Relativistic f Values for the Resonance Transitions of Li- and Be-Like Ions*

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Relativistic Hartree-Fock calculations indicate that the dipole oscillator strengths for the $2s \rightarrow 2p_{3/2}$ and $2s \rightarrow 3p_{3/2}$ transitions of the Li sequence and those for the $2s^2\,{}^1S \rightarrow 2s2p_{3/2}\,P_1$ transitions of the Be sequence deviate appreciably for $Z > 40$ from values extrapolated from low-Z ions.

Dipole oscillator strengths (f values) and excitation energies for the resonance transitions in highly stripped ions are urgently needed in the study of controlled thermonuclear reactions, both for estimating the energy loss through impurity ions in the plasma and for plasma diagnosis.[1,2] Experimental and theoretical data available in the literature[3,4] are mostly for ions with low nuclear charge Z, i.e., $Z < 30$.

To study the relativistic effects in high-Z ions, we have calculated from the relativistic Hartree-Fock wave functions the f values for the $2s \rightarrow 2p$ and $2s \rightarrow 3p$ transitions of the Li sequence, and the $2s^2\,{}^1S_0 \rightarrow 2s2p\,{}^{1,3}P_1$ transitions of the Be sequence. For the Li sequence, single-configuration wave functions were used. Excitation energies calculated from these wave functions for the Li-like ions of low Z are in excellent agreement ($\sim 1\%$ or better) with experimental values. For the Be sequence, however, it is well known that strong configuration mixing exists in the ground state.[4] In addition, for the $2s2p\,{}^{1,3}P_1$ state, we expect that the LS coupling scheme would be adequate only for low-Z ions, and we must provide for a gradual change into the jj coupling scheme as Z increases. We have, therefore, used multiconfiguration wave functions for both the ground and the excited states. The ground-state wave function is given by ($1s^2$ omitted for brevity)

$$\Psi_{J=0} = \alpha(2s_{1/2})^2 + \beta(2p_{1/2})^2 + \gamma(2p_{3/2})^2, \tag{1}$$

and the excited-state wave function by

$$\Phi_{J=1} = \alpha'(2s_{1/2}'2p_{1/2}') + \beta'(2s_{1/2}'2p_{3/2}'), \tag{2}$$

where J is the total angular momentum, $(2s)^2$, $(2s_{1/2}'2p_{3/2}')$, etc., denote appropriate Slater determinants of the four-component orbitals, and α, β, etc., are configuration-mixing coefficients to be determined by the variational method. Details of the computational method have been given elsewhere.[5] We simply note that the orbitals for the ground and excited states are determined separately by the variational method, and that Ψ and Φ are correct antisymmetrized eigenfunctions of J as indicated in Eqs. (1) and (2). The variational determination of the mixing coefficients α' and β' automatically include intermediate coupling. We shall show that the values of the coefficients indeed shift toward the jj coupling limits as Z increases.

It is more convenient to look into the relativistic effects in each of the two factors in the definition of the f value, i.e., the excitation energy E and the line strength S. In terms of these, f is defined in the length form as

$$f = ES(3gR)^{-1}, \tag{3}$$

where $R = 13.6$ eV and g is the degeneracy of the initial state. As is discussed below, the relativistic effects in f could come from those in E or in S.

The excitation energies were calculated by taking the differences in the total energies, which include the usual terms in the Dirac Hamiltonian, the nonrelativistic Coulomb repulsion between the atomic electrons, and the Breit interaction term.[6] The Lamb shift and other radiative corrections were not included. Sample results on E and S are shown in Table I.

Li sequence.—We find that both E and S for the $2s \rightarrow 2p_{1/2}$ and $2s \rightarrow 3p_{1/2}$ transitions deviate only moderately from nonrelativistic results even for high Z, so that the relativistic effects in the f values are minor. For the $2s \rightarrow 2p_{3/2}$ transitions, however, E increases rapidly for large Z, though S remains close to the nonrelativistic value throughout. Hence, the combined effect is a substantial increase of the f values for high Z (Fig. 1). On

TABLE I. Excitation energy E and line strength S for the resonance transitions of the Li- and Be-like ions.

Z	Ion	Transition	E (eV) Relativistic [a]	E (eV) Nonrelativistic [a]	Z^2S Relativistic [a]	Z^2S Nonrelativistic [a]
Li sequence						
10	Ne^{7+}	$2s \rightarrow 2p_{\frac{3}{2}}$	16.22	15.92	52.37	52.45 [b]
		$2s \rightarrow 3p_{\frac{3}{2}}$	140.7	140.4	11.49	11.60
42	Mo^{39+}	$2s \rightarrow 2p_{\frac{3}{2}}$	214.6	77.61	37.89	39.11
		$2s \rightarrow 3p_{\frac{3}{2}}$	3271	3124	10.56	12.43
74	W^{71+}	$2s \rightarrow 2p_{\frac{3}{2}}$	1715	138.6	33.71	37.71
		$2s \rightarrow 3p_{\frac{3}{2}}$	11668	9977	7.003	12.48
Be sequence						
10	Ne^{6+}	$2s^2 \rightarrow 2s2p\,^1P_1$	28.31	28.10	57.44	57.32
42	Mo^{38+}	"	251.9	136.0	40.16	41.90
74	W^{70+}	"	1758	243.0	33.80	40.33

[a]Present calculation. The nonrelativistic results are from the Hartree-Fock wave functions equivalent to those for the relativistic calculations.

[b]Nonrelativistic S values for the Li sequence are divided according to the statistical ratio $p_{3/2}:p_{1/2}=2:1$.

the other hand, for $2s \rightarrow 3p_{3/2}$ transitions, the relativistic S decreases rapidly for high Z compared to the nonrelativistic S values while E remains close to the nonrelativistic E values. The combined result is that the relativistic f values for high-Z ions are smaller than the nonrelativistic values. As shown in Fig. 1, the sum of the f values for the $2s$ to $2p_{1/2}$, $2p_{3/2}$, $3p_{1/2}$, and $3p_{3/2}$ transitions agrees well with the corresponding sum of the nonrelativistic f values. For low Z (<30), our relativistic f values are in excellent agreement with those recommended by Smith and Wiese.[3] Their recommendation is based on a large number of empirical and theoretical data available for the low-Z ions.

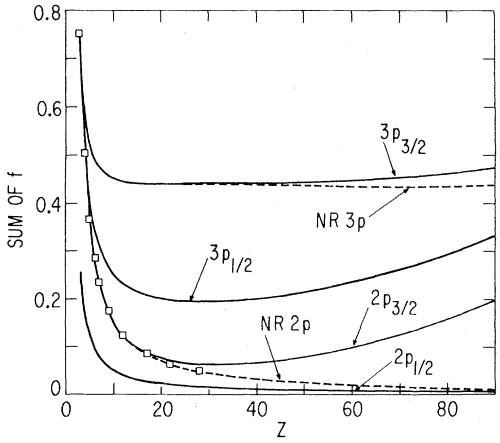

FIG. 1. Z dependence of the sum of the f values for the $2s_{1/2} \rightarrow np_j$ transitions of the Li sequence. Solid curves represent the results from the relativistic Hartree-Fock wave functions, and broken curves are those from the nonrelativistic (NR) Hartree-Fock wave functions. Squares are the values recommended by Smith and Wiese (Ref. 3).

Be sequence.—As is expected from the hydrogenic degeneracy (in energy) of the $2s_{1/2}$ and $2p_{1/2}$ orbitals, we find that the importance of the $(2p_{1/2})^2$ configuration [Eq. (1)] in the ground state remains fairly constant as Z increases. On the other hand, the weight for the $(2p_{3/2})^2$ configuration decreases rapidly for high Z (Table II) as the difference in the energies of the $2s_{1/2}$ and $2p_{3/2}$ orbitals widens. The wave function Φ [Eq. (2)] leads to two $J=1$ eigenstates. In the low-Z region, these two states correspond to the $^3P_1$ and $^1P_1$ states, and correspondingly, the values of the mixing coefficients α' and β' are very close to the LS coupling limits[7] (Table II). For

TABLE II. Configuration-mixing coefficients for the Be sequence [cf. Eqs. (1) and (2)].

		Ground state			2nd $J=1$ state [a]	
	Z	α	β	γ	α'	β'
Ne^{6+}	10	0.968	0.147	0.205	−0.572	0.820
Mo^{38+}	42	0.986	0.141	0.089	−0.200	0.980
Xe^{50+}	54	0.989	0.138	0.054	−0.102	0.995
W^{70+}	74	0.992	0.126	0.024	−0.038	0.999

[a]The LS coupling limit is $\alpha'=-0.577$ and $\beta'=0.816$ (Ref. 7).

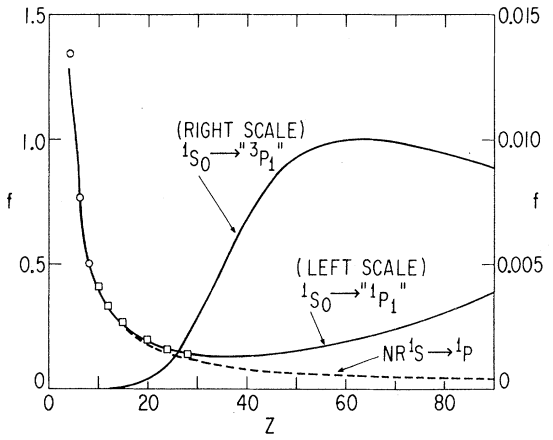

FIG. 2. Z dependence of the f values for the $2s^2\,{}^1S_0 \rightarrow 2s2p\,P_1$ transitions of the Be sequence. Solid curves represent the results from the relativistic multiconfiguration Hartree-Fock wave functions (lower $J=1$ state denoted by "$^3P_1$" and the upper one by "$^1P_1$"). The broken curve represents the results from the nonrelativistic multiconfiguration Hartree-Fock wave functions ($2s^2+2p^2\,{}^1S$ for the ground state and $2s2p\,{}^1P$ for the excited state). Circles are theoretical values from correlated wave functions (Ref. 4) and squares are those recommended by Smith and Wiese (Ref. 3). Note the different scales for the $^3P_1$ and $^1P_1$ transitions.

high-Z ions, however, the values of α' and β' shift to the jj coupling limits (e.g., $\alpha'=0$ and $\beta'=1$ for the second $J=1$ state). It is clear from Table II that the intermediate coupling scheme must be introduced (either by a relativistic variational approach as we have done or by a suitable perturbation method[8]) for ions of $10<Z<50$. We found that the relativistic f values for the transitions to the upper $J=1$ state (corresponds to the $^1P_1$ state for low Z) exhibit basically the same Z dependence on E and S as those observed in the $2s \rightarrow 2p_{3/2}$ transitions of the Li sequence (see Table I). For the transitions to the lowest $J=1$ state (corresponds to the $^3P_1$ state for low Z), we find that both E and S are much smaller than those for the upper $J=1$ state, resulting in f values smaller by a factor of 20 to 10^9 compared to the "allowed" transitions to the upper $J=1$ state (Fig. 2). The transitions to the lowest $J=1$ state remain "weak" even for $Z>50$ where the two $J=1$ states are very close to the jj coupling limits. In Fig. 2, the relativistic f values for the $2s^2\,{}^1S_0$-$2s2p$ second P_1 transitions are compared with the recommended values of Smith and Wiese.[3] The departure of our f values from the recommended values for the first few members of the sequence is an indication that the limited number of orbitals we have used in Eqs. (1) and (2) is insufficient to represent the electron correlation effects.

Details of our relativistic calculations will be reported later. We are very grateful to Dr. A. W. Weiss for communicating to us many unpublished results for comparison.

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