YAC: An Atomic Data Calculation Tool

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Abstract

A convenient and flexible graphical user interface has been developed for the YAC atomic physics code. [The YAC code computes opacities and detailed spectral information using a relativistic atomic model (Dirac equation) that is accurate for medium and high-Z plasmas.] Combining HDF5 (Hierarchical Data Format 5) with Java technology, the YAC user interface features database searching, data presenting and plotting on various computer platforms. The interface is designed to support multiple plasma models (LTE, Corona, CRE) and multi-component plasmas. As an illustration of the usefulness of the tool, an aluminum plasma spectrum is generated and compared with experiments. Good agreement is obtained. By visualizing the output, a deeper understanding of the spectrum structure is acquired through the YAC tool.

Outline

Overview of Existing Codes

Non-relativistic (include relativistic effects):

SUPERSTRUCTURE

- ❖ Cowan's code
- ❖ MCHF by F. Fischer

Relativistic:

- ❖ GRASP by Grant

HULLAC by Klapisch, Bar-shalom

In our group:

JATBASE, RSSUTA

YAC: develop an integrated package similar to HULLAC

❖: Public available

Hartree-Fock-Slater Atomic Structure

N-electron Hamiltonian:

$$H = \sum_{i=1}^{N} H_D(i) + \sum_{\substack{i,j \\ i<j}}^{N} \frac{1}{r_{ij}}$$

Atomic state function:

$$\Psi = \sum_{r=1}^{n_c} c_r \Phi_r$$

Dirac equation:

$$F_{n\kappa} = a_P^{-1/2}(r) P_{n\kappa}(r)$$

$$\frac{d^2}{dr^2} F_{n\kappa}(r) + \xi(r) F_{n\kappa}(r) = 0$$

Self-consistent potential:

$$V(r) = -\frac{Z}{r} + V_e(r) - \zeta \frac{3}{2}\left(\frac{3}{\pi}\rho(r)\right)^{1/3}$$

Transition oscillator strength:

$$S_{ij} = \left| \sum_{rs} C_{ri} C_{sj} \sum_{\alpha\beta} < \Phi_r \| Z^L \| \Phi_s > \tilde{M}^L_{\alpha\beta} \right|^2$$

$$gf_{ij} = \frac{1}{[L]} \omega S_{ij}$$

Average Configuration Approximation

Relationship between configuration rates and orbital rates

$$Q_{c\to c'} = q_{n\alpha}^{n_\alpha} \left[1 - \frac{q_{j\beta}}{g_{j\beta}}\right]^{n_\beta} \left[\frac{q_{j'\gamma} - \delta_{\alpha\gamma}}{g_{j'\gamma} - \delta_{\alpha\gamma}}\right]^{n_\gamma} Q_{\alpha\beta\gamma}$$

Electron collisional excitation:

$$Q(n_\alpha l_\alpha - n_\alpha l_\beta) = \frac{8\pi a_0^2}{(2l_\alpha+1)E} \sum_{ll'} \left[\sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{D}^2_\lambda + \sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{E}^2_\lambda + \sum_\lambda \sum_{\lambda'} (-1)^{\lambda+\lambda'+1} \begin{Bmatrix} l' & l & \lambda \\ l_\beta & l_\alpha & \lambda' \end{Bmatrix} \tilde{D}_\lambda \tilde{E}_{\lambda'} \right]$$

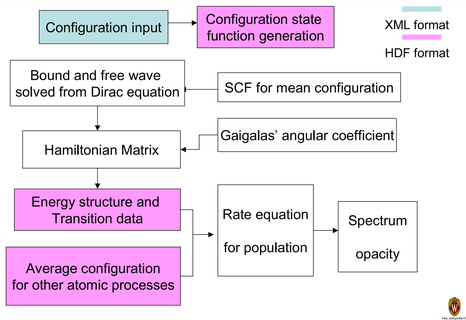
Electron collisional ionization:

$$Q(n_\alpha l_\alpha) = \frac{8a_0^2}{(2l_\alpha+1)E} \int_0^{(\varepsilon-I)/2} d\varepsilon' \sum_{ll'} \left[\sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{D}^2_\lambda + \sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{E}^2_\lambda + \sum_\lambda \sum_{\lambda'} (-1)^{\lambda+\lambda'+1} \begin{Bmatrix} l' & l & \lambda \\ l'' & l_\alpha & \lambda' \end{Bmatrix} \tilde{D}_\lambda \tilde{E}_{\lambda'} \right]$$

Autoionization:

$$A(n_\alpha l_\alpha n_\gamma l_\gamma - n_\beta l_\beta) = \frac{2\pi}{h} \sum_T \left[\sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{D}^2_\lambda + \sum_{\lambda=0} \frac{1}{2\lambda+1} \tilde{E}^2_\lambda + \sum_\lambda \sum_{\lambda'} (-1)^{\lambda+\lambda'+1} \begin{Bmatrix} l_\gamma & l & \lambda \\ l_\alpha & l_\beta & \lambda' \end{Bmatrix} \tilde{D}_\lambda \tilde{E}_{\lambda'} \right]$$

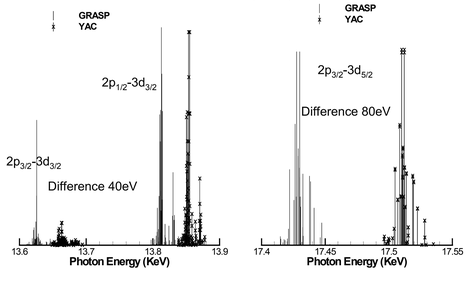
YAC Code Structure



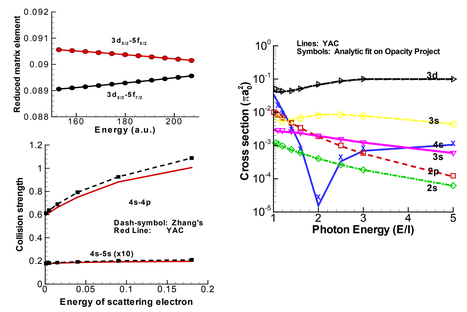
Comparing with GRASP Calculations

Cu-like U 2p-3d transition from initial configuration $1s^22s^22p^63s^23p^63d^94p^2$

Relative difference looks much smaller (0.3%)



YAC Results and Comparison with Other Calculations



Application to Hard X-ray Emission

- Experiment on hard X-ray emission from laser-produced U plasma
- Hydrodynamic simulation using the Bucky code

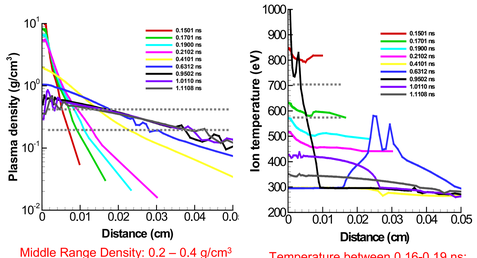
1 ns square pulse

24 OMEGA beams on each side

Each with an energy of 500J

Total laser energy 11.6 kJ

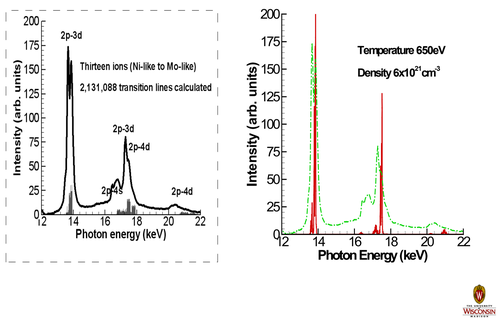
Hydrodynamic Simulations from BUCKY



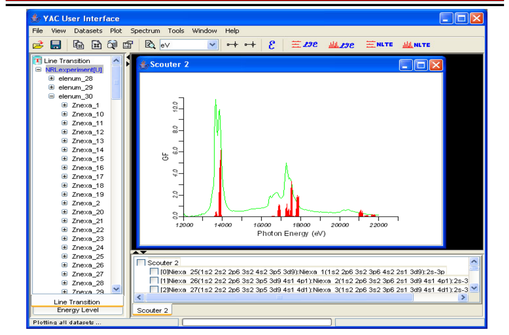
Middle Range Density: 0.2 – 0.4 g/cm^3 (6×10^{21}-1.2×10^{22})

Temperature between 0.16-0.19 ns: 600-700eV

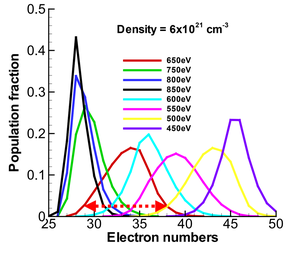
Transitions for Thirteen Ions and Synthetic Emission Spectrum



Screen Shot of YAC User Interface



CRE Quasi-Steady State Population



For temperatures much lower or higher than 650 eV, the dominant ions are shifted to the lower or higher ion stages, which generate considerably lower or higher 2p-3d transition and cannot explain the observations.

Summary

- We are developing an integrated package for the calculation of a variety of atomic processes.
- The code structure and formalism are described, and calculations are compared with other theoretical results.
- The code is used with the hydrodynamic code to analyze hard X-ray emission from laser produced Uranium plasmas. Further study is needed to resolve the disagreement.
- Future code developments include detailed level-by-level calculations for other atomic processes.