

Implementation of a Super-Shell Refinement Algorithm for Plasma Opacities

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The spectral fidelity of opacity spectra generated using Super-Transition Array (STA) formalism is strongly dependent by the choice of super-shell structure. We report on an algorithm where a parent super-configuration (SC) is iteratively refined into daughter SCs until the probabilities of the parent and daughter SCs are equal within a small tolerance. This naturally leads to an SC-dependent super-shell structure, avoiding redundant refinement of SCs that are already converged using a small number of super-shells. We further discuss some modifications of the scheme necessary to accelerate convergence of STA spectra when orbital relaxation, or finite-state effects, are considered. Benchmark calculations illustrating computational efficiency using LLNL's LTE opacity code OPUS will be showcased and discussed. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-868727.

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