Accurate MCHF/MCDF Transition Rates

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1 Introduction

With today's powerful workstations and high performance architectures, it has been possible to improve considerably the accuracy to which atomic properties can be predicted. This is done by using systematic methods, where wave functions for a series of models including more and more physical effects are obtained from expansions defined in terms of an orbital basis of increasing size. Typically, the first model is one that includes only valence correlation. But often core-polarization is also important in which case a core-valence calculation is need. In some instances, even core-core correlation produces a small correction. By monitoring convergence within the different models and comparing the converged results themselves, an uncertainty estimate can be obtained. These methods can be used both for non-relativistic MCHF calculations where Breit-Pauli corrections are added in configuration interaction (CI) calculations, or for MCDF calculations starting with the Dirac-Coulomb Hamiltonian, adding Breit and leading QED corrections in relativistic CI.

2 Iso-electronic Sequences

A number of iso-electronic sequences have been explored using MCDF. In fact, the recently implemented non-orthogonal methodology allowing for separately optimized initial and final state wave functions was first tested on the Mg-like sequence [1].

The same MCDF procedures have been applied to the study of the Be-like E1 transitions $2s^2\ ^1S - 2s2p\ ^{1,3}P_1$. For low-$Z$, the transition rates in Babushkin (length) and Coulomb (velocity) gauges do not show good agreement [2, 3], though in C III the former is in excellent agreement with Breit-Pauli [4] and recent experiment [5]. Table 1 shows some results for the sequence. For the intercombination line (IC) the difference in gauges is decreasing with Z whereas for the allowed resonance transition, the difference is only one or two units in the fourth decimal place for all Z. A detailed analysis (in preparation) also shows that the frequency dependent Breit correction is important for high-Z.

Other sequences investigated recently using MCHF with Breit-Pauli are the $2s^2\ ^1S - 2s3p\ ^{1,3}P_1$ allowed and intercombination lines for $Z \leq 10$ [6, 7]. The experimental data for these transition rates have been analyzed semi-empirically [8] and values predicted for the sequence. Except for N IV, our computed values are in closer agreement to the semi-empirical predictions than experiment itself.

3 Spectrum Calculations

Many variational studies have concentrated on accurate, single line, benchmark calculations. The MCHF+BP and MCDF programs also permit the study of portions of a spectrum. In the latter,

Table 1: Transition energies (in cm^{-1}) and rates (in s^{-1}) for the $2s^2\ {}^1S_0 - 2s2p\ {}^3P_1$ intercombination (IC) and $2s^2\ {}^1S_0 - 2s2p\ {}^1P_1$ allowed dipole (E1) lines in the Be isoelectronic sequence. In the table [x] denotes powers of ten.

Z		ΔE_{IC}	A^l_{IC}	A^v_{IC}	ΔE_{E1}	gf_l	gf_v
7	MCDF	67 301	5.586 [2]	8.597 [2]	131 029	0.6113	0.6118
	Exp	67 272			130 694		
8	MCDF	82 104	2.212 [3]	3.074 [3]	159 154	0.5122	0.5124
	Exp	82 079			158 798		
9	MCDF	96 899	6.961 [3]	9.041 [3]	187 224	0.4414	0.4416
	Exp	96 861			186 841		
10	MCDF	111 730	1.862 [4]	2.305 [4]	215 350	0.3882	0.3884
	Exp	111 705			214 952		
11	MCDF	126 640	4.410 [4]	5.275 [4]	243 625	0.3470	0.3471
	Exp	126 612			243 208		
12	MCDF	141 662	9.508 [4]	1.118 [5]	272 133	0.3141	0.3142
	Exp	141 631			271 687		
⋮							
24	MCDF	341 252	2.772 [7]	2.824 [7]	667 962	0.1623	0.1623
	Exp	341 120			667 150		
25	MCDF	360 178	3.773 [7]	3.834 [7]	709 557	0.1578	0.1578
	Exp	359 970			708 770		
26	MCDF	379 363	5.041 [7]	5.118 [7]	753 366	0.1539	0.1540
	Exp	379 130			752 502		
27	MCDF	398 983	6.631 [7]	6.721 [7]	799 649	0.1505	0.1505
	Exp	398 720			799 040		
28	MCDF	418 964	8.583 [7]	8.689 [7]	848 677	0.1474	0.1476
	Exp	418 720			847 494		

orbitals may be optimized for a series of levels. Using this option, the $3s^2 3p^3$, $3s3p^4$, $3s^2 3p^2 3d$ levels of selected elements of the iso-electronic sequence in the range $22 \leq Z \leq 32$ were computed along with E1 transitions between these levels [9]. Some lifetimes for levels of Fe XII, which all show remarkable agreement in length and velocity forms, are reported in Table 2.

In Table 3 we report excitation energies of selected levels from Fe XII ions, comparing them with previous theory and experiment. When both are available, the present MCDF results are generally in better agreement with experiment.

4 Complex Systems

The MCHF+BP and MCDF programs have also been applied to the study of forbidden transitions among the twelve (12) lowest levels of $3d^5$ of Fe IV. A re-examination of the data for these levels was suggested by Rubin *et al* [11] as a result of an analysis of the the flux of Fe IV ($3d^5\ {}^4P_{5/2} - 3d^5\ {}^6S_{5/2}$) in the Orion Nebula, using the Goddard High-Resolution Spectrograph. From a theoretical point of view, an accurate *ab initio* calculation is extremely complex. The MCHF+BP approach was restricted to the mixing of the four lowest terms, ${}^6S$, ${}^4G$, ${}^4P$, and ${}^4D$, each with a correlated expansion. The resulting Breit-Pauli calculations required almost four hours on a Cray T3E computer with 32 nodes. Still missing, was the mixing with other quartets and the doublets. In the MCDF approach, the expansions grow in size rapidly with the orbital set (there being more relativistic

Table 2: Excitation Energies and Lifetimes of levels of $3s3p^4$

Fe XII Levels		Energy (cm^{-1})		Lifetime (s)	
No.	J^P	Calc.	Exp.	Length	Velocity
6	5/2 +	274620	274373	6.11(–10)	6.17(–10)
7	3/2 +	284131	284005	5.70(–10)	5.78(–10)
8	1/2 +	288431	288307	5.40(–10)	5.49(–10)
9	3/2 +	341076	340020	2.75(–10)	2.78(–10)
10	5/2 +	342949	341703	3.02(–10)	3.05(–10)

Table 3: Excitation energies for a few selected levels of the $3s^23p^3$, $3s3p^4$, and $3s^23p^23d$ configurations for Fe XII ions. All energies (in cm^{-1}) are displayed with respect to the $3s^23p^3\ ^4S_{3/2}$ ground–state level.

Level	Designation of states	J^P	Huang *et al.* Ref. 9	Fawcett Ref. 10	This work	Experiment
1	$3s^23p^3\ ^4S$	3/2 −	0	0	0	0
2	^2D	3/2 −	45375		42667	41555 ±1
3	^2D	5/2 −	49932		47130	46088 ±1
4	^2P	1/2 −	78297		75532	74108 ±1
5	^2P	3/2 −	84503		81792	
6	$3s3p^4\ ^4P$	5/2 +	274625	274344	274620	
7	^4P	3/2 +	284157	283556	284131	
8	^4P	1/2 +	288345	287737	288431	
9	^2D	3/2 +	345263		341076	339761 ±10
10	^2D	5/2 +	347176		342949	
21	$3s^23p^23d\ ^4D$	5/2 +	460430	453305	454327	
22	^4D	7/2 +	470196		463593	
23	^2G	7/2 +	509637		496836	
24	$3s3p^4\ ^2P$	3/2 +	516954		507969	
25	$3s^23p^23d\ ^4P$	5/2 +	528771	512530	517607	513708 ±10

orbitals) and so the correlation effects had to be restricted. Only after the inclusion of the Breit correction were computed levels in the observed order. Thus spin-orbit alone cannot predict the energy structure. The transition rates for transitions within these levels, vary over orders of magnitude. There appears to be good agreement between our theories for some transitions, particularly for the M1 transitions where the $\Delta S = 0$ and $\Delta L = 0$ selection rules are obeyed.

Heavy atoms also are of great interest. They differ from light atoms in that a fully relativistic Dirac-Fock-Breit formalism may be necessary and correlation exhibited by the mixing of configuration states is very strong. We are currently extending the MCDF codes for larger, more efficient correlation studies. At the same time, open f-shells appear. Correlation studies of such states in MCDF will be extremely difficult because of the size of the expansions that occur in jj-coupling. In fact, only the core electrons are "relativistic": it may be possible to describe the outer electrons in the Breit-Pauli scheme. This approach is being investigated. The MCHF package has been extended to include an arbitrary number of f electrons. For this purpose, an efficient method is used for finding algebraic expressions for matrix elements. It is based on second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique [13]. Coefficients of fractional parentage are replaced by the far fewer "reduced" coefficients of fractional parentage. Codes based on this formalism have been found to be, on average, 2-6 times faster.

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