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# RELATIVISTIC MASS SHIFT CALCULATIONS WITH THE GRASP2K PACKAGE

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The tensorial form of the relativistic mass shift operator (RMS) to the lowest order in (m/M) [1,2] (in a.u.)

$$H_{MS} = \frac{1}{2M}\sum_{i,j}^{N}\left(\mathbf{p}_i\cdot\mathbf{p}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\mathbf{r}_i)\mathbf{r}_i}{r_i^2}\right)\cdot\mathbf{p}_j\right)$$

is derived and is implemented in the GRASP2K package [3,4]. The inclusion of this relativistic operator allows to investigate more consistently mass shift effects in the full relativistic approach [5].

Calculations including single (S), double (D) and triple excitations (T) are performed for Li I (see Table). The new results are compared with the corresponding values obtained with the same relativistic wave functions and the uncorrected operator adopted in [6], and with the non relativistic Multiconfiguration Hartree-Fock results [7].

**Table**. Specific mass shift parameter $S_{sms}$ in a.u. for Li I for $1s^2\ 2s\ ^2S_{1/2}$.

| $AS_n$ | SD | | SDT | | MCHF [7] |
|---|---|---|---|---|---|
| | OLD | NEW | OLD | NEW | |
| n=5 | 0.3010343291 | 0.3008225633 | 0.3013767853 | 0.3011648528 | |
| n=6 | 0.3010361585 | 0.3008243666 | 0.3014579841 | 0.3012459847 | |
| n=7 | 0.3019544951 | 0.3017423943 | 0.3024396569 | 0.3022273237 | |
| n=8 | 0.3018617523 | 0.3016497153 | 0.3024115843 | 0.3021992791 | |
| n=9 | 0.3017987398 | 0.3015867742 | 0.3023512554 | 0.3021390203 | |
| n=10 | 0.3018561821 | 0.3016442119 | 0.3024141615 | 0.3022019200 | 0.30205339864 |
| n=11 | 0.3018280421 | 0.3016160885 | | | |

Results for other levels and heavier systems will be presented to illustrate the interest of the present code extension.

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