Building Tools for Atomic Data Calculations

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UW-FTI atomic physics capability

• Atomic properties computed using state-of-the-art models (Z=1-92)
• Plasma state computed using state-of-the-art equilibrium and non-equilibrium models (1 eV – 100keV)
• Rosseland and Planck opacities computed in tabulated form
• Spectral analysis of measured and computed spectra

Tasks

• Harden atomic physics modeling software
• Create database of requested data
• Complete processing tools to generate data, access data, and visualize data
• Complete analysis tools to compare data to experiment

Theoretical Atomic Models

• Hydrogen-like model
  Radiative and collisional properties are calculated by assuming only one electron (nl or nlj) in the system that has an effective charge state.
  
• Average Atom model – self-consistent potential, TFD
  Assuming only one pseudo-atom in the plasma.

• Unresolved Transition Array method (UTA)
  A single profile is used to represent a cluster of transition arrays.

• Detailed Configuration Accounting (DCA)
  The radiative and collisional properties are done on the configuration level.

• Detailed Term Accounting (DTA)
  The most complex method that explicitly calculates the radiative and collisional properties under LS or JJ or intermediate coupling scheme.

Plasma Models to Obtain Atomic State Populations

• LTE Model (Local Thermal Equilibrium) -- Collisional ionization and three-body recombination
• Corona Model -- Collisional ionization and radiative recombination
• Collisional Radiative Equilibrium (CRE) Model

Non-LTE Model

Assumptions:

• Consider collisional and radiative atomic processes at the ion stage level

\[ \frac{dN_i}{dt} = \sum_j \left( w_{ij} - n_j \sum_k \sigma_{kj} \frac{n_k}{N} \right) \]

• Rate coefficients use semi-classical formulas, such as Lotz's for electron ionization, Kramer's for radiative recombination.
• Screened hydrogen-like atomic data are used for rate coefficient calculations.
• Local thermal equilibrium (LTE) approximation for energy levels in each ion stage.

Using accurate atomic energy levels, oscillator strengths from either UTA or DSSUTA model or high-Z RACUTA model, enable us to calculate high-Z non-LTE opacities.
Radiative rates taken into account, therefore <Z> in more accurate than LTE calculations of <Z> for high temperature low density plasmas.

RSSUTA compares favorably to TOPS

JATBASE User Interface (2001)

The YAC Code

JATBASE

• Detailed LSJ, LS coupling radiative atomic data (E, gf) for Z=1-18
• Large scale EOS and opacity calculations
• Format compatible with hydro codes
• Non-relativistic unresolved transition array method
• Storage in text data format

YAC

• Implement all physics already in JATBASE
• Relativistic unresolved transition array method (RSSUTA)
• More detailed drift-down information
• Better user interface
• 3D graphics visualization
• Universal Hierarchical Data Format (HDF)

Features of computer codes

Atomic data processing tools

• JATBASE (completed) -- Jiankui Yuan’s Ph.D. thesis
• YAC (In progress) -- Stand alone application to process data
• WEBATOM (In progress) -- Web interface to data

Relativistic Single-Configuration UTA method

Wave functions are solved from the Dirac equation:

\[ \left( i \hbar \gamma \cdot p + m + \beta \cdot \lambda \right) \psi = \alpha \psi \]

Cross sections are calculated under the configuration average approximation:

\[ \sigma = \sum_i \frac{d\sigma}{d\Omega} \]

Vertex line shape, natural, Doppler, Stark and UTA broadening

Atomic Data Package Framework