 2. Oscillator strengths versus the reciprocal of the nuclear charge for the $2s\,^2S \rightarrow 6p\,^2P^\circ$ transition in the lithium isoelectronic sequence. ◇, QDO, polarization (present paper); +, QDO, mean value (present paper); □, critical compilation (Reference 40); ×, Coulomb approximation (Reference 41).

and for the final states the uncertainties vary from ±0.0001 the for $2p$ state to ±0.0039 for the $7p$ state. Therefore, a relative variation in the IP as small as 0.008% implies a relative variation of about 0.13%, the quantum defect of the initial state and a relative change as high as 12.26% for that corresponding to the $7p$ state.

In Table V, we give our QDO f values for Mg X together with the absolute variations corresponding to the uncertainty of ±250 cm^{-1} in the ionization potential. From this table some remarks can be inferred.

(i) For each transition, the three sets of f values show the same absolute variations. The absolute variations in the f values are independent of the form of the dipole matrix element used in the calculation of the oscillator strengths.

(ii) The f value for the resonance transition is practically insensitive to the uncertainty in the ionization potential.

(iii) The relative dependence of the f values on the uncertainties of the IP increases with the principal quantum number of the final state of the transition. The relative variations run from about 0.09% for the $2s\,^2S \rightarrow 3p\,^2P^\circ$ transition to about 0.5% for the $2s\,^2S \rightarrow 7p\,^2P^\circ$ one. In Figs. 1 and 2 we have plotted f values versus the reciprocal of the nuclear charge for the entire isoelectronic sequence.

The dependence of the oscillator strengths, for the resonance transition $2s\,^2S - 2p\,^2P^\circ$ on the reciprocal of the nuclear charge, Fig. 1, is essentially given by a parabola. The f values extend smoothly to the hydrogen value as $1/Z \rightarrow 0$ which is, in this case, zero because the principal quantum number remains unchanged in this transition.

Different dependence of the f value on the nuclear charge is encountered in the remaining transitions $2s\,^2S \rightarrow np\,^2P^\circ$, $n = 3-7$. As an example we only show that corresponding to $n = 6$, Fig. 2. In these cases severe cancellations in the transition integral occur for the neutral atom, and therefore, the $1/Z$ dependence curve starts our with a very small f value at the highest value for $1/Z$. With the exception of the ion Ne VIII in the $2s\,^2S \rightarrow np\,^2P^\circ$ $n = 5,6,7$ transitions, the QDO results exhibit a correct decreasing trend reaching the hydrogen value as $1/Z \rightarrow 0$. This anomaly in the f values of the Ne VIII ion is also found in the Coulomb approximation results of Lindgård and Nielsen[42] for the same transitions.

V. CONCLUSIONS

Several conclusions can be drawn from Sec. IV. We only summarize here the most relevant ones.

The QDO set of the geometric mean of the dipole length and the dipole velocity results seems to be more correct than the individual dipole length and dipole velocity f values. However, as the nuclear charge increases along the isoelectronic sequence, and as the principal quantum number of the final state of the transition is higher, both formulations give similar results.

Core-polarization effects are more important for the first four atomic species of the isoelectronic sequence (Li I–C IV) than for the remaining ions. In general, when these effects are explicitly introduced in the QDO procedure a better agreement with experiment is reached than when they are neglected.

A small change in the ionization potential implies important variations in the quantum defects; however, the corresponding QDO f values are practically insensitive to the uncertainty in the ionization potential.

The f value versus the reciprocal of the nuclear charge curve shows a correct trend, the oscillator strength smoothly approaching the hydrogen value as $1/Z$ tends to zero. From the presented figures, additional f values for very highly charged ions may be obtained by just reading those off the curves.

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