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RELATIVISTIC CONFIGURATION INTERACTION OF ENERGY LEVELS AND WAVELENGTHS OF HE-LIKE LITHIUM.

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Abstract. In recent years, there have been extensive spectroscopic studies, both experimental and theoretical, of helium isoelectronic sequence. Such an analysis requires information for a wide range of atomic parameters, including energy levels and wavelengths. Our target is to extend the calculation and present a complete and accurate data for helium-like ions. We expect that our extensive calculations will be useful to experimentalists for identifying the fine-structure levels.

1. Theoretical method

FAC is a fully relativistic code created by Ming Feng Gu which higher efficiency enables user to carry out large-scale computations and allows finding various atomic parameters (Gu., 2008). We employed FAC code to perform the whole three different calculations: FAC, Relativistic Configuration Interaction (RCI) and Many Body Perturbation Theory (MBPT).

The configuration-interaction (CI) method which is based on the variational principle represents one of the approaches for treating many-electron systems. Non-relativistic CI techniques have been used extensively in atomic and molecular systems calculations. However, the generalization to relativistic configuration-interaction (RCI) calculations also presents theoretical as well as technical challenges. While, the MBPT approach starts from the Rayleigh-Schrödinger perturbation theory of a multiconfigurational model space. The self-consistent-field approximation and the Breit interaction Hamiltonian as well as QED effects have been included in the calculations to improve the generated wave functions: Manai et al. 2019.

We review the theoretical background used by the FAC code. Then, the computational details of the calculation of the $1s^2, 1s2l, 1s3l, 1s4l, 1s5l$ and $1s6l$ configurations of He-like lithium which give rise to the lowest 71 fine structure levels. The number of levels of the fine structure which we considered is larger than that in Aggarwal et al. 2010 and Kramida et al. 2018. Then, the transition energy $[cm^{-1}]$ and wavelengths $\lambda[\mathring{A}]$ are presented.

Accurate energy levels calculations among the lowest 71 levels arising of $1s^2$ and

$1snl$ ($n \leq 6$, $l \leq (n-1)$) configurations of He-like lithium have been carried out through the relativistic configuration interaction (RCI) approach, the second-order many body perturbation theory ($MBPT$). We provide accurate calculations of energy levels and wavelengths of types of transitions ($E1$, $E2$, $M1$ and $M2$) for He-like lithium.
Finally, a discussion of our results and a comparison with available theoretical and experimental data are presented.

1. 1. RESULTS

In table.1, the use of the $MBPT$ approach significantly improves the value of the energy levels. The maximum difference relative to the NIST data: Kramida et al. 2018 becomes 651 cm^{-1} while the majority of values of energy levels of RCI method are decreased by approximately 5000 cm^{-1}.
From figure.1, the average relative deviation of wavelengths don't exceed 5% for the three methods compared to the results from NIST: Kramida et al. 2018. For the MBPT calculations we have $-0.47 \pm 0.90\%$, for the RCI calculations we have $2.62 \pm 1.70\%$ and for the FAC calculations we have $3.13 \pm 1.60\%$.
The present results are in good agreement with already published data in the literature, theoretical: Aggarwal et all. 2010 and experimental data: Kramida et al. 2018. Several new energy levels were found out where no other theoretical or experimental results are available. We expect that our extensive calculations will be useful to experimentalists for identifying the fine structure levels: Cantu et al. 1977.
We present the average relative deviation between our different methods and the experimental data as by the following equation:

$$[(E_{theory} - E_{NIST})/E_{NIST}] \times 100 \tag{1}$$

Table 1: Restriction of values of energy levels in (cm^{-1}) of He-like lithium chosen arbitrarily, calculated by different methods: FAC, RCI and $MBPT$. Experimental data from the $NIST$ database are also represented.

Index	Configuration	Level	Our work			NIST
			$E_{FAC}(cm^{-1})$	$E_{RCI}(cm^{-1})$	$E_{MBPT}(cm^{-1})$	$E_{NIST}(cm^{-1})$
0	$1s^2$	$^1S_0$	0.00	0.00	0.00	0.00
1	$1s\,2s$	$^3S_1$	468653.14	476659.81	475809.66	476034.98
2	$1s\,2p$	$^3P_1^o$	488226.11	495893.34	492877.69	494261.17
3	$1s\,2p$	$^3P_2^o$	488227.61	495895.88	492883.62	494263.44
4	$1s\,2p$	$^3P_0^o$	488230.97	495897.79	492875.37	494266.57
5	$1s\,2s$	$^1S_0$	489275.25	496473.66	490308.45	491374.60
6	$1s\,2p$	$^1P_1^o$	499233.39	506243.71	501688.74	501808.59
7	$1s\,3s$	$^3S_1$	547214.25	557219.00	554216.70	554754.45
8	$1s\,3p$	$^3P_1^o$	551896.98	561999.88	559309.39	559500.35
9	$1s\,3p$	$^3P_2^o$	551897.37	562000.70	559311.02	559501.42
10	$1s\,3p$	$^3P_0^o$	551898.11	562000.85	559308.59	559502.32

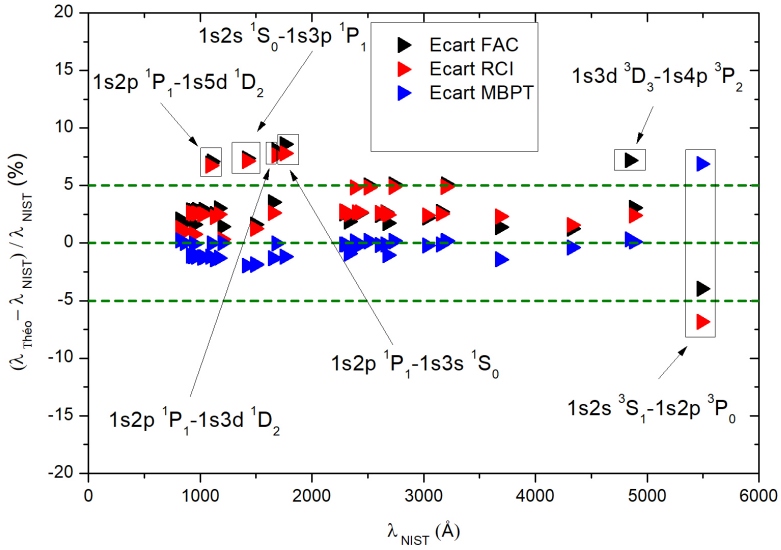

Figure 1: The average relative deviation of wavelengths calculated by different methods (FAC, RCI and MBPT) compared to NIST wavelengths.

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