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Computing radiation parameters for atoms and multicharged ions within relativistic energy approach: Advanced code

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Abstract content
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We present the results of computing radiation (transitions probabilities, oscillator strengths etc) parameters of atoms and ions on the basis of advanced computer code within relativistic approach to calculation of the in spectra of multicharged ions, based on energy approach and relativistic many-body perturbation theory [1]. The key feature of the presented basis theory is an implementation of the optimized one-particle representation [3] into the frames of the S-matrix energy formalism. It provides a consistent approach to minimize gauge-non-invariant contributions to gf values and thus it make our approach significantly more advantagable in comparison with standard Hartree-Fock (HF), Dirac-Fock (DF) methods. We have carried out calculating energies, radiation and Auger transition probabilities for Li- and Zn-like ions (Z=10-70). It is checked that all gf values, obtained within our approach in different photon propagator gauges (Coulomb, Babushkin, Landau) are practically equal. As example in table below we list our results (REA) on gf of the 4s2(1S0)- 4s4p (1P01) transition in some Ne-Zn-like ions. For comparison the HF, DF, DF (with fitting to experiment) and model potential (MP) calculation data are presented too (look [1] and refs. therein).
[1] A.V.Glushkov, L.N.Ivanov, E.P.Ivanova, in Autoionization Phenomena in Atoms (Moscow State Univ.) 55 (1986); L.N.Ivanov, E.P.Ivanova, E.V.Aglitsky, Phys.Rep. 166, 315 (1988); A.V. Glushkov, L.N. Ivanov, Phys.Lett.A 170, 33 (1992); O.Yu. Khetselius, Int.J.Quant.Chem.109, 3330 (2009).

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