Z dependence of gf values

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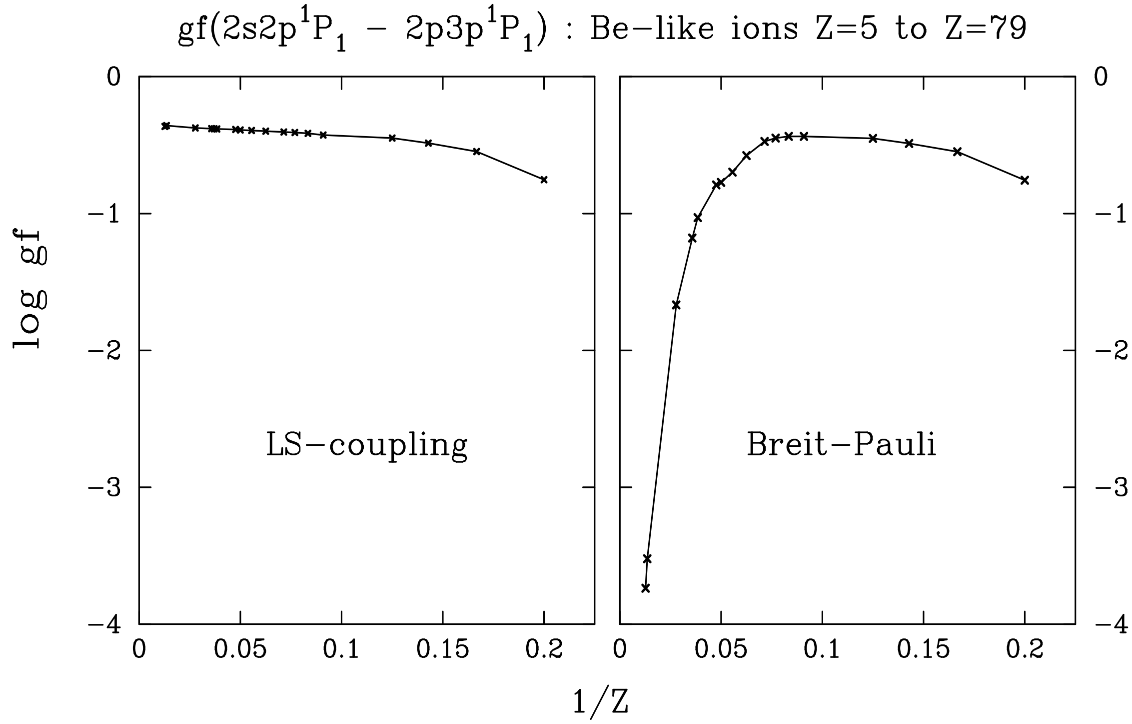
Introduction

In the 1980s I worked with Mike Seaton and Keith Berrington on the beryllium sequence. We calculated energies, gf values and ionisation cross sections as part of the Opacity Project (Tully et al. 1990). The OP codes assumed LS coupling and on comparing our gf values with those of Brian Fawcett (1984) I noticed some striking differences which are shown in Figure 3 of the paper by Seaton et al. (1992). I suggested then that these were the result of relativistic effects which Fawcett took account of since he used Robert Cowan's code that includes the Breit-Pauli approximation. The Configuration Interaction Version 3 (CIV3) program first appeared over 30 years ago (Hibbert 1975). In the 1990s Alan Hibbert provided me with an updated version of CIV3 which allows one to use either LS coupling or the Breit-Pauli approximation. The program can also calculate numerical orbitals, but these make no allowance for relativistic effects. It has always been my intention to compare Fawcett's results with those produced by CIV3. In addition, I also wanted to find out how the gf values behave for much heavier ions than nickel, which is where Fawcett's tabulation stops. I began work on this a few weeks before the present symposium was due to begin. In order to compute oscillator strengths with CIV3, atomic orbitals are needed. Most of these I obtained by using CIV3 together with Enrico Clementi & Carla Roetti's (1974) tables for the ground state ($1s^2\,2s^2\ {}^1S_0$). Their tabulation ends at Z = 36 so I extended it using CIV3. In this way I obtained numerical data for ten orbitals (1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f) in seventeen Be-like ions from boron (Z = 5) to gold (Z = 79).

Electric dipole transition 5 → 26

The labelling in Table 1 is for the lowest 26 levels of Be-like nickel and corresponds to what Marita Chidichimo and I published in 2004, having used CIV3 with orbitals 1s to 4f. While the first 10 levels remain the same throughout the entire sequence, this is no longer true for some of the others. The inclusion of relativistic effects means that levels can no longer be classed as singlet or triplet, and in some cases the mixing is so severe that the LS labels used in Table 1 are incorrect. Level $i = 26$, which Fawcett calls $2p3p\,{}^1P_1$, is shown by CIV3 to be more triplet than singlet. The OP results for the gf value being considered here, increase slightly with Z and tend to a finite limit point at $Z = \infty$. However, Fawcett's Breit-Pauli results, which go no further than Z = 28, decrease in a dramatic fashion as Z increases from 12 to 28. The question I asked myself was, Does the f value eventually increase?, as Zhang & Sampson's (1989) TABLE III shows it does for some transitions between the ground and upper levels in Ne-like ions. In order to explore the region beyond $Z = 28$, I used CIV3 for 17 ions, ranging from Be-like boron (Z = 5) to Be-like gold (Z = 79). The LS and BP results from CIV3 are shown here in the pair of adjoining figures, where log gf is plotted against Z^{-1}. The present results confirm the conclusion one can draw from Fawcett's tabulated data: namely that gf for this transition continues to fall as Z increases and never rises.



Comparing CIV3 and MCDF

Those who have worked a lot with the Breit-Pauli approximation tell me that it should provide reliable atomic data for transitions in heavy elements whose atomic number does not exceed about 30. Table 2 shows f-values for 17 electric dipole transitions and compares results from CIV3 with those that Zhang & Sampson (1992) got by using Ian Grant's Multi Configuration Dirac-Fock (MCDF) code, see Grant et al. (1980). It can be seen that for krypton ($Z = 36$) the differences are insignificant, whereas for tungsten ($Z = 74$) they are more than a few percent with seven of them being factors of between 3 and 12. The biggest difference is interesting because it is the only transition in W and Au for which the MCDF result exceeds CIV3's. Also, the oscillator strength 0.0037(5-6) is one of the smallest for Be-like W, there being only two that are smaller, namely 0.0001(3-9) and 0.0009(5-7).

References

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Table 1.

i	$E(i)$	Label	
1	0.000000	2s2s	$^1S_0$
2	3.432912	2s2p	$^3P^o_0$
3	3.796753	2s2p	$^3P^o_1$
4	4.970093	2s2p	$^3P^o_2$
5	7.743286	2s2p	$^1P^o_1$
6	9.538940	2p2p	$^3P_0$
7	10.47998	2p2p	$^3P_1$
8	10.97400	2p2p	$^3P_2$
9	12.54077	2p2p	$^1D_2$
10	14.67029	2p2p	$^1S_0$
11	95.54187	2s3s	$^3S_1$
12	96.18140	2s3s	$^1S_0$
13	97.18019	2s3p	$^3P^o_0$
14	97.18506	2s3p	$^3P^o_1$
15	97.56921	2s3p	$^1P^o_1$
16	97.60059	2s3p	$^3P^o_2$
17	98.49597	2s3d	$^3D_1$
18	98.55103	2s3d	$^3D_2$
19	98.64575	2s3d	$^3D_3$
20	99.26904	2s3d	$^1D_2$
21	99.87031	2p3s	$^3P^o_0$
22	100.0547	2p3s	$^3P^o_1$
23	100.9955	2p3p	$^3D_1$
24	101.4067	2p3s	$^3P^o_2$
25	101.7371	2p3p	$^3D_2$
26	101.7393	2p3p	$^1P_1$

Table 2.

Z	1-3	1-5	2-7	3-6	3-7	3-8	3-9	5-6
	A1-E1	A1-E2	D1-B1	E1-A2	E1-B1	E1-C1	E1-C2	E2-A2
28	0.0021	0.1487	0.0616	0.0172	0.0141	0.0274	0.0019	0.0003
	0.0021	0.1499	0.0626	0.0174	0.0142	0.0281	0.0019	0.0003
36	0.0052	0.1362	0.0605	0.0142	0.0127	0.0317	0.0018	0.0001
	0.0053	0.1375	0.0616	0.0143	0.0128	0.0328	0.0018	0.0001
74	0.0354	0.3083	0.1518	0.0174	0.0263	0.1184	0.0001	0.0003
	0.0088	0.2630	0.1331	0.0075	0.0228	0.1044	0.0001	0.0037
79	0.0736	0.4190	0.2055	0.0306	0.0354	0.1625	0.0001	0.0000
	0.0086	0.2958	0.1498	0.0070	0.0255	0.1189	0.0001	0.0040

Z	5-10	5-7	5-8	5-9	4-7	4-8	4-9
	E2-A3	E2-B1	E2-C1	E2-C2	F1-B1	F1-C1	F1-C2
28	0.0327	0.0002	0.0104	0.0511	0.0119	0.0265	0.0160
	0.0339	0.0002	0.0108	0.0519	0.0120	0.0265	0.0167
36	0.0283	0.0005	0.0126	0.0462	0.0092	0.0150	0.0242
	0.0292	0.0005	0.0128	0.0468	0.0092	0.0148	0.0251
74	0.0531	0.0031	0.0194	0.1240	0.0121	0.0131	0.0744
	0.0475	0.0009	0.0058	0.1077	0.0044	0.0049	0.0659
79	0.0706	0.0063	0.0367	0.1694	0.0221	0.0234	0.1010
	0.0528	0.0008	0.0054	0.1218	0.0041	0.0045	0.0743

Table 1. Ni XXV level energies in Ryd units relative to the ground state. Theoretical results from Tully & Chidichimo (2004)

Table 2. Electric dipole oscillator strengths for the beryllium sequence. Comparing present results from CIV3 (Breit-Pauli approximation) with those obtained by Zhang & Sampson's (1992) who used MCDF, the multi configuration Dirac-Fock code of Grant et al. (1980). Z is the atomic number and transitions can be identified by means of Table 1. The labelling used by Zhang & Sampson is given in order to simplify comparison with their TABLE II. Agreement is good for ions with $Z \leq 36$. However for tungsten (Z=74) and gold (Z=79) the MCDF f-values are smaller than those predicted by CIV3, except for transitions 3-9 and 5-6.