Relativistic multireference many-body perturbation theory for open-shell systems with multiple valence shell electrons*

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Accurate electronic structure and collision data are crucial to understanding astrophysical and laboratory plasmas. Recent efforts through the development and implementation of accurate relativistic many-body theoretical methods have greatly improved the accuracy of such data. In this presentation, a relativistic multireference many-body perturbation theory (MR-MBPT) for accurate predictions of term energies, spectroscopic transitions, and electron impact excitation cross sections in multielectron systems will be outlined.

An important feature in the relativistic many-body algorithm is the highly correlated state-specific many-electron wavefunctions that accurately account for relativity and for static as well as dynamic correlation energy corrections arising from the effective electron-electron interaction - the instantaneous Coulomb and Breit interactions - in addition to the QED corrections. The perturbation theory employs a general class of configuration-interaction wave functions as reference functions, and thus is applicable to multiple open valence shell systems with near degeneracy of a manifold of strongly interacting configurations.

The relativistic MR-MBPT is employed to construct the effective Hamiltonians for accurate representation of the N-electron target and (N+1)-electron scattering Hamiltonian matrices in relativistic R-matrix close-coupling theory. The effective many-body Hamiltonian R-matrix close-coupling calculations were successfully applied to the near-threshold electron impact excitation of electric dipole-allowed and spin-forbidden transitions in systems of astrophysical importance [1,2].

High-accuracy relativistic MR-MBPT calculations were carried out on the ground and excited levels of Al, Si, P, S, Cl, Zn, Ga, and Ge isoelectronic systems in which the near degeneracy of a manifold of strongly interacting configurations mandates a multireference treatment [3-6]. Transition rates associated with E1/M1/E2/M2/E3 radiative decays and lifetimes of a number of excited levels were calculated and compared with laboratory measurements to critically evaluate recent experiments.

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