Atomic structure and transition rates using BSR

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Atomic structure calculations is an important and well developed field of physics with many successful methods such as Multiconfigurational Dirac-Hartree-Fock, but highly excited atomic states still a major challenge to most methods.

In this work the BSR-codes [1], R-Matrix theory with a B-spline basis for bound state and continuum functions, is used for several calculations involving Rydberg series and quasi-bound states. In combination with MCHF-calculations[2] for low lying states this gives a good basis for describing a "complete" system efficiently. Such calculations has many applications. As shown in this work it can be used for systems with highly excited states treating both radiative and and non radiative processes, such as autoionization, that are important in plasma diagnostics. Also since many states are included simultaneously a large amounts of data can be extracted from one calculation. Many applications have been proposed, for example Stark effect[3] calculations where a complete Rydberg series needs to be included.

We first present calculations on neutral Helium to show the capability and limitations of the program. Several $1sn'l'$ Rydberg series along with a few bound states above the ionization limit were investigated. Results agree very well with experimental data, especially for highly excited states and many levels in the series can be predicted accurately.

Lundberg *et al.* [4] discuss the Boron I system and mainly the problems within the $2s^2ns^2S$ Rydberg series. The $2s2p^2\ ^2S$ perturber is heavily mixed with several states in the series causing the *ab initio* calculation to fail placing this state in the correct position relative to the Rydberg series. This also gives rise to an error in the lifetime of the states. Taking advantage of BSR, calculations of these states can be done, along with several quasi-bound states. The lifetime of these states will also be presented.

In further studies dielectronic recombination (DR) and autoionization in Carbon II are considered. C. Jupén *et al.* [5] discuss oscillations observed in the plasma of the fusion reactor at JET research facility. These seem to be the result of DR and autoionization at the edge of the plasma involving in particular the $1s2s2p(^3P)4s\ ^4P$ states. Transitions between lower lying states and these quasi-bound states must be understood as well as the autoionization rates to be able to give a theoretical description of this process.

References

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