TASK QUARTERLY 2 No 1 (1998), 97-100

REPORT ON MULTICONFIGURATION--INTERACTION CALCULATIONS OF TRANSITIONS IN LEAD

PAWEŁ HORODECKI AND JÓZEF E. SIENKIEWICZ

Chair of Theoretical Physics and Mathematical Methods
Technical University of Gdansk
Narutowicza 11/12, 80-952 Gdansk, Poland

Abstract: Relativistic multiconfiguration-interaction calculations of the dipole magnetic and quadruple electric transitions in the lead atom have been calculated. The computer program GRASP2 (General Relativistic Atomic Structure) has been used.

1. Introduction

In this short report we present theoretical foundation on which the computer program GRASP2 is based. We also present results of our calculations. Detailed comparison with experiment can be found in [1].

2. Theoretical Method

In this chapter we present relativistic multiconfiguration calculations of the electric and magnetic transitions (rank 2 and 1, respectively) in $6p^2$ configuration of Pb by means of the GRASP2 code [2]. This is the newest version of a fully relativistic program GRASP [3] based on the Dirac-Fock theory [4] which is appropriate for the description of heavy atoms like lead. The multiconfiguration Dirac-Fock theory (MCDF) implemented in the program consists of two main elements. The first one is a representation of the atomic state function (ASF) as a linear combination of relativistic configuration state functions (CSF):

$$|\Gamma PJM\rangle = \sum_{r=1}^{n} c_{r\Gamma} |\gamma_r PJM\rangle. \tag{1}$$

Any CSF $|\gamma_r PJM\rangle$ is constructed as a Slater determinant of relativistic one electron orbitals being eigenstates of total angular momentum and parity operators.

The label γ_r represents all information (occupation of different subshells, coupling schemes and seniority numbers) required to define CSF uniquely. The second element, which is an essential ingredient of the MCDF approach, is the Dirac-Coulomb Hamiltonian:

$$\hat{H}^{DC} = \sum_i \hat{h}_i + \sum_{i<j} \frac{1}{\left|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j\right|}. \tag{2}$$

Here the first part of the Dirac-Coulomb Hamiltonian represents an electron in the potential of the nucleus V_{nuc}:

$$\hat{h}_i = c\sum_{k=1}^{3} \alpha_k^i \hat{p}_k^i + \left(\beta^i - 1\right)c^2 + V_{\text{nuc}}\left(\hat{r}_i\right) \quad i = 1,\ldots,N. \tag{3}$$

In the MCDF method the radial parts of functions $|\gamma_r PJM\rangle$ (1), as well as the mixing coefficients c_{rt} are generated by the selfconsistent field (SCF) of the above Hamiltonian.There is an optional possibility in the program to take into account the transverse Breit interaction and leading radiative corrections as perturbations correction only.

The MCDF method is an *ab initio* method appropriate for heavy atoms.The problem is to attain the convergence of the SCF procedure, which is an essential difficultly for larger number of the fields accounted for in the CSF.

The computational method, described above, allows to calculate eigenvalues and eigenfunctions of the atomic Hamiltonian $\hat{H}^{DC}$. The eigenvalues or the atomic energy levels and the eigenfunctions are observed experimentally through the electromagnetic radiation emitted or absorbed during transitions between two energy levels. These transitions occur due to the interaction between an atom and an electromagnetic field. Usually this interaction is treated as a perturbation of the Hamiltonian $\hat{H}^{DC}$ and leads to the well known formulas for transition probabilities [5]. In the present calculation the Breit corrections have been included. The effect of thefinite size of the nucleus has also been taken into account via the choice of the Fermi model (with parameters $a = 9.89059\times10^{-6}$ and $c = 1.25946\times10^{-4}$ in Bohr radii). All calculations have been performed in average level scheme [3], for which the energy functional is averaged over a set of states with different total angular momentum.

3. Numerical calculations and results

The choice of the configurations for which the calculations were carried out has been based partly on the literature. It is obvious that only even parity configurations should contribute to the basic $6p^2$ configuration. The $6p^4$ configuration has been found to be the most important [6, 7].

Thus we have performed the calculations for the following cases:

MCDF 1 $6p^2 + 6p7s$

MCDF 2 $6p^2 + 6p^4 + 6s^16p^3 + 6p7s$

MCDF 3 $6p^2 + 6p^4 + 6p7p$

MCDF 4 $6p^2$.

The excited configuration of opposite parity 6p7s together with the most important admixture $6s6p^4$ [8] has been included to get the resonant E1 transitions as a by-product and to see how much the small basis approximation is consistent with the fact that the Hamiltonian commutes with the parity operator.The larger sets of configurations have not been considered here due to the convergence problems.

The calculated transition probabilities are presented in Tables 1 and 2. In the case of the electric transitions (Table 2) both the results in Coulomb (V) and Babushkin (L) gauges have been included (see [5] for details). The coefficient γ introduced here provides some information about the level of consistency between the two gauges. As one may expect, the results of MCDF1 are similar to the results of MCDF4. Not that big discrepancies are consequence of finite basis approximation together with the SCF approach.

Table 1. *Magnetic dipole transitions for different calculations: A^{M1} is the spontaneous emission probability per unit time, λ is the transition wave length.*

Transition	A^{M1}						
	λ (nm)	MCDF 1	MCDF 2	MCDF 3	MCDF 4	MCDF 5	MCDF 6
$^1S_0 \rightarrow {}^3P_1$	461.9	95.81	71.74	66.78	97.97	73.07	99.61
$^1D_2 \rightarrow {}^3P_2$	925.3	12.07	9.07	9.06	12.83	9.36	11.69
$^3P_1$	733.2	14.30	10.56	10.52	15.29	10.91	13.63
$^3P_2 \rightarrow {}^3P_1$	3532.2	0.49	0.47	0.45	0.47	0.47	0.57
$^3P_1 \rightarrow {}^3P_0$	1278.9	4.33	3.96	4.29	4.78	4.11	4.05

Table 2. *Electric dipole transitions for different calculations; A^{E2} is the spontaneous emission probability per unit time, λ is the transition wave length, V and L indicate respectively the Coulomb and Babushkin gauges.*

Transition		A^{E2}					
	λ (nm)	MCDF 1	MCDF 2	MCDF 3	MCDF 4	MCDF 5	MCDF 6
$^1S_0 \rightarrow {}^1D_2$ V	1248.6	0.04	0.02	0.008	0.03	0.02	0.06
L		0.23	0.06	0.15	0.19	0.06	0.31
$^3P_2$ V	531.5	2.33	1.73	3.10	2.43	1.79	2.43
L		57.05	21.21	24.41	59.51	21.06	55.52
$^1D_2 \rightarrow {}^3P2$ V	925.3	0.74	0.63	0.61	0.77	0.66	0.74
L		0.80	0.49	0.57	0.95	0.51	0.62
$^3P_1$ V	733.2	0.68	0.59	0.48	0.71	0.61	0.68
L		0.62	0.37	0.33	0.74	0.38	0.49
$^3P_0$ V	466.0	0.45	0.49	0.42	0.43	0.51	0.52
L		0.72	0.70	1.10	0.80	0.71	0.65
$^3P_2 \rightarrow {}^3P_1$ V	3532.2	14.2×10^{-4}	16.6×10^{-4}	16.1×10^{-4}	12.5×10^{-4}	16.9×10^{-4}	18.3×10^{-4}
L		18.3×10^{-4}	15.5×10^{-4}	15.6×10^{-4}	18.9×10^{-4}	15.7×10^{-4}	17.4×10^{-4}
$^3P_0$ V	938.9	0.41	0.38	0.24	0.43	0.41	0.39
L		0.15	0.13	0.18	0.19	0.14	0.11
$\sum_i \frac{\lvert A_i^V - A_i^L \rvert}{A_i^V + A_i^L}$		0.3617	0.3435	0.3805	0.3808	0.3422	0.3627

4. Conclusion

Computer program GRASP2 has been used to obtain numerical values of dipole forbidden transitions in the neutral lead atoms. Calculated results can be compared with experimental and theoretical data.

Acknowledgements

Numerical calculations have been performed in Computer Centre in Gdansk TASK. This work has been partially supported by State Committee for Scientific Research under the project No. 2 P03B 009 12.

References

[1] Horodecki P., Kwela J. and Sienkiewicz J. E., submitted to Can. J. Phys.

[2] Parpia F. A., Grant I. P. and Froese C. Fisher, private communication

[3] Dyall K. G., Grant I. P., Johnson C. T., Parpia F. A., Plummer E. P., Comput. Phys. Commun., **55** (1989) 425

[4] Grant I. P., Comput. Phys. Commun. **17** (1979) 149

[5] Grant I. P., J. Phys . B: Atom. Molec. Phys., **7** (1974) 1458

[6] Flambaum V. V., Sushkov O. P., J. Quant. Spectrosc. Radiat. Transfer. **20** (1978) 569

[7] Biémont E., Hasen J. E. , Phys. Scr. **33** (1986) 117

[8] Dembczyński J. , Rebel H., Physica **125** C (1984) 341