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Contribution Invited talks

Recalculation of astrophysical opacities: overview, methodology and atomic calculations

Atomic Opacities

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Content

The Opacity Project was launched in 1983 with the goal of calculating astrophysical opacities using state-of-the-art atomic physics based on the coupled channel (CC) approximation employing the powerful R-Matrix (RM) method [1]. Over the next decade, a suite of extended RM codes were developed to compute large-scale bound-bound transition strengths and bound-free photoionization cross sections with unprecedented accuracy. One of the primary features of OP was the precise delineation of *intrinsic* autoionizing resonance profiles whose shapes, extent and magnitudes are determined by myriad channel couplings in the (electron+ion) system. However, CC-RM calculations are of immense complexity and require substantial computational effort and resources. For the often dominant inner-shell transitions they could not be completed owing to computational constraints on the then available high-performance supercomputing platforms. Simpler approximations akin to distorted-wave (DW) type methods used in other opacity models, that neglect channel couplings, were therefore employed to compute most of the OP data.

In recent years a renewed effort has been under way as originally envisaged using the CC-RM methodology [2], stimulated by two independent developments. The first was a 3D Non-LTE analysis of solar elemental abundances that were up to 50% lower for common volatile elements such as C, N , O and Ne [3]. It was suggested that an enhancement in opacities could resolve the discrepancy, particularly in helioseismological models. The second was an experimental measurement of iron opacity at the Sandia Z-pinch device, under stellar interior conditions prevalent at the base of the solar convection zone, that were 30-400% higher in monochromatic opacity compared to OP [4]. The Z results also found nearly half the enhancement in mean opacity needed to resolve the solar abundances problem.

The pilot CC-RM calculations [2] for an important iron ion Fe XVII resulted in 35% enhancement relative to the OP Rosseland mean opacity at the Z conditions. While the enhancement is consistent with subsequently reported results from other opacity models [5,6], there are also important differences in (i) atomic physics, (ii) equation-of-state, and (iii) plasma broadening of autoionizing resonances. The calculations are of immense complexity and require substantial computational effort and resources. The Fe XVII calculations were carried through to convergence by including n = 3 and n = 4 levels of the target ion Fe XVIII. They showed large enhancements in photoionization cross sections, as successive thresholds are included, due to coupled resonance structures and the background. The extensive role of photoionization-of-core (PEC) or Seaton resonances associated with strong dipole transitions in the core ion Fe XVIII is especially prominent. Several sets of the pilot calculations have been carried out: relativistic Breit-Pauli R-Matrix (BPRM) calculations including 60 fine structure levels up to the n = 3 thresholds, non-relativistic calculations including 99 LS terms up to the n = 4 threshold, as well as BPRM calculations with 218 fine structure levels (in progress). One of the aims is to benchmark existing DW cross sections and monochromatic opacities in the non-resonant background and the high energy region above all coupled excitation thresholds.

In addition to the converged CC-RM atomic calculations, we are also investigating occupation probabilities from the Mihalas-Hummer-Dappen equation-of-state employed in the OP work which are orders of magnitude lower for excited levels than other models. A new theoretical method and computational algorithm for electron impact broadening of autoionizing resonances in plasmas, as function of temperature and density, is described. Finally, issues related to completeness and accuracy would be addressed, particularly “top-up” background opacity contributions to the CC-RM opacities from high-n configurations [5-7].

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