QED Calculations of the Interelectron Interaction in Li-like Ions

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Investigations of heavy few-electron atoms provide an excellent opportunity for testing QED in strong Coulomb fields. A remarkable high experimental precision has been reached in Lamb-shift measurements of Li-like ions. The uncertainty obtained e.g. for the $2p_{1/2}$ - $2s$ transition energy in Li-like Ni and Zn [1], Ag and Xe [2, 3] and U [4] is by an order of magnitude smaller than the QED contribution of second order in the fine structure constant α. To achieve that level of accuracy in theoretical predictions rigorous calculations of all Feynman diagrams of order α^2 had to be carried out [5, 6, 7].

Traditional approaches for calculating energy levels in high-Z Li-like ions such as relativistic many-body perturbation theory, multiconfigurational Dirac-Fock, and the relativistic configuration-interaction method account for the correlation and the relativistic corrections but do not provide a rigorous treatment of the QED effects, which is required in high-Z systems. Since correlation effects cannot be separated from the QED radiative corrections *ab initio* calculations valid up to order α^2 must be carried out starting from the complete set of QED-Feynman diagrams. Two-electron QED corrections of order α^2 for a Li-like ion consist of three sets of Feynman diagrams, each of which is separately gauge invariant: the self-energy screening diagrams, the vacuum-polarization screening diagrams and the two-photon exchange diagrams. The two-photon exchange diagrams do not require any renormalization. Explicit expressions for the energy shifts can be derived either by means of the two-time Greens-function method [5, 6] or within the lineprofile approach [7].

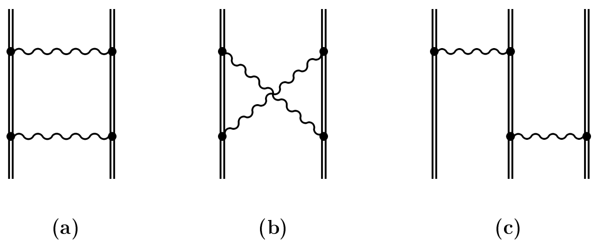

Figure 1: The two-photon exchange diagrams.

Numerical calculations have been performed in Feynman and in Coulomb gauge, respectively. The numerical values obtained exhibit an excellent agreement. The direct and the exchange parts are found to be separately gauge invariant on the level of the numerical accuracy. The results of the numerical calculation of the two-photon exchange corrections are presented in Table 1 for the $2p_{1/2}$-$2s$ transition energy in Li-like ions within the range of nuclear charge numbers $50 < Z < 100$ [5]. The estimated numerical accuracy is about 0.005 eV. Some results obtained from complete QED calculations including all available two-electron QED corrections of order α^2 are presented in Table 2. A detailed description of the formalism and of the QED effects included can be found in Refs. [6, 7]. The values from Ref. [7] also account partially for three-photon interactions. A comparison is made between theoretical calculations and experimental results for the $2p_{1/2}$-$2s$ transition in high-Z Li-like ions. The overall agreement with the experimental data reveals a significant improvement of the accuracy in the theoretical predictions.

Z	$2p_{1/2}$	$2s$	$2p_{1/2}$-$2s$
50	-13.398	-8.234	-5.164
60	-15.155	-8.953	-6.202
70	-17.547	-9.899	-7.649
80	-20.827	-11.146	-9.681
83	-22.046	-11.598	-10.448
90	-25.449	-12.823	-12.626
92	-26.596	-13.226	-13.370
100	-32.244	-15.146	-17.098

Table 1: Two-photon exchange correction to the $2p_{1/2}$-$2s$ transition energy in heavy Li-like ions (in eV).

Z	Ref. [6]	Ref. [7]	experiment	
30	57.384(4)(4)	57.34(1)	57.384(3)	[1]
47	99.43(1)(1)		99.438(7)	[2]
50	107.90(1)(2)		107.911(8)	[3]
70	176.44(6)(7)	176.52(10)		
80	220.93(15)(11)	220.92(20)		
92	280.48(11)(20)	280.36(21)	280.59(9)	[4]

Table 2: Theoretical predictions and experimental results for the $2p_{1/2}$-$2s$ transition energy in heavy Li-like ions (in eV).

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