Modified Version of the Coupled Perturbation Theory for Calculations of Atomic Properties

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For calculation of various physical parameters of atoms in external fields, we propose an improved version of the coupled many-particle perturbation theory in which the major part of intra-shell correlations is determined by the solution of the separate one-electron equations. The rest of the correlation correction is caused mainly by the change of the inter-shell interactions induced by an external field. The latter correction can be determined by means of iterative solution of the set of equations for corrections to radial orbitals. The use of expansions on the Sturmian - Hartree - Fock virtual orbitals in this approach is essential because it allows us to avoid all the troubles caused by the integration over continuum and, hence, to attain the high accuracy of the results and simplicity of the calculations. E. g., we obtain for the scalar part of the polarizability:

$\alpha_0 =$,

where σ_{nl} is a population of *nl*-shell, $\lambda_\nu^{(nl)}$ and $|\nu_{nl}>$ are the eigenvalues and the eigenvectors of the generalized eigenvalue problem (Sturm-type solutions) for the modified Hartree - Fock equation [1]. $T(n,l,k; n',l',k')$ are expressed through the double sum on ν, ν' of productes of the radial elements containing only the square-integrable functions. The expression (1) does not involve any integrations over the continuous spectrum.

[1] A.I. Sherstyuk, JETP Lett. **38** (1983) 665.