§13. New Trends to Access Atomic and Molecular Data

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Easy access to reliable Atomic and Molecular Data and Particle Surface Interactions (AM/PSI) are essential in fusion energy research. With regard to data production, both large scale advanced calculations as well as benchmark experiments for validation are needed. The Coordination Research Centre at NIFS (CR), member of the IAEA Data Centre Network[1], is a leader in producing, evaluating and diffusing AM/PSI data[2].

New trend to provide AM/PSI data, is to combined with usual numerical databases, web calculation tools, to quickly compute missing data. Joint-projects among Data Centres, as the IAEA Code Centre Network[3], develop to provide access to any information relevant for modelers in fusion plasma science. Data exchange is also an important issue, and NIFS is involved in the development of XSAMS[4], an XML schema for atoms, molecules and solids, organizing its last meeting in March 2010.

In this scope, large scale calculations of excitation cross section by electron impact from Xe I to VIII have been performed using the on line Los-Alamos Physics codes[5]. Atomic structures are calculated using the Hartree-Fock method. For each ionization stage, the configuration file comprises more than 20 configurations. Cross sections are calculated for 21 energy points on a log mesh from 1.01 to 1000 thresholds using the first order many body theory (FOMBT). Data provided are level energies and statistical weights of fine-structure levels of the ground and excited configurations, oscillator strengths and electron-impact excitation cross-sections.
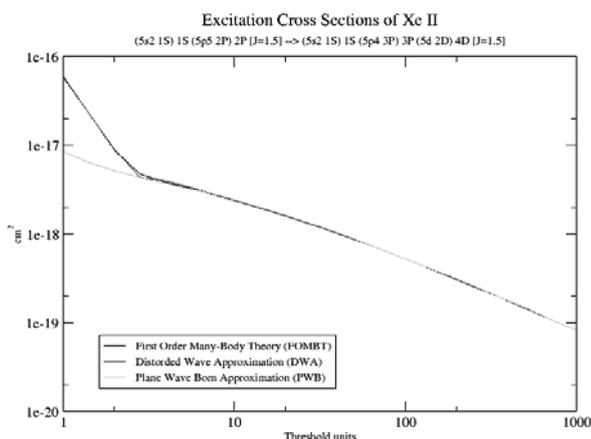

Fig. 1

Comparisons with the FOMBT theory and the distorted wave approximation (DWA) show a very good agreement (fig. 1), with some exceptions at low energies (fig. 2). Logically, for the plane wave Born approximation, agreement is always good at high energies.
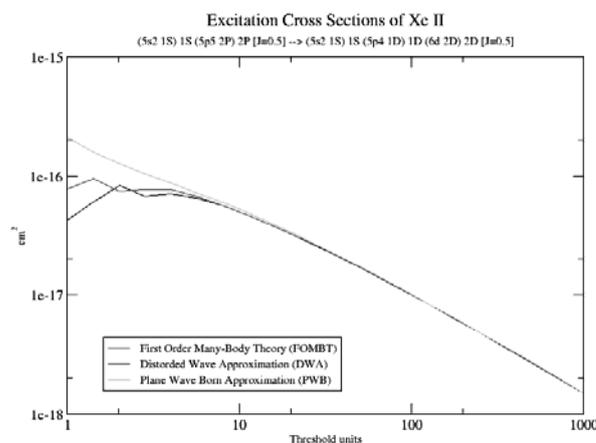

Fig. 2

Some other comparisons with the HULLAC code show also a good agreement (fig.3)
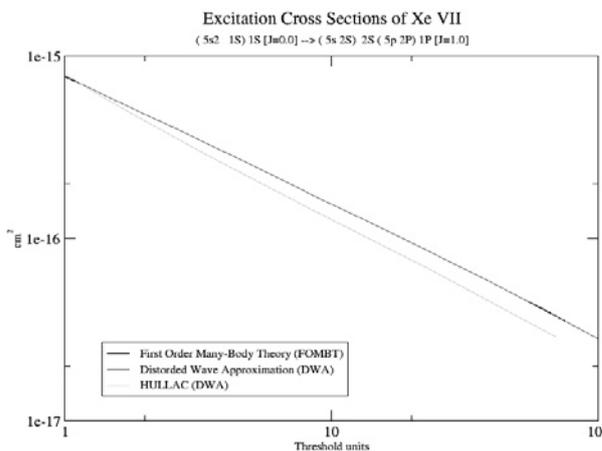

Fig. 3

Data will be available at NIFS[5], taking advantage of the development of the new web data service. Data are provided in tabular and graphical mode, as well as using the XML format XSAMS.

[1] http://www-amdis.iaea.org/DCN
[2] http://dbshino.nifs.ac.jp
[3] http://www-amdis.iaea.org/CCN
[4] http://www-amdis.iaea.org/xml
[5] http://aphysics2.lanl.gov/tempweb/lanl/