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Submitted on 1 Jan 1987

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MCDF CALCULATIONS OF RELATIVISTIC EFFECTS IN LITHIUM-LIKE IONS

P. INDELICATO

National Bureau of Standards(1), Gaithersburg, MD 20899, U.S.A.
and Laboratoire de Physique Atomique et Nucléaire(2), Université Pierre et Marie Curie, F-75231 Paris Cedex 05, France

Résumé: Dans ce travail est présenté le calcul complet des énergies des niveaux 1s² 2s et 1s² 2p dans la séquence isoélectronique du lithium. Ce calcul est réalisé suivant la méthode Dirac-Fock Multiconfigurationnelle (MCDF). Les contributions relativistes à l'énergie de chacun de ces niveaux ainsi que les corrections radiatives sont calculées en détail, et contribuent significativement à l'énergie totale. Les énergies de transition fournies par ce calcul sont en très bon accord avec les résultats expérimentaux disponibles entre Z=20 et Z=54.

Abstract: In this paper we report on a complete Multiconfiguration Dirac-Fock calculation of 1s² 2s and 1s² 2p level energies in the lithium isoelectronic series. Relativistic effects on correlation energies and radiative corrections are calculated in detail and shown to significantly contribute to level total energy. Available experimental data between Z=20 and Z=54 and our theoretical predictions are in very good agreement.

With the increasing availability of very precise high Z data for transition energies in few electron ions, it has become increasingly interesting to undertake fully relativistic calculations. The study of many bound electron systems in a relativistic model is still a challenge since such a problem has no simple exact hamiltonian form. We have recently shown /1/,/2/ (work hereafter referred as paper I and II) that it is possible to obtain fairly accurate values for n=1 and n=2 level energies in heavy heliumlike ions by ab initio Multiconfiguration Dirac-Fock calculations.

In this work we have used the method described in paper I to evaluate 1s² 2s and 1s² 2p level energies in lithiumlike ions. At this stage all significant configurations up to 2s 3d² or 2p 3d² have been included for both core and outer electrons. The three electron problem in the relativistic case is much more difficult than the two electron one. The number of jj configurations to achieve reasonable precision is far bigger (54 for the 1s² 2p ) than in the case of heliumlike systems, and one has to be careful in the evaluation of the 2p1/2-2p3/2 separation. In non relativistic calculations both levels have the same correlation effect. But in a relativistic MCDF calculation, as 2p1/2 and 2p3/2 radial wave-functions are computed separately, they have not the same non relativistic limit, and thus configurations like 2p3 do not contribute identically to both levels /3/. As correlations can be expanded in a double series in 1/Z and Za /4/, we have circumvented this difficulty by doing all calculations twice, a being taken once to be 0 (non relativistic limit). The spurious non-relativistic contribution can then be subtracted and replaced by exact non relativistic results. To obtain these non-relativistic values we have used a 1/Z expansion, writing \( \Delta E_{\text{corr}} = \Delta E_0 + \Delta E_1 (1/Z) \). The value of \( \Delta E_0 \) is known exactly /5/ and the value of \( \Delta E_1 \) has been evaluated by using the exact lithium result /6/. It has been checked that this procedure does not lead to sizeable uncertainty for Z\geq20, by comparing the \( \Delta E_1 \) value deduced from configuration interaction calculation (A Weiss, unpublished results).

(1) Correspondence address : Building 221, Room 141, Gaithersburg, MD 20899, U.S.A.
(2) Permanent address : CNRS UA-771, Université Pierre et Marie Curie, 4, Place Jussieu, F-75231 Paris Cedex 05, France
The results of this calculation are shown in figure 1. One can see that electrostatic correlations are strongly affected by relativistic contributions (particularly for the $1s^2 2p_{1/2}$ level). In fact these relativistic effects are stronger and show up for smaller Z than in the heliumlike ion case.

The correlations being taken into account, one as to include radiative corrections. The approximation for self-energy screening described in paper II has been extended to the three electron case. All calculations were done using experimental values for the nuclear radius and mass when available and a semi-empiric formula [7] otherwise. For the sake of completeness these calculations include finite nuclear size correction to the hydrogenic self-energy [7] as well as $\alpha(Z\alpha)^3$ contribution to vacuum polarization (Wichman and Kroll contribution), because they give important contributions at high Z.

![Graph](image)

**Figure 1:** Relativistic effects in electrostatic correlations. NR=Non relativistic, * means j=1/2.

Fundamental constants are those of the 1986 adjustment [8]. To convert our values from eV to Å one should use $C=12398.4245$ eVÅ, and to cm$^{-1}$, $C'=8065.54092$ cm$^{-1}$/eV. The fine structure constant is taken as $\alpha=1/137.0359895$ and the conversion from atomic unit to eV is done using 1 Hartree=27.21139634 eV. Reduced mass correction and approximate specific mass shift are also taken into account.
Figure 2: Comparison between theoretical and experimental $2p_{3/2}-2s_{1/2}$ transition energy (eV). Differences between experiment and theory are plotted altogether with experimental uncertainties (dotted lines).

Figure 3: Comparison between theoretical and experimental $2p_{3/2}-2p_{1/2}$ transition energy (eV). Differences between experiment and theory are plotted altogether with experimental uncertainties (dotted lines).

This work is the first to include all these corrections altogether with very precise correlation contribution. Theoretical transition energies can then be directly be compared with experiment, both being of the same accuracy. Recent measurements performed using both Tokamak plasma /9/
and beam foil spectroscopy (S Martin private communication) experiments are available up to 
Z=36 and Z=54 respectively (the latter results being very crude however). The accuracy of these 
measurements is of ±0.02 Å between Z=20 and Z=36. Figures 2 shows comparison between the 
Tokamak set of data and this work for 2p3/2-2s separation. The overall agreement is excellent and 
confirms the quantitative predicting power of the MCDF method. Transition energies are displayed 
in table 1.

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<th>22</th>
<th>24</th>
<th>26</th>
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Table 1: Comparison between theoretical and experimental transition energies (eV).

Acknowledgements.

Part of this work has been done using the CS² computer facility at the National Bureau of 
standards. The author wishes to thank Prof. J. P. Briand, Dr. R. D. Deslattes, Dr. J. P. Desclaux, 
and Dr. Y. K. Kim for many helpful discussions, and A Weiss for communication of unpublished 
results.

References.