

New approach to calculation of the neutral and highly-ionized atoms structure and oscillator strengths

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In the theory of radiative and nonradiative decay of the quasistationary states of multielectron atom it's well known an energy approach (c.f. [1]), based on the adiabatic Gell-Mann and Low formula for the energy shift with electrodynamic scattering matrix. This approach represents the decay probability as an imaginary part of energy shift dE . The method is a consistently electrodynamic one, allowing for the uniform consideration of a variety of induced & spontaneous processes. Their contributions, interference effects are represented by successive corrections of the electrodynamic perturbation theory (EDPT). Here we present new calculation scheme for the atomic oscillator strengths (OS), based on the energy approach with the use of the new ab initio method for construction of the wave functions in the transition matrix elements [4]. It refines the analogous method developed in [2]. In the "4" EDPT order there are diagrams, whose contribution into imaginary part of radiation width $\text{Im}dE$ accounts for the core polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (noninvariant one). The minimization of the corresponding functional $\text{Im}dE$ leads to the integrodifferential equation which can be solved using the standard numerical code (c.f. [2-5]). In result one can receive the optimal basis. To check efficiency of new procedure there have been calculated the oscillator strengths for some Na- and Fr-like ions. Results for the resonance 3p-3s transition in SVI: $gf(\text{exp.})=0,66-0.002$; $gf(\text{this work})=0,67$; $gf(\text{noninv. part})=0,1\%$. It is important to turn attention on the smallness of the gauge noninvariant part to the OS. This means that the results of calculations within traditional approach in the forms of "length" & "velocity" are practically equal for chosen representation. It's proved the theorem, generalizing the known Grant theorem [4].

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