



**International Atomic Energy Agency**

**Electron and Radiative Processes  
for Atoms and Ions With  
Application to Fusion Research**

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**Nuclear Data Section**

# Overview

- **Introduction: Fusion plasmas and data needs**
- **Atomic structure**
- **Electron impact excitation**
- **Ionization processes: electron impact, photo- and auto- ionization**
- **Applications to collisional radiative model**

# Introduction

# Fusion plasmas

- **Main constituents are hydrogen isotopes**
- **Impurities from variety of sources**
- **Must model entire plasma for ionization stages, spectrum analysis**
- **Different plasma regimes: LTE, coronal, CR**
- **Large datasets needed for CR model**

# Plasma regimes

- **At high density, collisions dominate all processes, upward and downward rates balance, plasma is in LTE. Populations from energies, statistical weights.**
- **At low density, excited states not populated. Only transitions from ground states need be followed. Common in astrophysics; coronal equilibrium.**

# Plasma regimes

- **Moderate densities require solving full set of rate equations, tracking populations of excited states. Large databases needed.**
- **Often plasma is in steady state; populations not changing. Otherwise, need to do time evolution.**

# Types of data needed

- **Atomic structure – energy levels, wave functions.**
- **Radiative processes.**
- **Collisional processes.**
- **Charge transfer processes.**
- **Plasma interaction with wall materials.**
- **Data for atoms, ions and molecules.**

# Atomic Structure

# Atomic structure

- **Relativistic versus non-relativistic.**
- **Notation and coupling schemes.**
- **Electron configurations.**
- **LS Terms.**
- **Fine structure levels.**
- **Mixing of basis states.**

# Relativistic and Non-relativistic

- **For heavy elements and for high charge states full relativistic treatment is needed**
- **Possibility of inclusion of some relativistic features in non-relativistic treatment; mass and darwin terms in radial wave function, spin-orbit interaction in energy levels**
- **For most fusion applications, modified non-relativistic approach is adequate**

# Hartree-Fock Method

- **Total wave function is an anti-symmetrized determinant product of one-electron orbitals (the "Slater" determinant)**
- **Begin with approximate orbitals for all electrons**
- **Use these orbitals, calculate potential and solve Schroedinger equation for one electron orbital**

# Hartree-Fock Method

- **With the new orbital, continue to next electron**
- **Continue through all electrons, giving new set of orbitals**
- **Iterate through process until all orbitals converge**
- **Large computer code developed by R.D. Cowan, updated and modernized by J. Abdallah, Jr.**
- **Interface allows use of structure code through Internet**

# Radial wave functions

- From structure calculation each radial wave function may be displayed
- As nuclear charge increases, radius decreases

# Configuration notation

- **Simplest specification is specification of principle and orbital quantum numbers with occupation number:  $1s^22s2p$  for example**
- **For compactness, often inner noble gas core is assumed, leading to above configuration abbreviated  $2s2p$**
- **This assumes non-relativistic; could also use  $jj$  coupling**

# Noble gas cores

- Noble gases: He, Ne, Ar, Kr, Xe closed shell systems
- Do not change angular coupling
- For simplicity, do not need to include explicit listing of noble gas core

Examples: C I has configuration  $1s^2 2s^2 2p^2$  which can be entered as  $2s^2 2p^2$

Al III may be entered as simple  $3s$ , dropping the entire Ne-like core

# On the web

- **Go to A+M home page:  
[www-amdis.iaea.org](http://www-amdis.iaea.org)**
- **Use link to LANL codes**
- **READ the information, then proceed to calculation.**
- **Select ion stage, continue.**
- **Select configurations. More than two configurations are permitted. Enter list of configurations. Note that noble gas cores need not be entered.**

# Configurations

- **Radial wave functions are calculated for configurations**
- **Radial wave functions are not changed for different couplings of angular momentum**
- **Influence of angular momentum coupling included through mixing of target states**

# Configuration energies

- For any structure calculation, energies of all shell may be displayed
- Koopman's theory:  
Energy of electron in a shell is equal to the ionization energy
- Theory rigorous for hydrogenic
- Approximate for complex systems, other electron orbitals change with removal of electron

# Configuration energies

- **Hydrogenic orbitals:**  
Ionization energy is  $Z^2/n^2$  where  $Z$  is the nuclear charge and  $n$  is the principle quantum number
- **Screening constants:**  
For an electron outside other orbitals, the inner electrons “screen” the nuclear charge, thus for Li-like, the 3s electron sees  $Z_{\text{eff}} = Z - \sigma$  where  $\sigma$  is a screening parameter

# Coupling of angular momentum

- **Electrons have orbital angular momentum and spin**
- **These couple vectorially**
- **There are a number of possible methods to couple**
- **We will follow LSJ coupling**

# LSJ coupling

- **Start from electron configurations**
- **Couple electron orbital momenta within a shell.**
- **Couple electron spins in shell**
- **Couple result to previous shell, continue through all shells**
- **Couple total orbital angular momentum and spin for total angular momentum**
- **Include target state interactions: Configuration mixing from Coulomb interaction, mixing of LS terms from spin-orbit interaction**

# Example

- Simple case first
- $C^{+4}$ , helium-like
- Consider 1s2p configuration
- Total orbital angular momentum,  $L$ , must be 1 ( $l_1=0, l_2=1$ )  $|l_1-l_2| \leq L \leq l_1+l_2$
- Total spin,  $S$ , can be 0 or 1 ( $s_1= s_2=1/2$ ) and  $|s_1-s_2| \leq S \leq s_1+s_2$
- Terms are 1s2p  $^1P$  and 1s2p  $^3P$ , using notation of  $^{2S+1}L$

# Example

- The  $^1P$  term can only have total angular momentum,  $J$ , of 1 ( $S=0$ ,  $L=1$ )  $|L-S| \leq J \leq L+S$
- The  $^3P$  can have  $J=0,1,2$  ( $S=1$ ,  $L=1$ ).
- Energy levels are:  $1s2p\ ^1P_1$ ,  $1s2p\ ^3P_0$ ,  $1s2p\ ^3P_1$  and  $1s2p\ ^3P_2$ .
- For more complex cases, the procedure is to couple within a shell, then couple to previous shells.

# Example

- Consider case of electron configuration of  $3s^2 3p^2 3d^2 4p$ . This requires coupling the 3p electrons first, then coupling the 3d electrons, coupling that result to the 3p result, and finally coupling the 4p electron.
- One sample level is:  
 $(3p^2 \ ^1D)^1D \ (3d^2 \ ^3F)^3H \ (4p^1 \ ^2P) \ ^4I$ .
- This single electron configuration gives rise to 604 fine structure levels.

# Mixing of target states

- **Configurations and LS terms form basis states**
- **Coulomb interaction causes mixing of configurations which have the same LS terms**
- **Spin-orbit causes mixing of LS terms which have the same configuration**
- **Mixing provides better description of energy levels**

# Example of Configuration Mixing

- Consider Be-like ion,  $\text{Fe}^{+22}$ .
- Consider configurations  $2s^2$ ,  $2s2p$ ,  $2p^2$ ,  $2s3p$  and  $2p3s$ .
- Configuration mixing occurs due to Coulomb interaction.
- Spin-orbit causes mixing of LS terms.
- List of make-up of energy levels:

# Make-up of Energy Levels

index	j	component	configuration
1	.0	9.8008E-01	( 2s2 1S) 1S
		2.3433E-02	( 2p2 3P) 3P
		1.9722E-01	( 2p2 1S) 1S
2	.0	1.0000E+00	( 2s1 2S) 2S ( 2p1 2P) 3P
3	1.0	9.8649E-01	( 2s1 2S) 2S ( 2p1 2P) 3P
		1.6382E-01	( 2s1 2S) 2S ( 2p1 2P) 1P
4	2.0	1.0000E+00	( 2s1 2S) 2S ( 2p1 2P) 3P
5	1.0	-1.6382E-01	( 2s1 2S) 2S ( 2p1 2P) 3P
		9.8647E-01	( 2s1 2S) 2S ( 2p1 2P) 1P
6	.0	-7.3820E-02	( 2s2 1S) 1S
		9.6485E-01	( 2p2 3P) 3P
		2.5221E-01	( 2p2 1S) 1S

# Consequences of Mixing

- Configuration can allow “double electron” jumps. Since the  $2s^2\ ^1S_0$  contains some of the  $2p^2\ ^1S_0$  state, it becomes possible to have a non-zero probability for a transition to occur between those states.
- LS term mixing can cause radiative transitions between “spin-forbidden” states

# Example of Effects of Mixing

- Consider He-like transition  $1s^2 \rightarrow 1s2p^3P_1$ .
- The  $1s2p^3P_1$  is actually a mixture of  $^1P_1$  and  $^3P_1$  with the mixing varying with nuclear charge. For C, the mixing coefficients are 0.99995 and 0.00041, while for Fe they are 0.95922 and 0.28266.
- For carbon this is a forbidden transition,  $gf = 1.1851e-05$

# Example of Effects of Mixing

- For iron it is allowed,  $gf = 6.3684e-02$
- This makes a difference in radiated power and for ionization balance
- For carbon, electron configuration overestimates radiated power, underestimates ionization rates
- For iron, configuration model is better

# Configuration vs fine structure

- **Configuration calculation mode gives no coupling of angular momentum**
- **CFG mode runs fast**
- **CFG has few levels**
- **Often CFG mode makes reasonable approximation to levels**
- **CFG mode has no mixing effects**

# Data Obtained From Structure Code

- **Energy levels**
- **Radial wave functions**
- **Effects of mixing (configuration and spin-orbit)**
- **Oscillator strengths**
- **Configuration and fine structure modes**

# Using GENIE

- **Go to A+M home page**
- **Select GENIE**
- **Use Transition Probabilities portion**
- **Enter ion stage**
- **For optical properties, select wavelength range (in angstroms)**
- **Select databases to search (default is all)**
- **View results. Now, do exercises**

# Electron Impact Excitation

# Transition processes

- **Excitation**
- **Ionization**
- **Autoionization**
- **Photoionization**
- **Inverse processes**
- **Both electron and ion impact may be important in above**
- **Charge transfer**
- **Molecular processes**

# General Formulation for excitation

$$Q = \sum |R(a, b)|^2$$

$$R(a, b) = \int dx_1 \dots \int dx_{N+1} u^*(x_i) \Psi^*(x_i^{-1}) \left[ \sum \frac{1}{r_{pj}} \right] u(x_j) \Psi(x_j^{-1})$$

# **Electron impact excitation considerations**

- **Requires solution of coupled equations representing target states and free electrons**
- **Common solution is to largely decouple to initial target and free electron, final target and free electron**
- **Choices are then in method of solution for target and for free electron**

# Common approximations

- **Plane-wave-Born**
- **Coulomb Born**
- **Distorted wave**
- **Close coupling**

# Allowed and forbidden transitions

- Dipole allowed,  $l_2 = l_1 \pm 1$ , are generally stronger, with  $l_2 = l_1 + 1$  the stronger
- Spin allowed are generally stronger, singlet-singlet or triplet-triplet
- $J_2 = J_1 \pm 1, 0$  but not  $J_2 = J_1 = 0$
- Mixing can change these general assumptions

# Plane wave Born

- **Two state method**
- **Free electrons are both plane wave, potential of target is completely ignored**
- **Cross sections can be calculated from generalized oscillator strength from target states**
- **Calculation is fast**
- **Accuracy best at high impact electron energies**

# Coulomb Born

- **Next level of approximation**
- **Free electrons are Coulomb functions, using  $Z-N$  bound electrons for effective charge**
- **Sampson et al. calculated for hydrogenic targets, then used screening parameters to extend to complex ions**
- **Best for several times ionized and not many equivalent electrons**

# Distorted wave

- **Take into account the actual potential from the target state in calculation of free electron**
- **Several methods for doing this, DWA, FOMBT**
- **Exchange effect on potential also treated in variety of ways**
- **Average approximation allows faster solution**

# Close coupling

- **Solve full set of coupled equations, bound and free**
- **May include many high lying states, above continuum, leading to resonances**
- **Long computing time required**
- **R-Matrix theory allows solutions within limited radius, matches energy solutions at boundary**
- **Most accurate theory**

# Collision strength

- Cross section generally of order of atomic dimension
- Cross section decreases with energy
- Cross section dependent on direction of transition
- Collision strength defined as:

$$Q_{ij} = \frac{\pi a_2^0}{g_i E_i (\text{Ryd})} \Omega(i, j)$$

# Rate coefficients

- Electron distribution is often Maxwellian
- Weighted integral of cross section gives rate coefficient:

$$R = \int F(E, T) v(E) \sigma(E) dE$$

# Rate coefficients

- **Can be generated from web interface**
- **Function of temperature, not individual electron energy**
- **Temperature grid automatically set by interface from range of impact energies used in cross section calculation**
- **Must have sufficient points for integration to make sense**

# Detailed balance

- In LTE, rates for upward and downward balance:  $n_i R_{ij} = n_j R_{ji}$
- Populations given by energies and statistical weights (assume Maxwellian electron distribution)
- Gives relationship between cross section and inverse:

$$R_{ji} = \frac{g_i}{g_j} e^{\frac{-E}{kT}} R_{ij}$$

# Resonances

- **Doubly excited levels may be formed and autoionize to a singly excited level**
- **Consider  $e + 1s^2 \rightarrow 1s2p + e'$  as the direct excitation**
- **At a particular energy a capture can take place:  $e + 1s^2 \rightarrow 1s3dnl$  giving a doubly excited state**

# Resonances

- **Autoionization can proceed:**  
 $1s3dnl \rightarrow 1s2p + e'$
- **Series takes place for different values of  $nl$ . Also, change the 3d shell to 3s, 3p, etc. Many resonances can occur**
- **Each resonance is at a definite, discrete energy, dictated by capture of the initial free electron into a specific state**

# Resources on the web

- **Several electronic databases, reviewed by D. Humbert, searched by GENIE**
- **LANL codes use DWA or FOMBT for electron impact excitation, configuration or fine structure**
- **Average approximation on A+M Unit home page for electron impact in configuration mode only**
- **Heavy particle collisions on Unit home page, bare nucleus on hydrogenic ion**

# Ionization Processes

# Electron impact ionization

- **Process similar to excitation, incoming free electron, outgoing free electron with different energy**
- **However, now there are two outgoing free electrons; causes complication**
- **Total energy after collision is  $E_T = E_i - \Delta E$ , where  $E_T$  total energy after collision,  $E_i$  is the impact energy and  $\Delta E$  is the ionization energy**

# Electron impact ionization

- **This energy is distributed between the two outgoing electrons**
- **For a given angular momentum of one outgoing electron, there is a range of angular momenta possible for the other, depending on the angular momentum of the target state**
- **These considerations give rise to a very large number of possible free electron wave functions needed to solve problem**

# Common approximations

- **Lotz formula. Well-known. Not bad accuracy for well-studied systems.**
- **Scaled Coulomb Born. Extension of the excitation method. Fits available. Accuracy acceptable for many systems.**
- **Distorted wave. Problem is now in two outgoing free wave functions, split of total energy between the two. Large increase of computational time**
- **Convergent close coupling (CCC) has been successfully applied to ionization**

# Scaled hydrogenic method

Reduced hydrogenic cross section :

$$Q_{nl}^{HR} = \left( \frac{Z}{n} \right)^4 \frac{Q_{nl}^H}{\pi a_0^2}$$

For complex ion,

$$Q(u) = \pi a_0^2 \left( \frac{n}{Z_{eff}} \right)^4 r_{nl} Q_{nl}^{HR}$$

# Scaled hydrogenic method

Note for hydrogenic ion, ionization energy is :

$$E^I (Ryd) = \left( \frac{Z}{n} \right)^2$$

Assume similar for complex ion to arrive at :

$$Q(u) = \frac{\pi a_0^2}{[E^I (Ryd)]^2} r_{nl} Q_{nl}^{HR} (u)$$

# Scaled hydrogenic method

- If scaled hydrogenic cross section,  $Q_{nl}^{HR}(u)$  is known, then cross section for arbitrary ion can be calculated
- Scaled cross sections calculated for 1s through 6g have been fitted as function of shell and impact energy
- Result is fit formula for scaled hydrogenic cross section
- Allows calculation of approximate cross section for any ion

# Scaled Hydrogenic Method

Fit form used :

$$Q_{nl}^{HR}(u) = \frac{1}{u} \left[ \left( C_1 + \frac{C_2 + C_3 l}{n} \right) \ln(u) + \left( C_4 + \frac{C_5 + C_6 l}{n} \right) \left( 1 - \frac{1}{u} \right) + \left( C_7 + \frac{C_8 + C_9 l}{n} \right) \left( 1 - \frac{1}{u} \right)^2 \right]$$

# Scaled hydrogenic

- In previous,  $u$  is the electron impact energy in threshold units
- Result is cross section for one shell of hydrogenic
- Possible to include angular coupling effects as well as mixing of target states
- The  $C_i$  are the fitting coefficients with the values:

# Fitting parameters

**$C_1$  1.5369**

**$C_2$  0.99656**

**$C_3$  -0.61916**

**$C_4$  2.4463**

**$C_5$  -2.4773**

**$C_6$  3.2151**

**$C_7$  -1.4512**

**$C_8$  1.7230**

**$C_9$  -0.47075**

# Distorted wave

- **Similar to calculation for excitation**
- **Difficulty is now there are two outgoing free electrons**
- **Energy splits between two, very many free electron orbitals needed**
- **Perform quadrature over outgoing electron energy split**
- **Computational time is significant**

# Close coupling

- **Application now made to ionization**
- **Convergent close coupling technique developed by Bray and Fursa has wide range of applications**
- **Still under development**
- **Difficulty handling partial filled shells**

# Photoionization

- **Photon causes ejection of electron**
- **Not very likely in fusion plasmas**
- **Inverse process is radiative recombination**
- **Competes with inverse of electron impact ionization, three body recombination**
- **Radiative recombination is often dominant recombination mechanism**

# Autoionization

- **May have ion suffer inner shell excitation**
- **Result may lie above continuum**
- **Result is autoionization**
- **Inverse process is di-electronic recombination**
- **Both may be very important in fusion plasmas**
- **May be calculated with DW theory, or automatically generated with CC methods**

# Autoionization and resonances

- Consider an initial configuration for Li-like ion of  $2s$  and impact energy  $E_i$ , below the energy necessary to excite the  $2s$  to the  $3s$  shell.
- Possible outcome is simultaneous excitation and capture to the  $3s^2$  configuration
- The  $3s^2$  may then autoionize to the  $2p$ , releasing the electron
- This is a resonance to the direct  $2s - 2p$  transition
- Requires precise energy match to allow capture with the excitation

# Collisional Radiative Models

# Collisional radiative model

- **With data in place can proceed to study of plasma**
- **May have interest in radiated power, spectrum, diagnosis of temperature, etc**
- **All require model of the plasma**
- **First need is the kinetics – determination of populations of all levels of all ion stages**

# Rate equations

Time evolution of populations :

$$\frac{dN_{i,j}}{dt} = \sum_k R_{i-1,k \rightarrow i,j}^I N_{i-1,k} - \sum_k R_{i,j \rightarrow i+1,k}^I N_{i,j} + \sum_k R_{i+1,k \rightarrow i,j}^R N_{i+1,k} - \sum_k R_{i,j \rightarrow i-1,k}^R N_{i,j}$$

# Special cases

- High density, approaches LTE
- Low density, goes to coronal
- Steady state, populations not changing:

$$\frac{dN_{i,j}}{dt} = 0$$

For all levels of all ion stages.

# Effective rate coefficients

- **Full model can involve very large problem, thousands of levels in each ion stage. Connections mean many millions of possible transitions. Solution of rate equations will be lengthy.**
- **Time dependent case will take longer, requiring solution in small time increments of the full rate equations.**

# Effective rate coefficients

- If solution is calculated over a two dimensional grid in temperature and density, solution for other temperature, density can be found; very good solution for steady state, acceptable for time dependent.
- For each calculated solution, save total population of each ion stage, total radiated power, radiated power per ion stage, total ionization and recombination rate coefficients for each ion stage. Can also store spectrum for each ion stage.

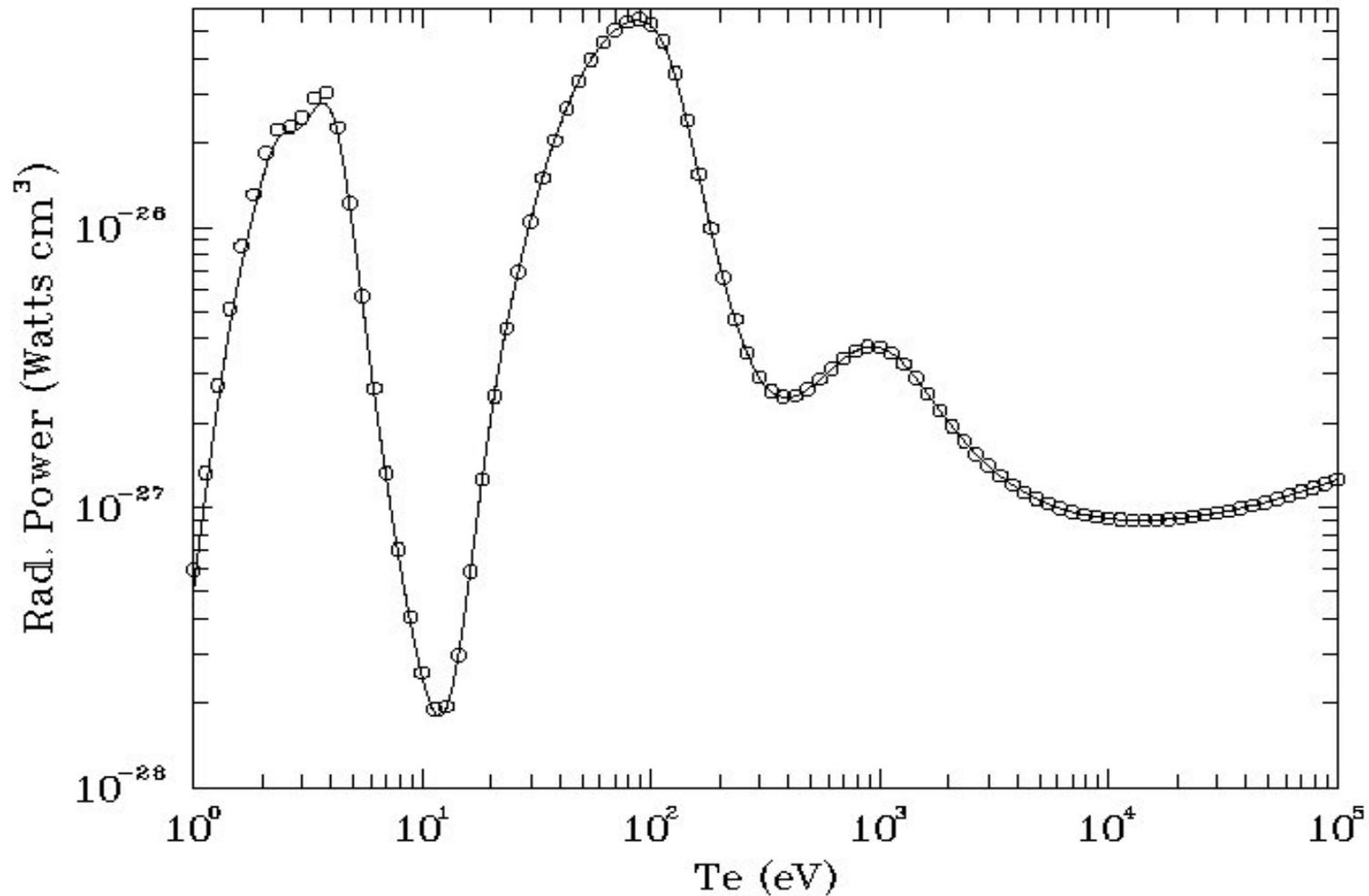
# Effective rate coefficients

- **For steady state solution, interpolate on total ion populations, total radiated power.**
- **For time dependent, interpolate on effective ionization and recombination rate coefficient. Then solve much simpler equations for ion stage populations, use with radiated power per ion stage to get total radiated power.**

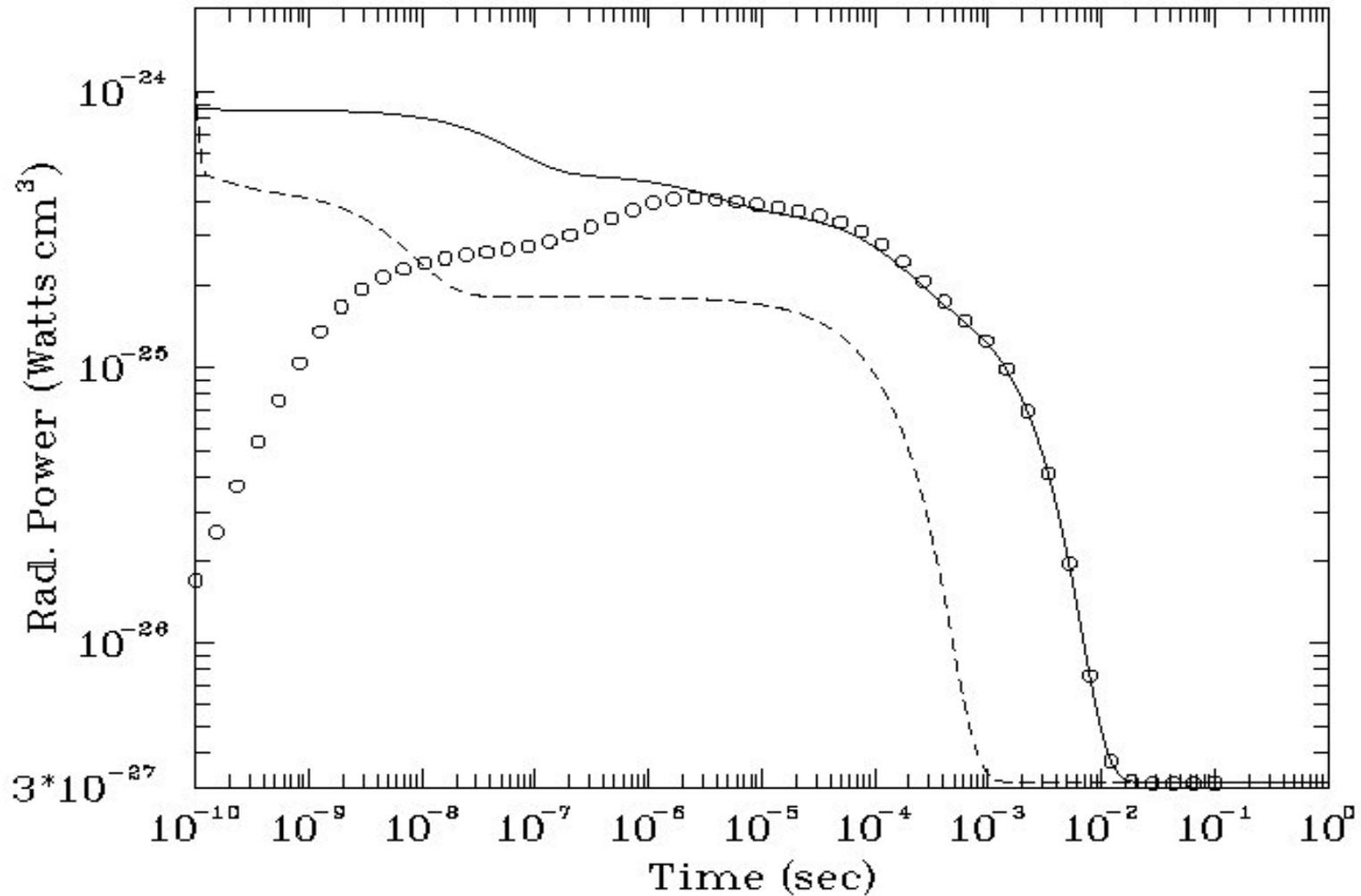
# Effective rate coefficients

- **Steady state solution is very good.**
- **Time dependent is good for overall time behaviour, not so good for early times far from steady state.**

# Steady state example



# Time dependent example



# Types of Time Dependent Problems

- **Initial equilibrium populations with changing temperature/densities.**
- **Initial ion stage out of equilibrium. Two cases; ionizing plasma, recombining plasma.**
- **At long time interval, should go to steady state solution, use as check on time dependent calculation.**

# Sensitivity to data

- **Many large scale properties of plasma relatively insensitive to details of calculation**
- **Most important aspect is building a complete set of data**
- **If processes are missing, disaster can occur; population builds up artificially and all results can be wrong**
- **Data should be consistent with same set of basis functions used**

# CR models

**On the web :**

**On Unit home page click on RATES**

**Can also go to temporary site:**

**<http://www-amdis.iaea.org/DATASENS/>**

# Data sensitivity

- **Go to DATASENS page**
- **First run baseline model**
- **May choose to view baseline results**
- **Have option to modify all data: select multiplier for each type of data and apply either in random manner, or uniformly**
- **Recalculate and compare results**

# Summary

# Plasma conditions

- **For fusion, not LTE**
- **For fusion, not coronal**
- **Collisional radiative model needed**
- **Large amounts of data for solution of rate equations required**

# Types of data presented

- **Atomic structure**
- **Electron impact excitation**
- **Ionization processes:**
  - Electron impact**
  - Photoionization**
  - Autoionization**

# Resources

- **Individual databases**
- **GENIE search engine**
- **Codes on Internet**

# Conclusion

**There are many data needed for modelling fusion plasmas. Many resources are available for such data. Often more data are needed, requiring continuing research in atomic, molecular and plasma interaction physics.**