Developments in CX data.

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ADAS-EU course – 26 – 30 Mars 2012

Outline

1. Motivation
2. Theoretical Methods
   - Molecular Quantal
   - Semi-classical
   - Classical CTMC
3. Results

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Motivation

- CXRS is used for plasma diagnostic (Ti, density, rotation...).
- Very accurate cross sections are required to adequately model the impurity density in plasmas.
- A wide range of energies is needed for cover thermal and neutral beam CX.
- Using different methods we can give cross sections data in a wide range of energies.

Different methods for B^{5+} + H calculation

Calculations peformed

↙ ↓ ↘

	Quantal	Semiclassical	Classical
capture	Yes	Yes	Yes
ionization	No(Yes*)	No(Yes*)	Yes
excitation	No(Yes)	Yes	No(Yes)
Energy interval (keV/amu)			
B^{5+}+H(1s)	$0.01 \leq E \leq 1$	$0.25 \leq E \lesssim 28.58$	$35.97 \lesssim E \leq 1000$
B^{5+} +H(2s)	$0.01 \leq E \leq 1$	$0.25 \leq E \lesssim 15.41$	$19.50 \lesssim E \leq 1000$

*: incluing pseudostates

Outline

Molecular Quantal Method

Common Reaction coordinate

Molecular Quantal Method

Common Reaction coordinate

- Electronic and nuclear motion are described by quantum mechanics.

$$H\Psi = E\Psi \begin{cases} \Psi(\mathbf{r}, \boldsymbol{\xi}) & \xrightarrow[\xi \to \infty]{} \quad \phi_i^A e^{i\mathbf{k}_i' \boldsymbol{\xi}} + \sum_f \frac{e^{ik_f' \xi}}{\xi} f_{if}'(\Theta)\phi_f^A \\ \Psi(\boldsymbol{r}, \boldsymbol{\xi}) & \xrightarrow[\xi \to \infty]{} \quad \sum_f \frac{e^{ik_f' \xi}}{\xi} f_{if}'(\Theta)\phi_f^B \end{cases}$$

Molecular Quantal Method

Common Reaction coordinate

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- Electronic and nuclear motion are described by quantum mechanics.

$$H\Psi = E\Psi \qquad \begin{aligned} \xi(\boldsymbol{r},\boldsymbol{R}) &= \boldsymbol{R} + \frac{1}{\mu}\boldsymbol{s}(\boldsymbol{r},\boldsymbol{R}) \\ \boldsymbol{s}(\boldsymbol{r},\boldsymbol{R}) &= f(\boldsymbol{r},\boldsymbol{R})\boldsymbol{r} - \frac{1}{2}f^2(\boldsymbol{r},\boldsymbol{R})\boldsymbol{R} \end{aligned}$$

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$$\Psi(\boldsymbol{r},\xi) = \sum_J \Psi^J(\boldsymbol{r},\xi) = \sum_J \sum_k \chi_k^J(\xi)\Phi_k(\boldsymbol{r},\xi)$$

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- $\{\Phi_k\}$ are Born-Oppenheimer eigenfunctions for R=ξ.

$$H_{elec}(\boldsymbol{r},\xi)\Phi_k(\boldsymbol{r},\xi) = E_k\Phi_k(\boldsymbol{r},\xi)$$

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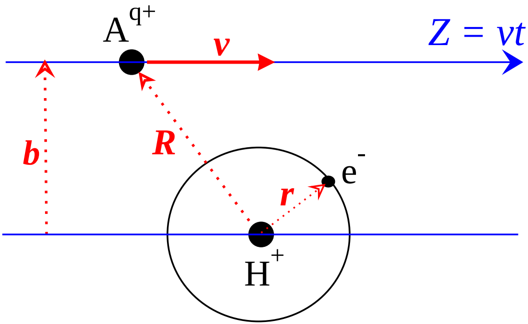
- Cross Section to the state j from the initial state i

$$\sigma_{ij} = \frac{\pi}{k_i^2}\sum_J (2J+1)|\delta_{ij} - S_{ij}^J|^2$$

Semiclassical Method

Eikonal approach At big impact energies ($E > 250 eV/uma$) nucleai motion can be approach by straight trajectories:

$$\boldsymbol{R}(t) = \boldsymbol{b} + \boldsymbol{v}\, t$$



Semiclassical Method

Eikonal ecuation

Electronic motion is described by $\Psi(\boldsymbol{r};t)$ that is solution of the eikonal equation:

$$i\left(\left.\frac{\partial\Psi(\boldsymbol{r};t)}{\partial t}\right|_{r}\right) = H_{el}\Psi(\boldsymbol{r};t)$$

H_{el} is the electronic Hamiltonian:

$$H_{el} = -\frac{1}{2}\nabla^2_{\boldsymbol{r}} - \frac{Z_p}{\boldsymbol{r}_p} - \frac{Z_t}{\boldsymbol{r}_t} + \frac{Z_pZ_t}{R}$$

Semiclassical Method

OEDM

$\Psi(\boldsymbol{r};t)$ is expanded in molecular orbitals (exact, variacional):

$$\Psi(\boldsymbol{r},t) = \mathrm{e}^{iU(\boldsymbol{r},R)} \sum_{j}^{N} a_j(t)\Phi_j(\boldsymbol{r};R)\exp\left[-i\int^{t} E_j(t')dt'\right]$$

with U=CTF.

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Coupled equation system:

$$\begin{aligned}\frac{\mathrm{d}a_k(t)}{\mathrm{d}t} &= \sum_j a_j(t)\left(\left\langle \Phi_k \middle| H_{el} - \mathrm{i}\frac{\partial}{\partial t}\middle| \Phi_j\right\rangle + \left\langle \Phi_k \middle| \frac{1}{2}(\nabla U)^2 + \frac{\partial U}{\partial t}\middle| \Phi_j\right\rangle + \right.\\ &- \left.\mathrm{i}\left\langle \Phi_k \middle| -\frac{1}{2}\nabla^2 U - \nabla U\cdot\nabla \middle| \Phi_j\right\rangle\right) \exp\left[-i\int_0^t (E_j(t') - E_k(t'))\mathrm{d}t'\right]\end{aligned}$$

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$$- \mathrm{i}\left\langle \Phi_k \left| -\frac{1}{2}\nabla^2 U - \nabla U\cdot\nabla \right| \Phi_j\right\rangle\Bigg) \exp\left[-i\int_0^t (E_j(t') - E_k(t'))\mathrm{d}t'\right]$$

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Semiclassical Method

AOCC

$\Psi(\boldsymbol{r}; t)$ is expanded in atomic orbitals:

$$\Psi(\boldsymbol{r}, t) = \sum_j^N a_j(t)\phi_j(\boldsymbol{r})f(\boldsymbol{R}, \boldsymbol{r})\exp\left[-i\int^t E_j(t')dt'\right] = \sum_j^N a_j(t)\chi_j(\boldsymbol{r}, t)$$

with f ETF.

where:

$$\begin{aligned} \left(-\frac{1}{2}\nabla^2 + V_p\right)\phi_k &= E_k\phi_k \quad \text{projectile} \\ \left(-\frac{1}{2}\nabla^2 + V_t\right)\phi_i &= E_i\phi_i \quad \text{target} \end{aligned}$$

Semiclassical Method

AOCC

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coupled equation system:

$$\mathrm{i}\sum_k \frac{\mathrm{d}a_k(t)}{\mathrm{d}t}\langle\chi_j|\chi_K\rangle=\sum_k a_k(t)\left\langle\chi_j\left|H_{el}-\mathrm{i}\frac{\partial}{\partial t}\right|\chi_k\right\rangle$$

Semiclassical Method

Cross Sections

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$$\sigma_{nlm}^{A,B}(v) = 2\pi \int |a_{nlm}^{A,B}(v, b, t \rightarrow \infty)|^2 b \mathrm{d} b.$$

Semiclassical Method

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$$\sigma_{nlm}^{A,B}(v) = 2\pi \int |a_{nlm}^{A,B}(v, b, t \to \infty)|^2 b \mathrm{d}b.$$

$$|S_{ij}|^2 = P_{ij}(b) = |a(v, b, t \to \infty)|^2$$

Classical CTMC Method

$E > 25$keV/amu

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Electronic motion is described by a statistical distribution of N punctual charges that do not interact:

$$\rho(\boldsymbol{r}, \boldsymbol{p}, t) = \frac{1}{N} \sum_{j=1}^{N} \delta\left(\boldsymbol{r} - \boldsymbol{r}_j(t)\right) \delta\left(\boldsymbol{p} - \boldsymbol{p}_j(t)\right)$$

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$\downarrow$ Liouville Equation:

$$\frac{\partial \rho}{\partial t} = -\left\{\rho, H_{el}\right\} = -\frac{\partial \rho}{\partial r} \cdot \frac{\partial H_{el}}{\partial p} + \frac{\partial \rho}{\partial p} \cdot \frac{\partial H_{el}}{\partial r}$$

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Obtainig the Hamilton Equations:

$$\left.\begin{aligned} \dot{r}_j(t) &= \frac{\partial H}{\partial p_j(t)} \\ \dot{p}_j(t) &= -\frac{\partial H}{\partial r_j(t)} \end{aligned}\right\}$$

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$$P_{c,e,i}(v,b) = \int d\boldsymbol{r}\int d\boldsymbol{p}\,\rho_{c,e,i}(\boldsymbol{r},\boldsymbol{p},t_{max}) = \frac{N_{c,e,i}}{N_{\text{Total}}}$$

$$\boxed{\sigma_{c,e,i}(v) = 2\pi\int_0^{\infty} db\, b\, P_{c,e,i}(v,b)}$$

Classical CTMC Method

Initial Conditions

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Initial Distributions $\rho(\boldsymbol{r}, \boldsymbol{p}, t \rightarrow -\infty)$:

Classical CTMC Method

Initial Conditions

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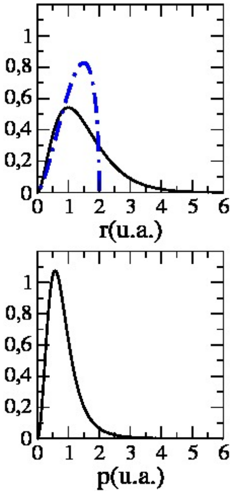
Initial Distributions $\rho(\mathbf{r}, \mathbf{p}, t \to -\infty)$:

- Microcanonical Distribution:

$$\rho^m(\mathbf{r}, \mathbf{p}; E_0) = \frac{(2|E_0|)^{5/2}}{8\pi^3 Z_H^3} \delta\left(\frac{p^2}{2} - \frac{Z_H}{r} - E_0\right)$$



Classical CTMC Method

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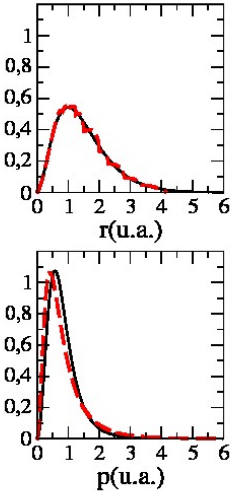
$$\rho(\boldsymbol{r}, \boldsymbol{p}) = \sum_{j=1}^{N_j} w_j \rho^m(\boldsymbol{r}, \boldsymbol{p}; E_j)$$



Classical CTMC Method

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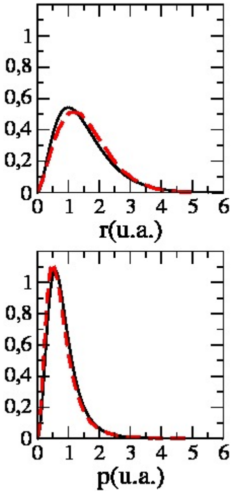
- Hydrogenic Distribution:

  $$\rho(\boldsymbol{r}, \boldsymbol{p}) = \sum_{j=1}^{N_j} w_j \rho^m(\boldsymbol{r}, \boldsymbol{p}; E_j)$$

- Continous Distributions

  Distributions: Gaussian, Rackovic, Cohen, Eichenauer, etc.

$$\rho(E) = K_1 e^{-K_2\left(\frac{Z_H}{\sqrt{-2E}} - 1.2\right)^2}$$



Outline

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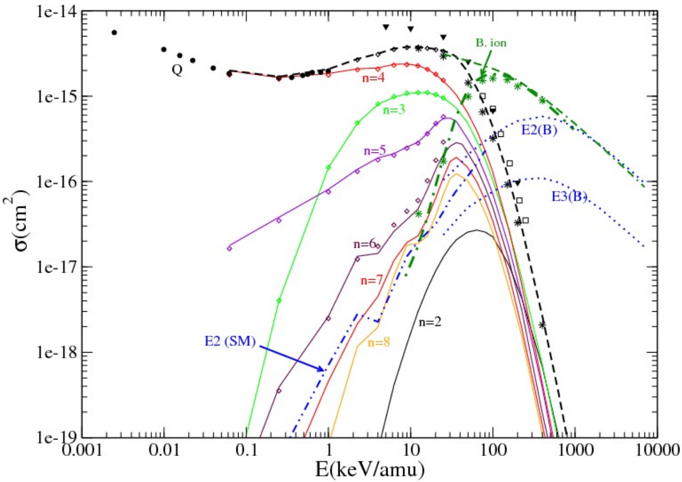
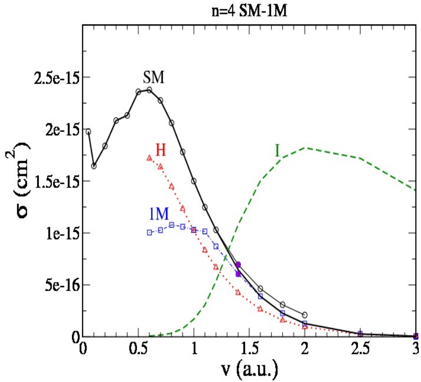
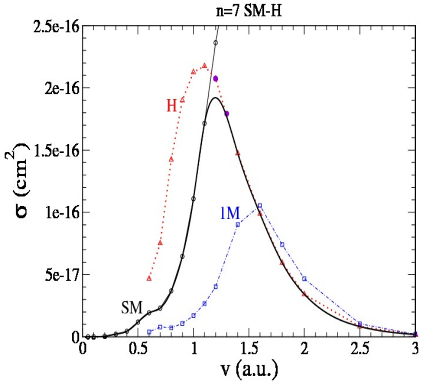
B^{5+} +H(1s) Cross Sections



L.F. Errea, F. Guzmán *et al.* PPCF **48** 1585(2006)

B^{5+} +H(1s) Cross Sections





ADAS comparison

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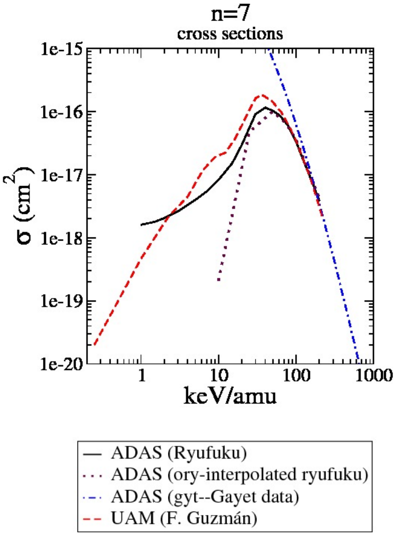
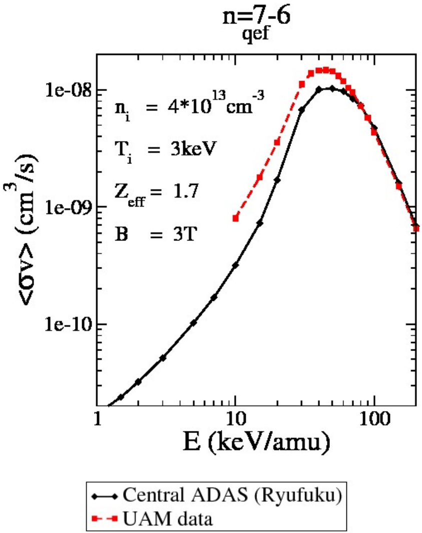
B^{5+} + H





ADAS comparison

Ne^{10+} + H and Ar^{18+} + H

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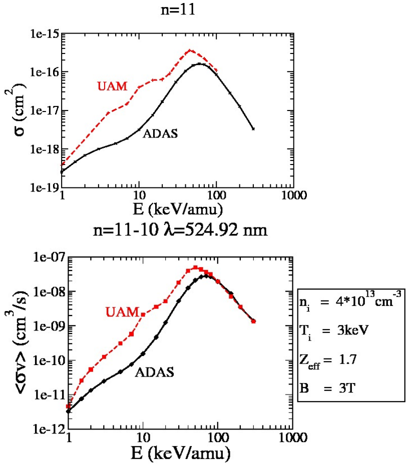
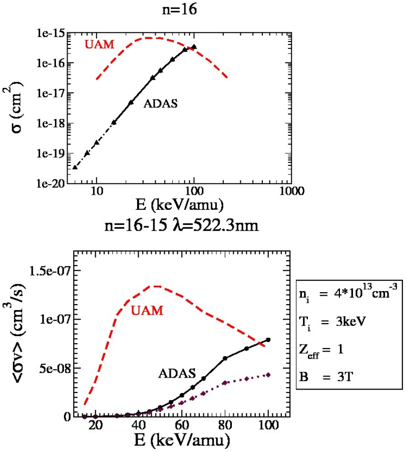
Ne^{10+} + H



Ar^{18+} + H



UAM: Errea *et al.* Nucl Inst. & Meth. Phys. Res. B **235**, 315 (2005)

New Calculations in AOCC

N^{7+} + H

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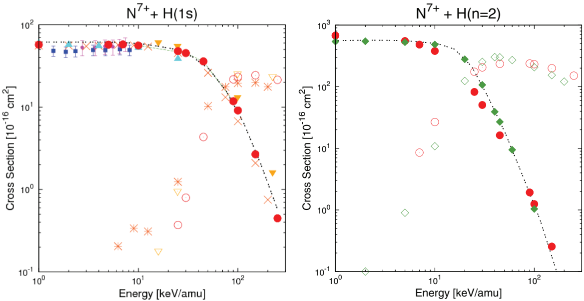

(a) (b)

Figure 1. Total cross sections for CX (full symbols) and ION (open symbols). (a) H(1s) target. Data presented in this work (AOCC●○, CTMC◆◇). For reference purposes we show experimental CX data from Meyer *et al* (1985) (■) and Dijkkamp *et al* (1985) (⬟) as well as results from various theoretical approaches: AO+ CX cross sections from Fritsch and Lin (1984) (▲), AOCC calculations with Gaussian-type orbitals (Toshima 1994) (CX×, ION✳), CTMC results for CX (▼) from Illescas and Riera (1999), scaled CX data (.....) calculated with ADAS315 (Foster 2008) and ION (▽) again from Illescas and Riera (1999). (b) H(n = 2) target.

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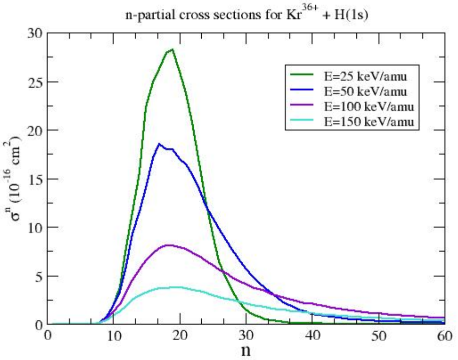
CTMC results

$Kr^{36+}+H$



Capture goes to high n's and follows the n^{-3} law.

Summary

- Different energy ranges require different theoretical methods. A wide range of energy cross sections can be achieved by overlapping different methods in its adequate energy.
- Adequate resembling of quantal initial conditions in each situation is needed for CTMC calculations.
- Cross sections accuracy is fundamental to obtain impurities densities by CXRS. There can be big differences between the different calculations in cross sections.
- Experimental methods which help in providing recommended cross sections are needed (next sesion!!) .

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ADAS-EU
ADAS for fusion in Europe

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