Atomic data and collisional-radiative modelling of neutral beams in eigenstates

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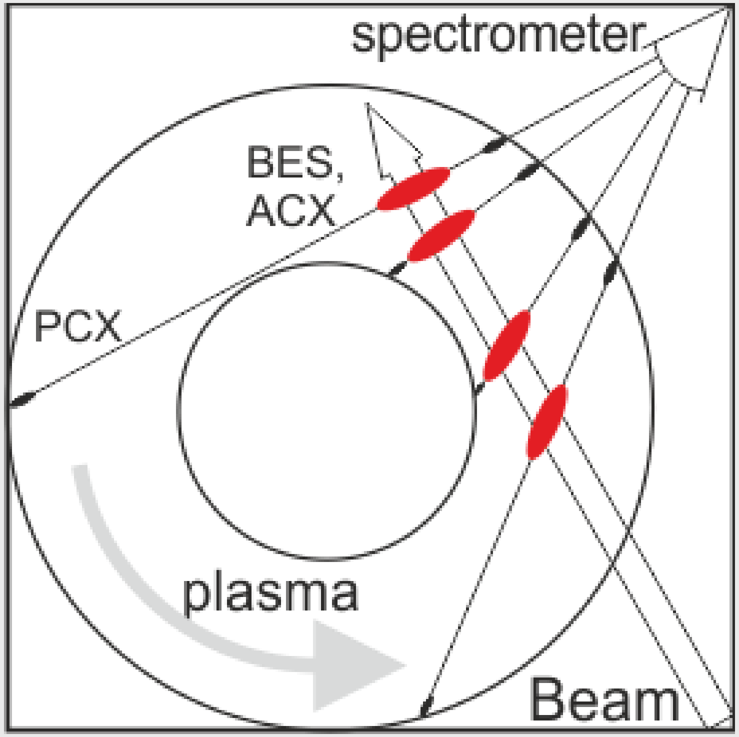
Contents

Injection of fast atoms and plasma spectroscopy



$$H_0 + \{e, H^+, X_z\} \rightarrow H^* + \{e, H^+, X_z\} \rightarrow \hbar\omega \quad (1)$$

$$H_0 + X_{z+1} \rightarrow H^+ + X^*_z(nl) \rightarrow \hbar\omega \quad (2)$$

$$H^+ + H_0 \rightarrow H^* + H^+ \rightarrow \hbar\omega \quad (3)$$

Plasma parameters:

- Density = $10^{13} \ldots 10^{14}$ cm^{-3}
- Beam energy = 20 .. 200 keV/u
- Temperature = 1..15 keV
- Magnetic field = 1.. 5 T

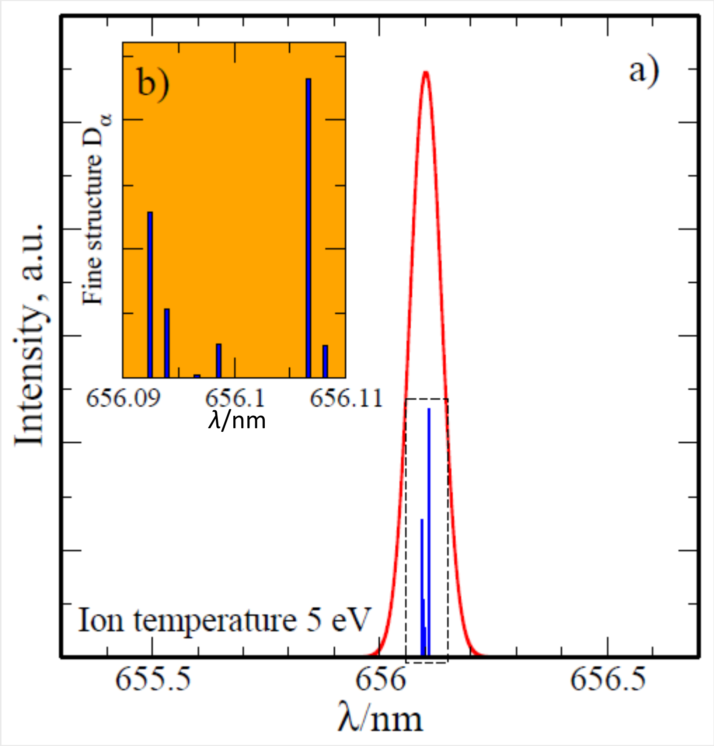
(1) beam-emission spectroscopy (BES)

(2) source of charge-exchange diagnostic

(3) source of fast ion diagnostic and main ion ratio measurements (ACX- active charge-exchange, PCX- passive charge-exchange)

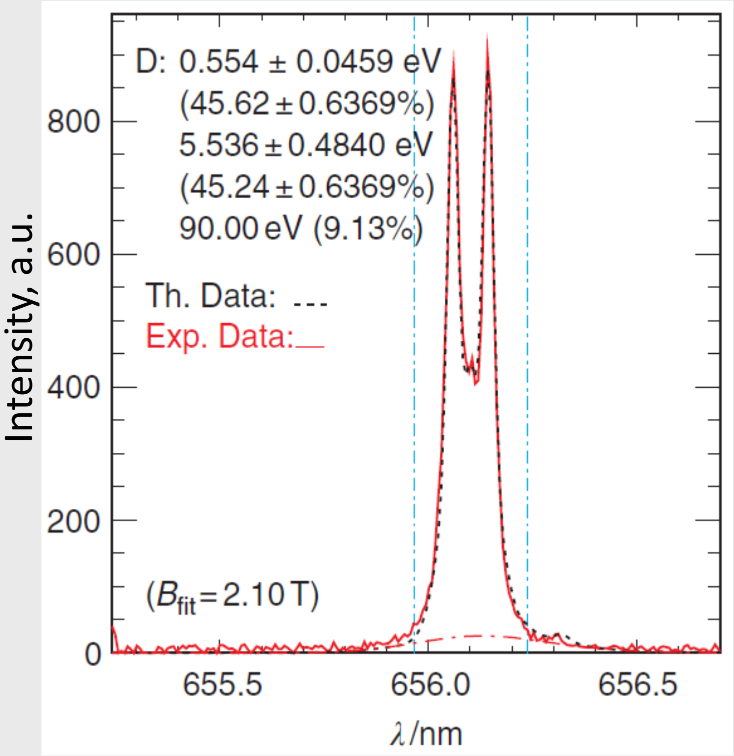
Example of the H_α line emission at the plasma edge

- Field-free D_α emission



(http://physics.nist.gov/asd, NIST)

- Measured D_α line emission



Mertens Ph. et al. PPCF 43 A349 (2001)

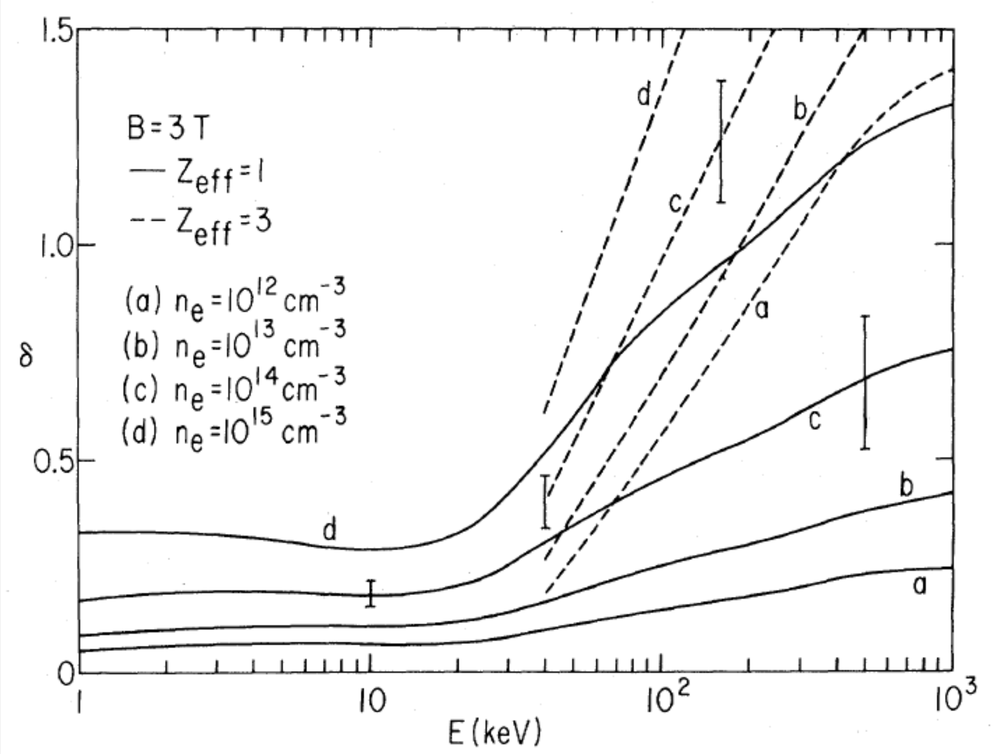
- Fine-structure of hydrogen atoms is never observed in fusion plasmas
  - Doppler effect due to the thermal motion of atoms
  - Zeeman effect due to the magnetic field

Excited states in the active beam diagnostics

- The role of the excited states in the beam penetration:

Janev R. et al. Phys. Rev. Lett. **52** 534 (1984)

- The first collisional-radiative model for the beam was introduced



$$I(x) = I_0 \exp\left(-\frac{x}{\lambda_0}\right),$$

$\lambda_0 = 1/(N_i \sigma_i \; \upsilon)$ – e-folding length,

N_i – is the ion density

σ_i - is the ionization cross-section

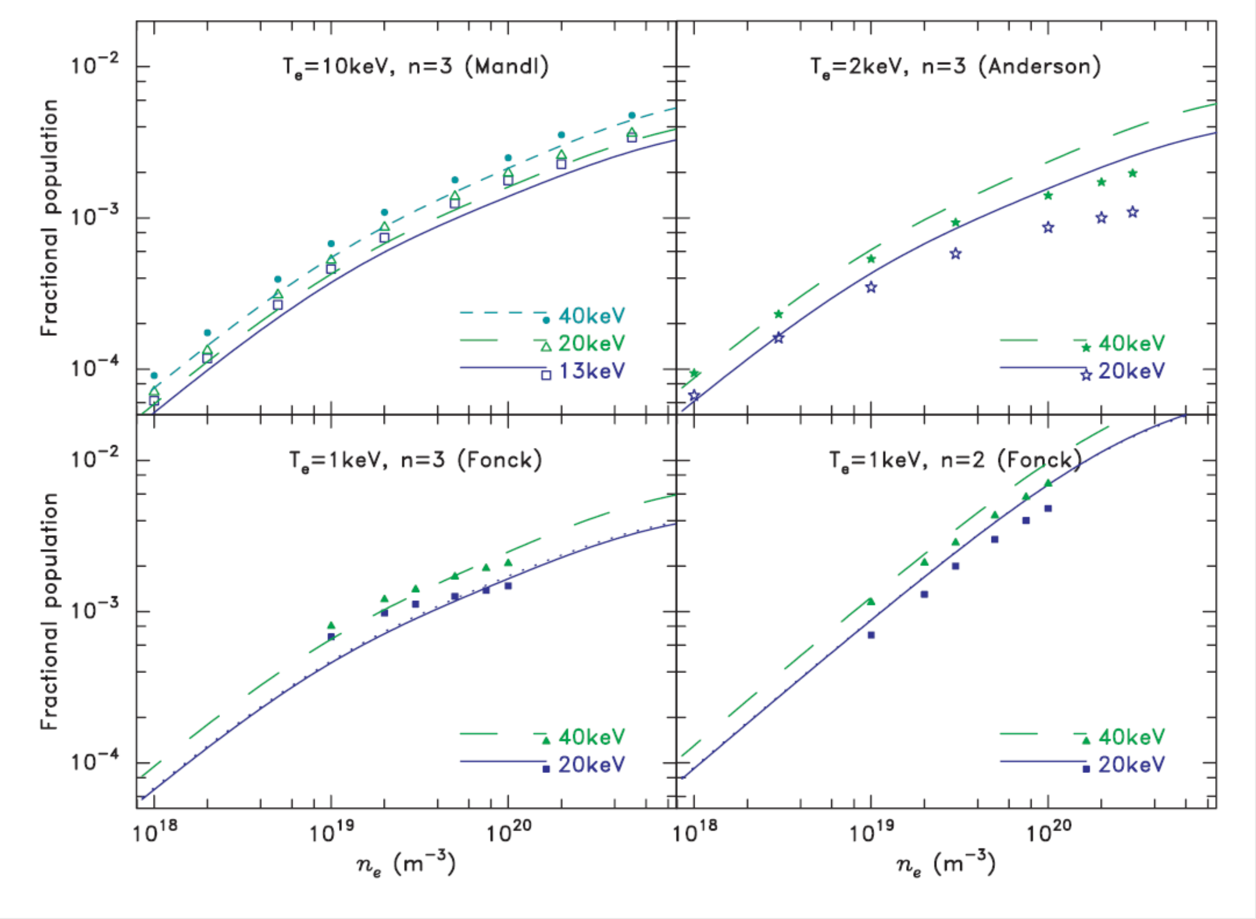
υ – is the beam velocity

x – is the distance along the beam

$$\delta = (\lambda - \lambda_0)/\lambda$$

- Increased (multi-step) ionization of beam atoms in the plasma → **stronger attenuation**

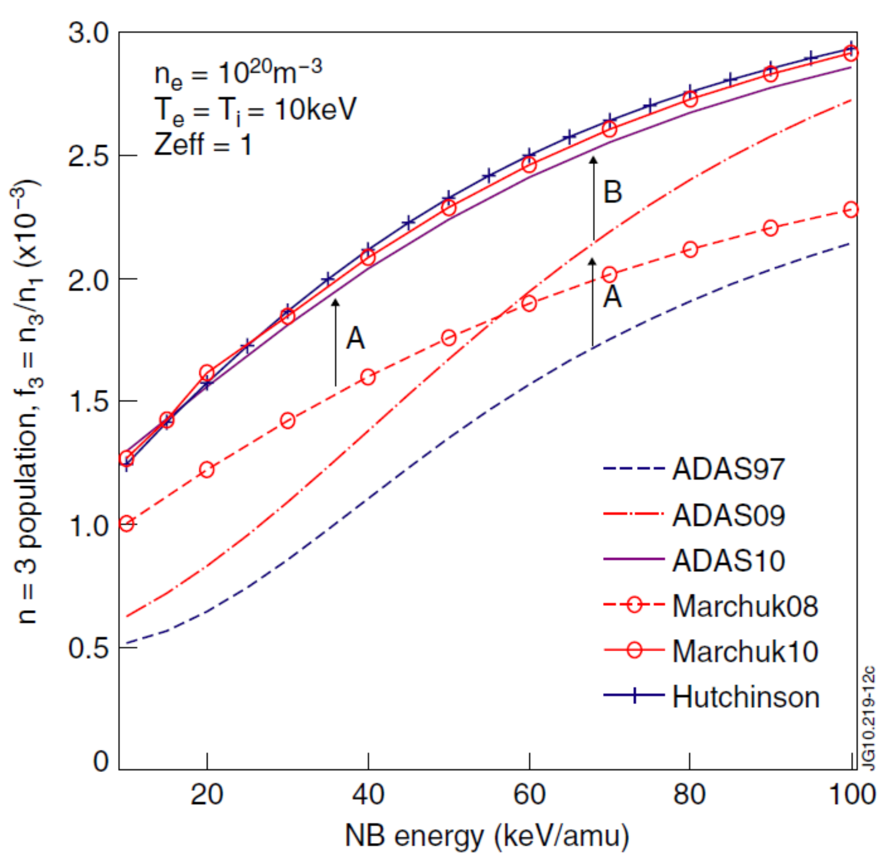
Problems in the CR models up to 2009



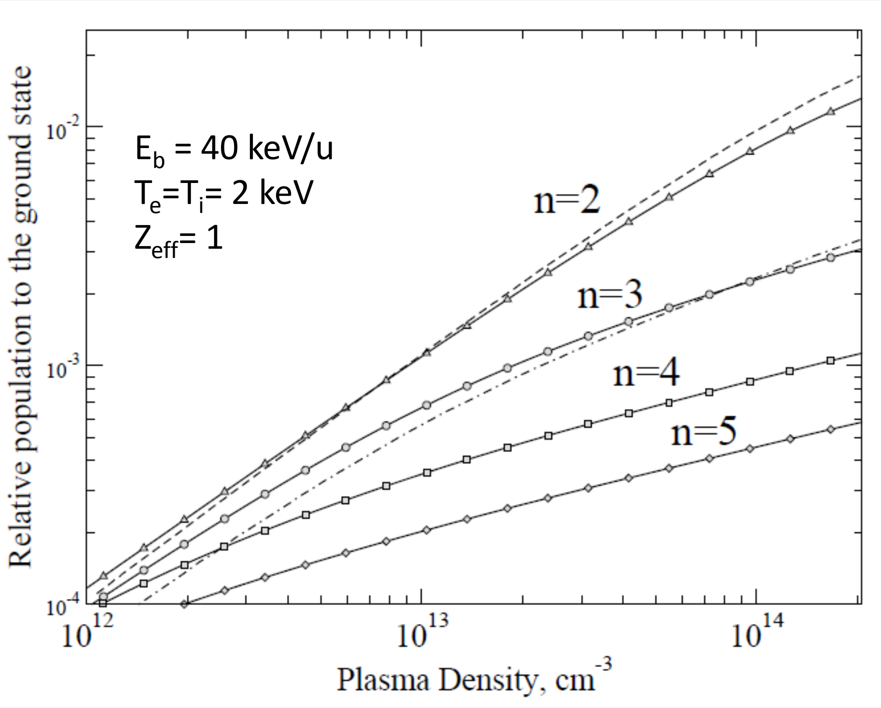
Hutchinson I. Plasma Phys. Contr. Fusion **44 71** (2002)

- The comparison in the emission of H_α line reveals the deviations up to the factor of 2-3

Status of statistical models



Delabie E. et al. PPCF **52** 125008 (2010)

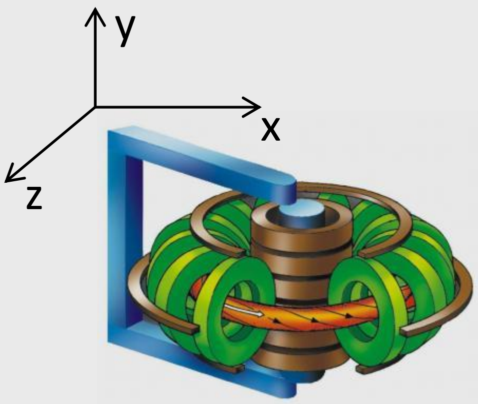


O. Marchuk and Yu. Ralchenko, “Populations of Excited Parabolic States of Hydrogen Beam in Fusion Plasmas”, Springer-Verlag in “Atomic Processes in Basic and Applied Physics” eds by Tawara and Shevelko(2012) https://link.springer.com/chapter/10.1007/978-3-642-25569-4_4

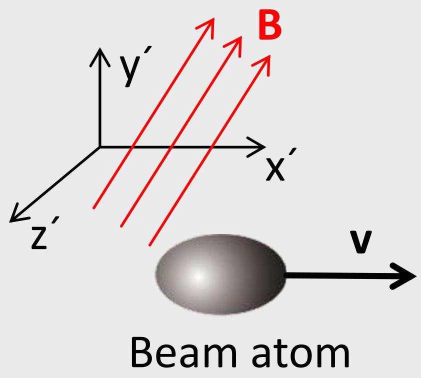
Solid lines with points – present calculations
Dashed line - Hutchinson I PPCF **44** 71 (2002)

- That is the first time that the population of excited states (n-states) of the beam agree within 20% for three different models in the density range of 10^{13}-10^{14}cm^{-3}:
  - Key component: ionization data from n=2 and n=3 states

Fields „observed“ by the H atom



(xyz) is the laboratory coordinate system



(x´y´z´) is the coordinate system in the rest frame of hydrogen atom

Lorentz transformation for the field:

$$\overrightarrow{F'} = \vec{F} + \frac{1}{c}\vec{v} \times \vec{B}$$

$$\overrightarrow{B'} = \vec{B} - \frac{1}{c}\vec{v} \times \vec{F} \qquad \text{(cgs)}$$

- In the rest frame of the atom the bound electron experiences **the influence of the crossed magnetic $\overrightarrow{B'}$ and electric $\overrightarrow{F'}$ fields**

- ❑ Example: B = 1 T, E = 100 keV/u → v = $4.4 \cdot 10^{8}$ cm/s → F **= 44 kV/cm**
- ❑ Strong electric and magnetic field in the rest frame of the atom is experienced by the bound electron
- ❑ External fields are usually considered as perturbation applied to the field-free solution

Linear Stark effect for the excited states

- Hamiltonian is diagonal in parabolic quantum numbers
- Spherical symmetry of the atom is replaced by the axial symmetry around the direction of electric field.

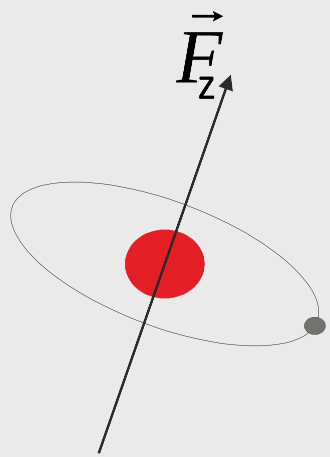
Parabolic quantum numbers:

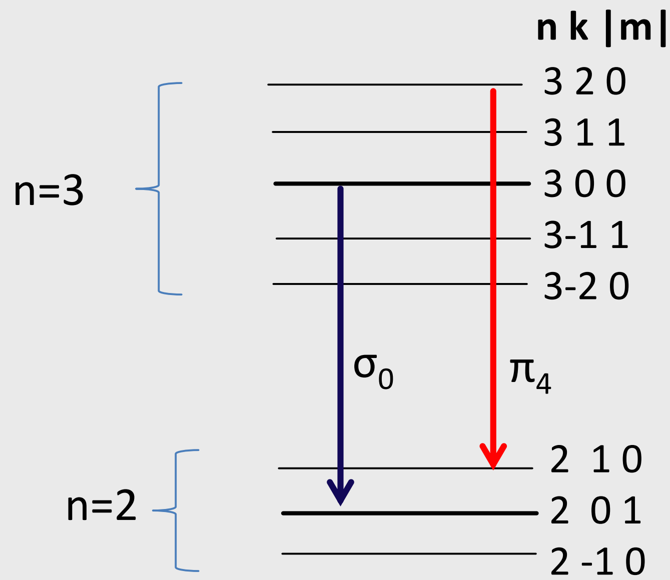
$n = n_1 + n_2 + |m| + 1, \; n_1, n_2 \geq 0$ (nkm)

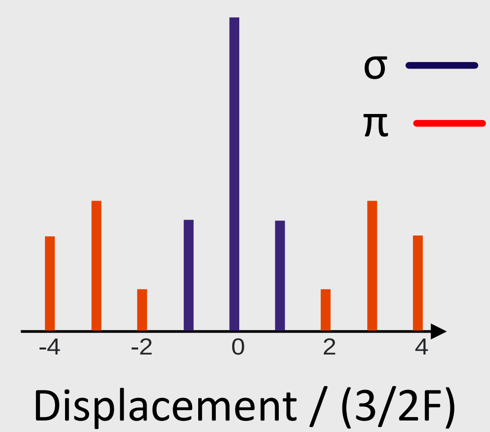
$k = n_1 - n_2$ – electric quantum number

m – z-projection of magnetic moment

$$E(nkm) = 3/2 \cdot F \cdot n \cdot k + O(F^2)$$







- The energy of the **m** –levels is not degenerated any more in the presence of electric field (multiplet structure)

Linear Zeeman-Stark for the excited states

- The angle between magnetic and electric field matters. In the case of H/D beam atom in the plasma

  $\overrightarrow{F'} = \vec{F} + \frac{1}{c}\vec{v} \times \vec{B}$ (translational electric field)

- In the case of the strong field approximation (with spin) the new energy of the levels

$$E^{\pm}(n,k) \approx \pm\Omega + k\sqrt{\left(\frac{3}{2}nF\right)^2 + \Omega^2}.$$

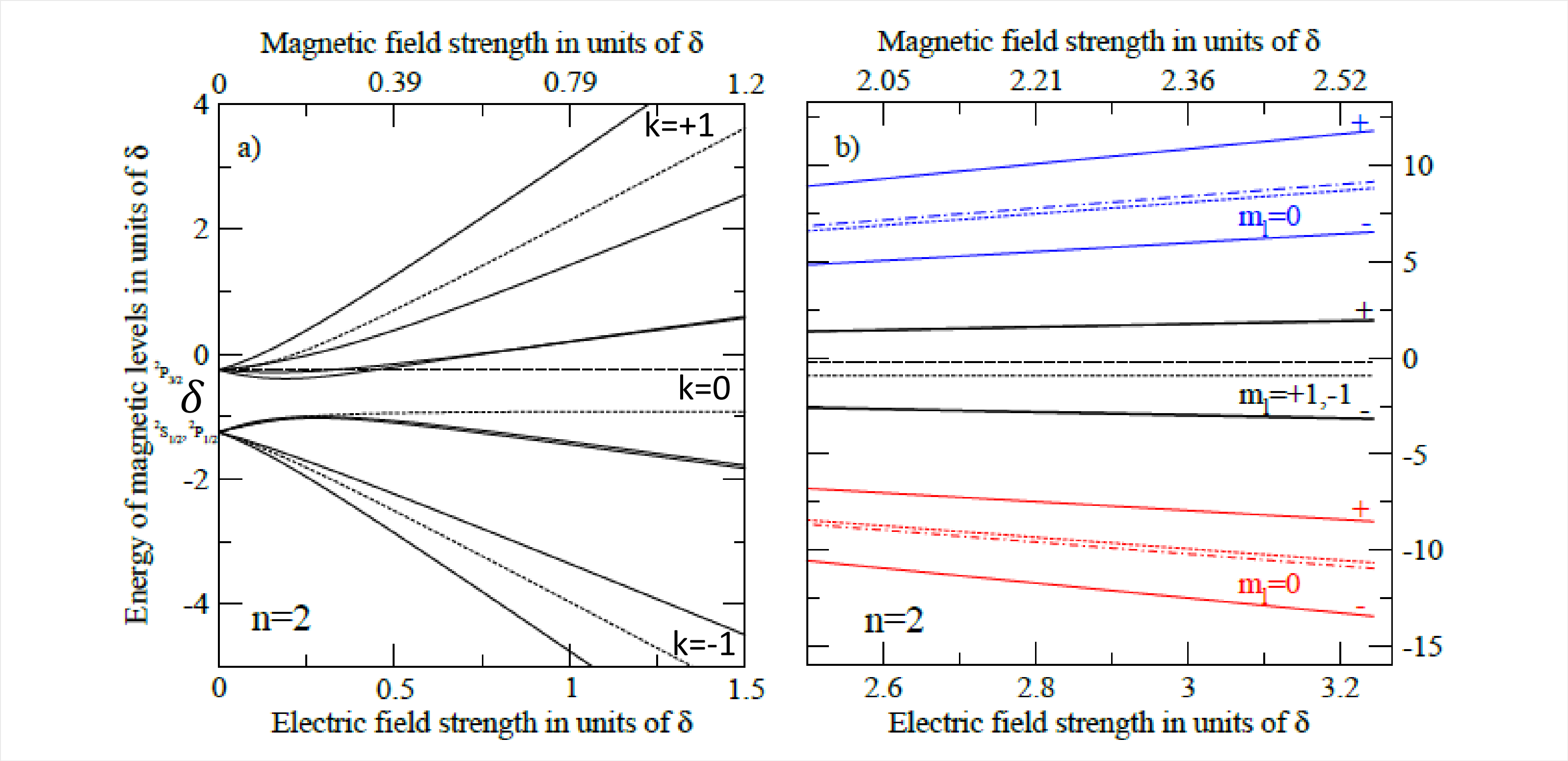
$\Omega = \frac{1}{2} \times \frac{B}{B_0}$, $B_0 = 2.35 \times 10^5\ T$

$F = \frac{E_L}{E_0}$, $E_0 = 5.142 \times 10^{11}\ V/m$

Parabolic quantum numbers:

$n = n_1 + n_2 + |m| + 1$; $n_1 \geq 0$, $n_2 \geq 0$; $k = n_1 - n_2$ electric quantum number

Energy levels of n=2 of H atoms in the plasma



R. Reimer et al, RSI (to be published)

a) point-point line – Stark effect + FS ; solid line – Zeeman Stark effect + FS
b) point-point line – Stark effect + FS; dashed-point line- Zeeman Stark effect ; solid line –Zeeman Stark effect + FS

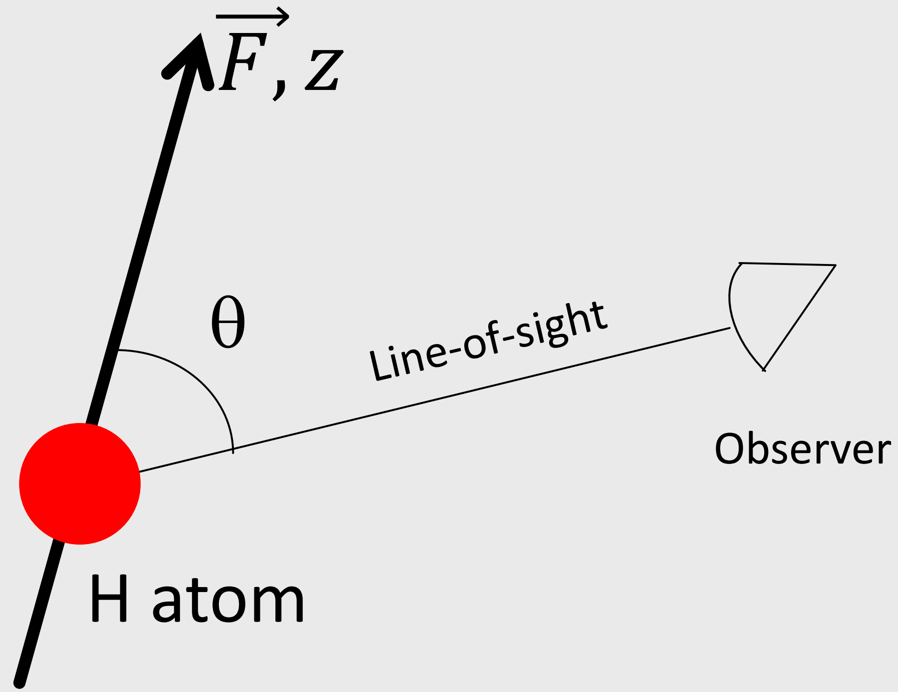
- The energy separation between different states is order of magnitude higher compared to the field free case → impact on the cross sections (LTE vs. nonLTE)

Polarization of spectral lines

For every observed line applies:

$$\varepsilon_{\pi} = I_{\pi} \times sin^2(\theta)$$

$$\varepsilon_{\sigma} = I_{\sigma} \times (1 + cos^2(\theta))/2$$



F – is the electric field strength

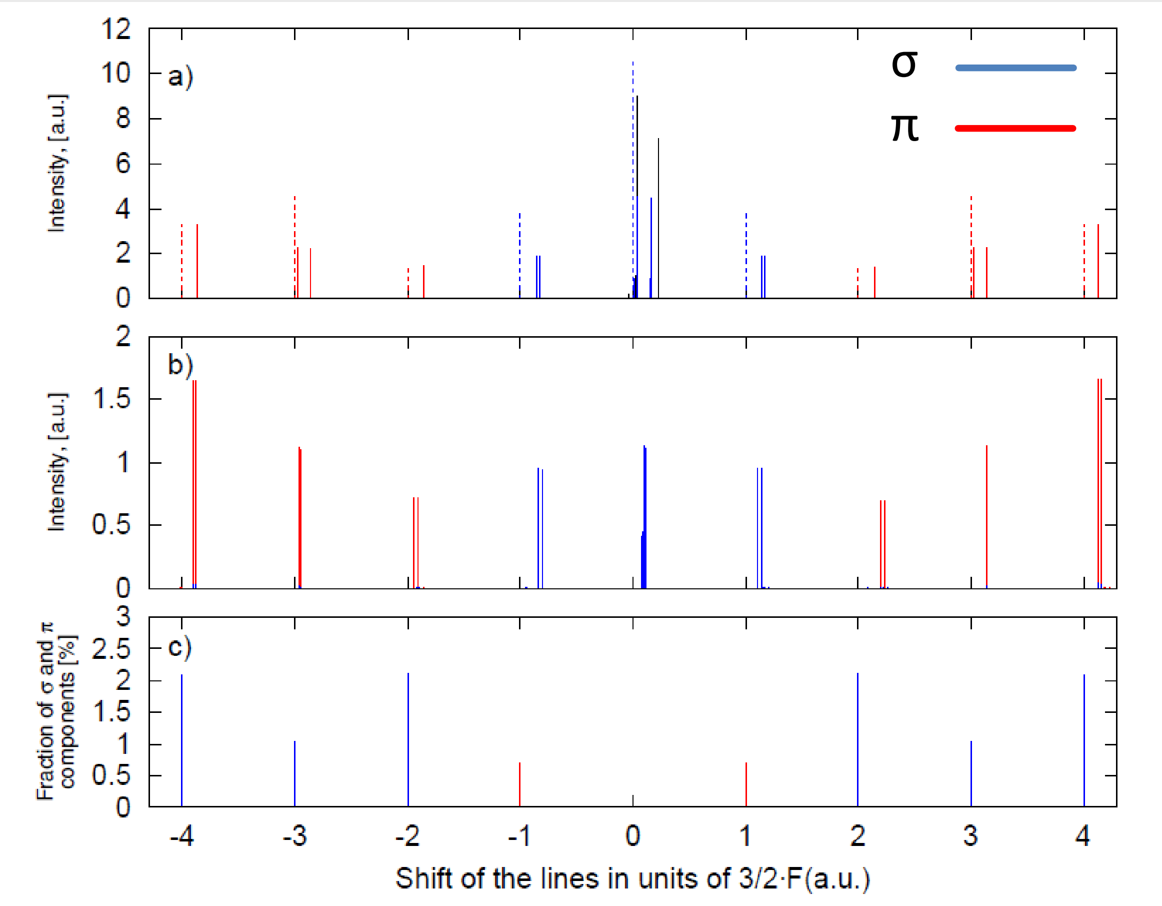
$\varepsilon_{\pi}, \varepsilon_{\sigma}$ are the experimental (observed) lines

I_{π}, I_{σ} - are the line intensities (calculation does not depend on the observation angle)

The π- transitions are the transitions which do not change the projection of angular momentum (magnetic quantum number m) onto the z axis, Δm=0

The σ- transitions are the transitions which change the projection of angular momentum onto the z axis, Δm=±1.

Comparison for the H_α multiplet between Zeeman–Stark and Stark effect



a) thin black lines –field free case;
dashed lines –Stark effect;
solid lines - Stark effect + FS

b) Zeeman-Stark effect + FS

c) Change in the polarization fraction

Lines are not of „pure“ polarization

E=10 keV, B=2 T

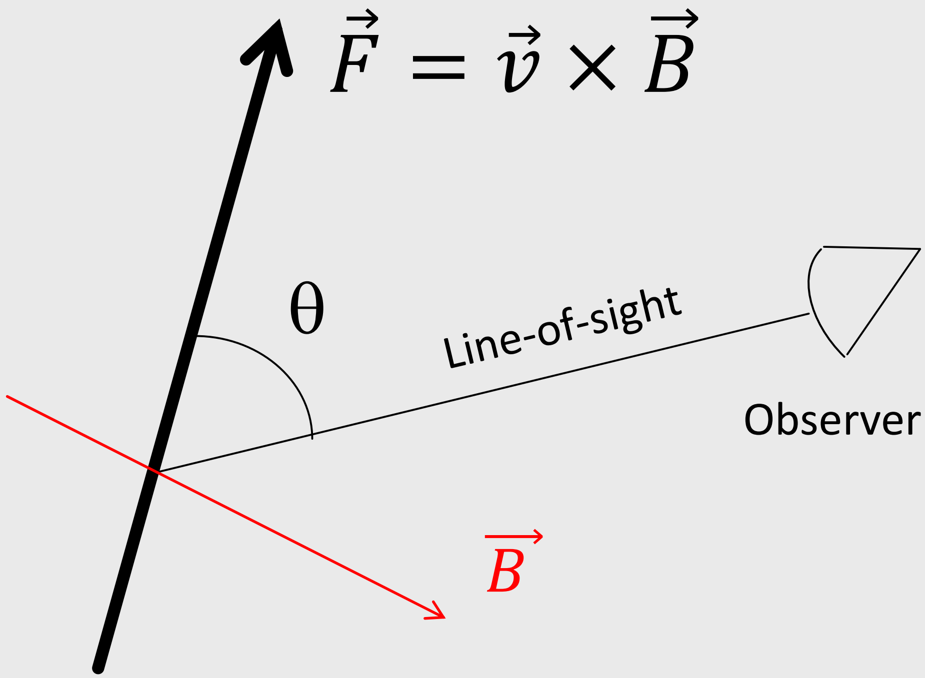
R. Reimer et al, RSI (to be pusblished)

- Zeeman effect affects the polarization fraction of Stark multiplet
  → impact on the pitch angle measurements
- The sum over all the σ and π components remains conserved

Why π− to σ− ratio is so important for fusion ?

- Vector $\vec{B}$ is unknown.
- Vector $\vec{v}$ is known (beam direction and beam velocity)
- Direction of $\vec{F}$ (angle θ) could be measured using the formula:

$$\left(\frac{\sum \varepsilon_\pi}{\sum \varepsilon_\sigma}\right) = \left(\frac{\sum I_\pi}{\sum I_\sigma}\right) \times \frac{2\,sin^2(\theta)}{1 + cos^2(\theta)}$$



Measured value - $\left(\frac{\sum \varepsilon_\pi}{\sum \varepsilon_\sigma}\right)$

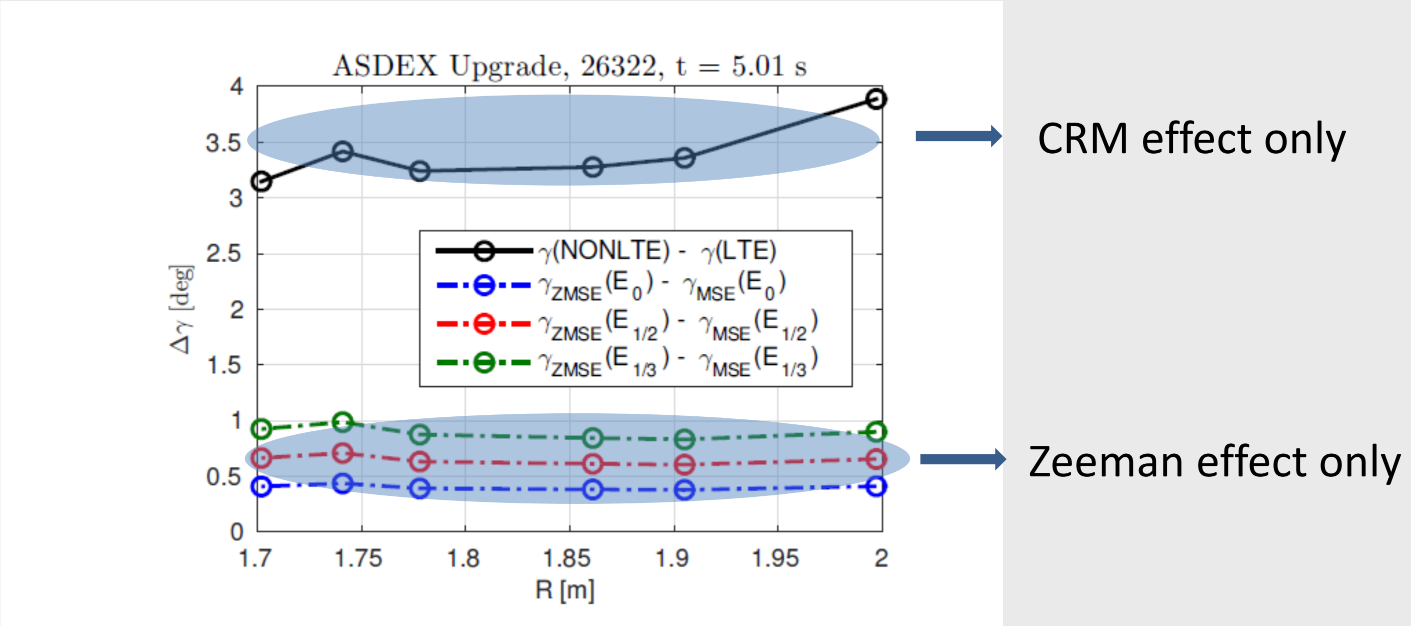
Atomic model value- $\left(\frac{\sum I_\pi}{\sum I_\sigma}\right)$

Only in statistical case: $\frac{\sum I_\pi}{\sum I_\sigma} = 1/2$

Atomic model must be able to calculate the line intensities without any assumption on statistical populations

Example of the impact of the Zeeman effect on the pitch angle measurements θ

$$T = \frac{\sum I_\pi}{\sum I_\sigma} \times \frac{2sin^2(\theta)}{1 + cos^2(\theta)}$$

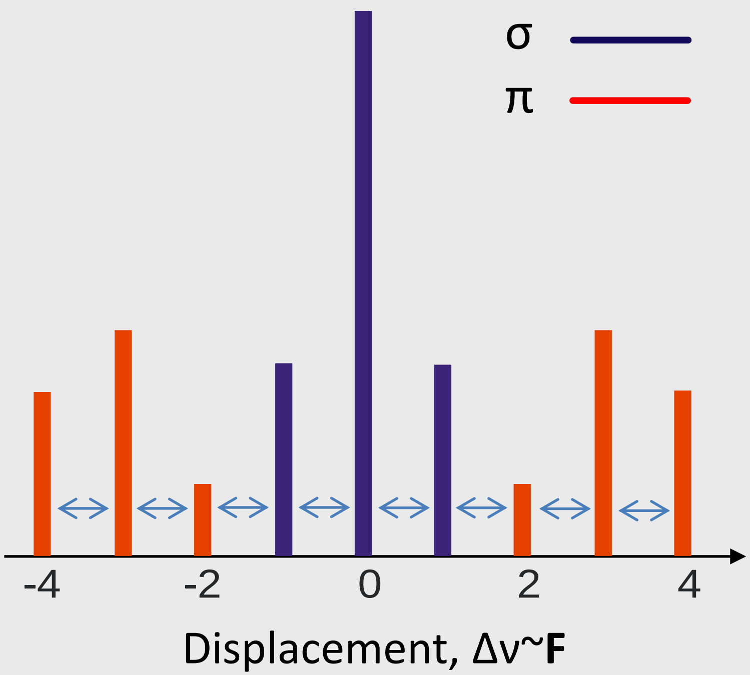


R. Reimer et al, RSI (to be pusblished)

- Atomic model modifies the derived angle of magnetic field on the order of up to 2-3°

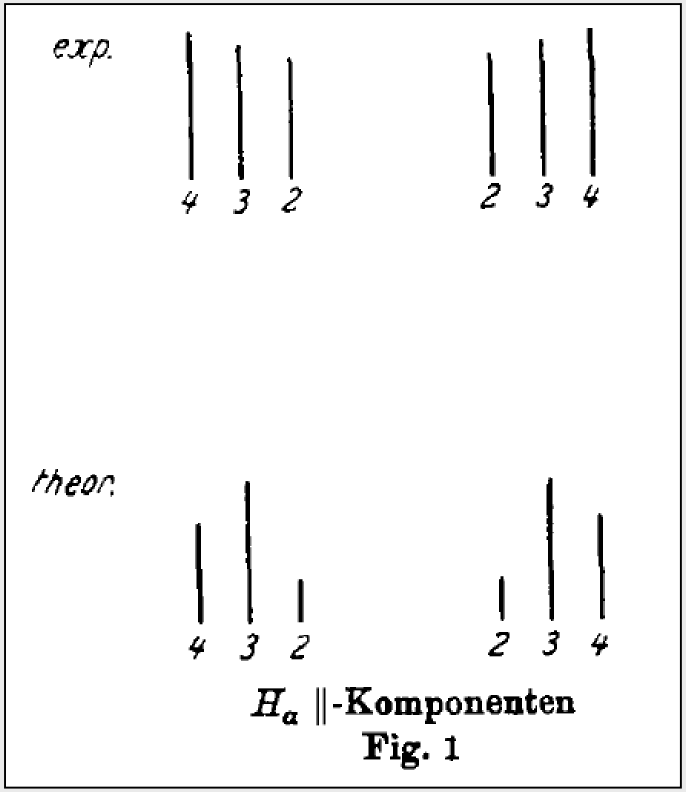
First atomic model of Hα Stark multiplet

- Lines separation and lines intensities



Separation is proportional to **|F|**

* 1st order perturbation theory only



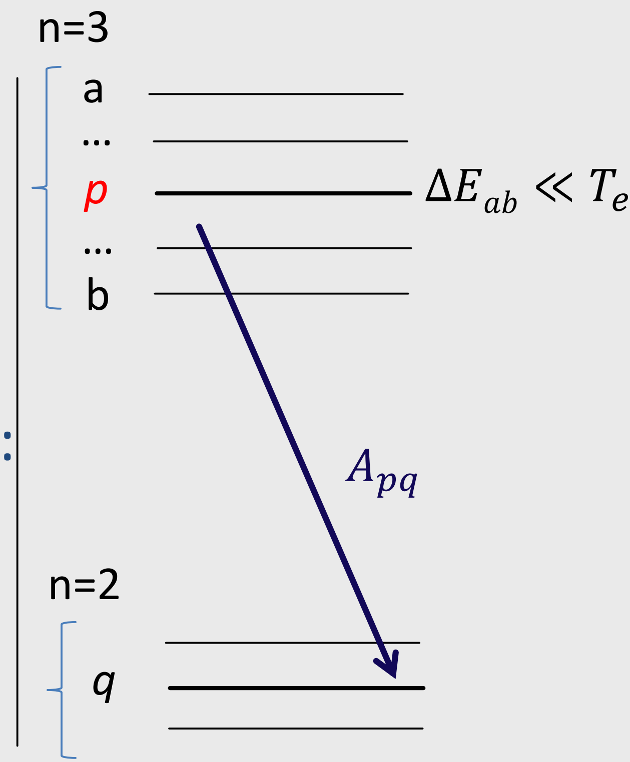
E. Schrödinger, Ann. der Physik **80(13)** 437 (1926)

Lines Intensity

$$I_{pq} \sim N_p \times A_{pq}$$

N_p is a population (density) of the state *p*

A_{pq} is a radiative decay rate p→q (1/s)



- Statistical assumption – statistical model:

  (Boltzmann distribution)

$$\frac{N_a}{N_b} = \frac{g_a}{g_b} \exp\left(-\frac{\Delta E_{ab}}{T_e}\right),$$

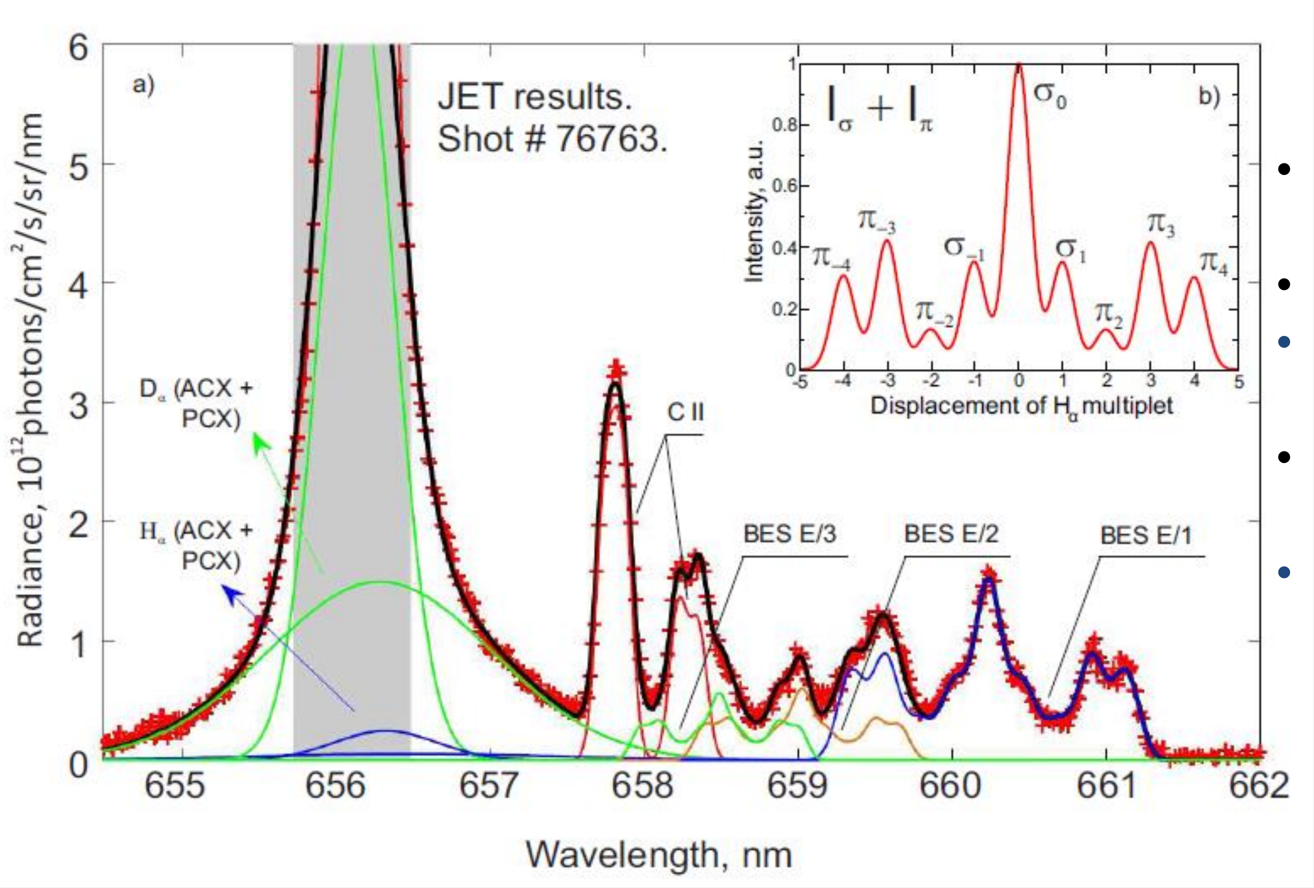
g_a – is the statistical weight of the state *a*,

$\Delta E_{ab} = E_a - E_b$ is the energy difference between the states *a* and *b*

T_e - is the plasma temperature

Beam emission spectra measured at JET $H_\alpha(n=3 \rightarrow n=2)$

Delabie E. et al. Plasma Phys. Contr. Fusion **52** 125008 (2010)



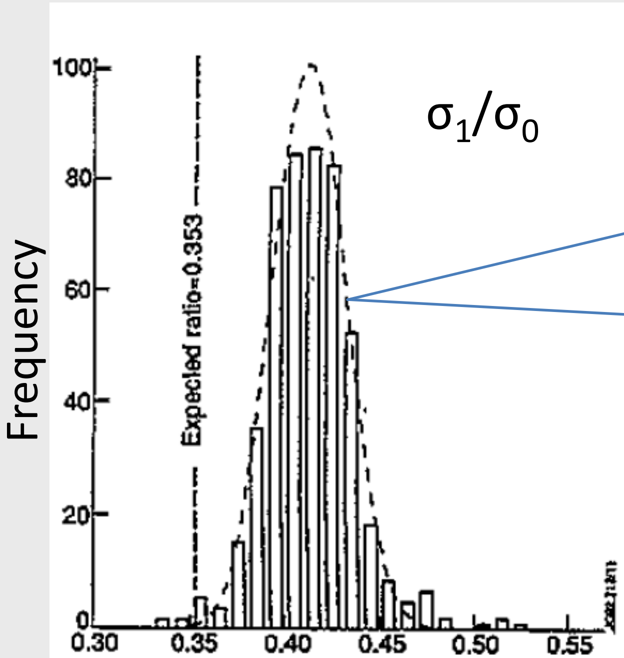
- 3 components in the beam (E/1, E/2, E/3)
- Passive light from the edge
- Emission of thermal H^+ and D^+
- Cold components of CII Zeeman multiplet
- Overlapped components of Stark effect spectra

- Intensity of MSE multiplet as a function of observation angle ϑ relative to the direction of electric field

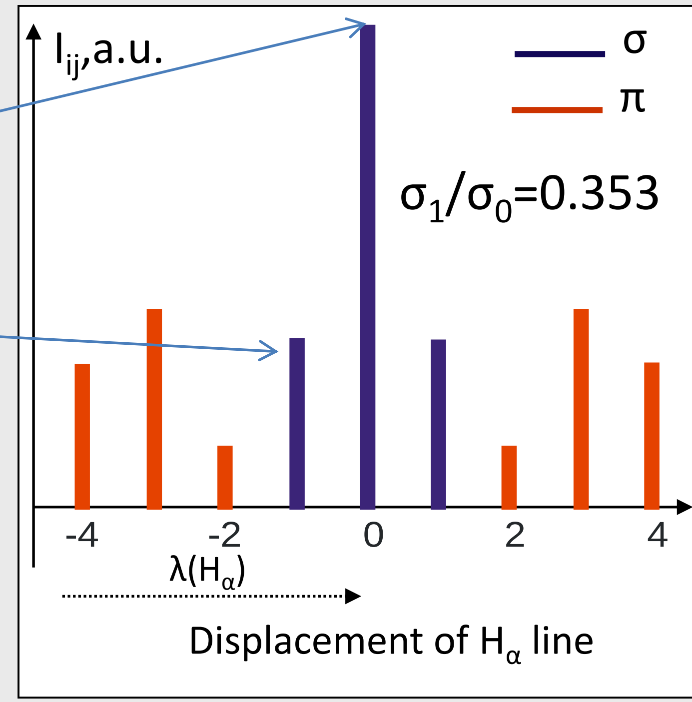
$$I(\theta) = I_\pi \sin^2(\theta) + I_\sigma(1 + \cos^2(\theta))/2$$

- Ratios among *π-(Δm=0)* and *σ- (Δm=±1)* lines within the multiplet are well defined and should be constant.

Measured intensities vs. statistical intensities



W. Mandl et al. PPCF **35** 1373 (1993)



- Observed line intensities with the same polarization show clear deviation from the statistical model.

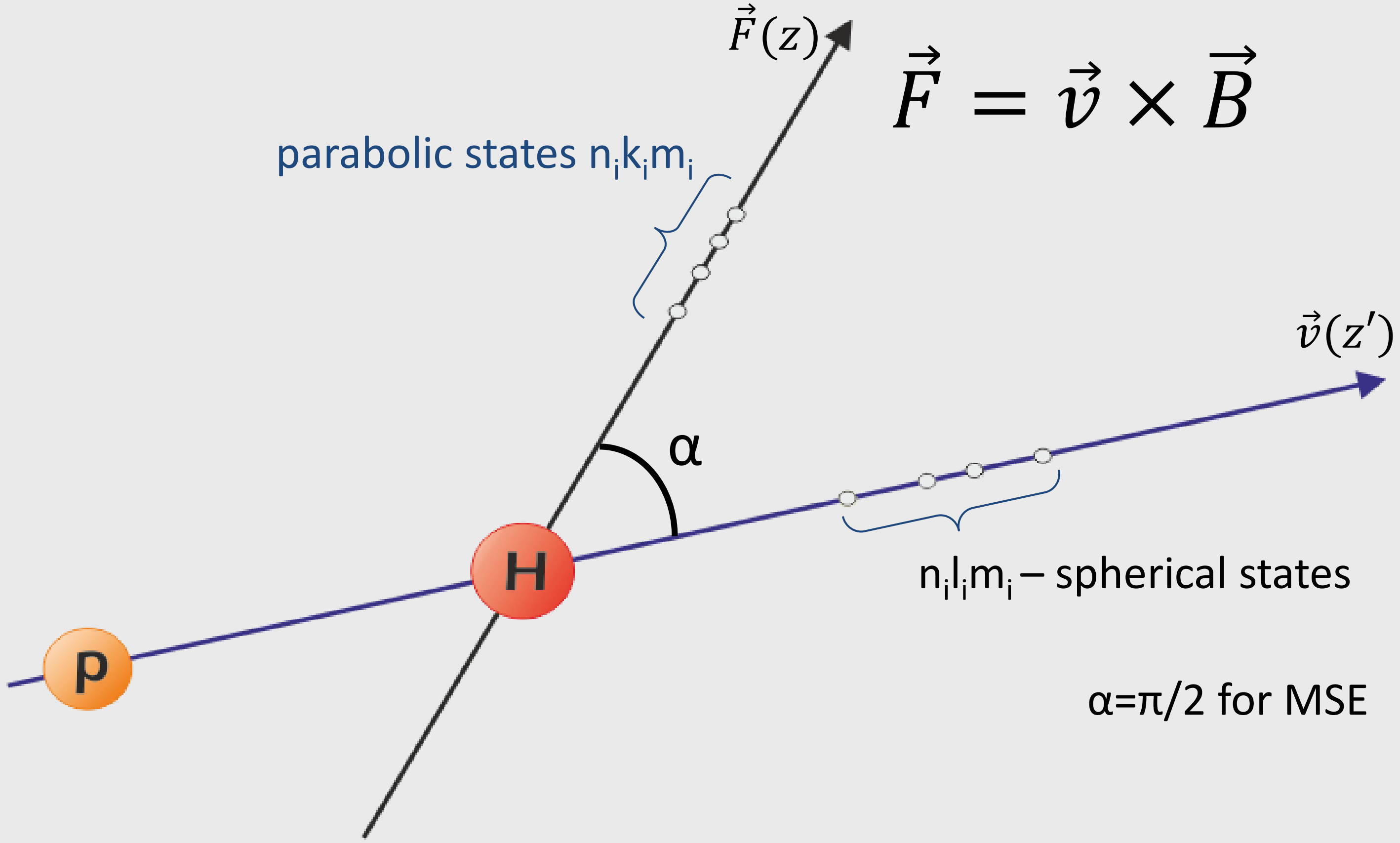
- **The non-statistical atomic models for fast atoms in parabolic (*eigen*) states must be developed.**

Atomic data in parabolic states (m-resolved)

- Radiative decays
  - Well known (Bethe & Salpeter)
- Electron-impact processes
  - Too high energies => small cross sections
- Proton-impact processes
  - The strongest but…

Problem: no cross sections/rate coefficients for transitions between parabolic states

Calculation of the cross sections in parabolic states



Calculations include two transformations of wavefunctions

- Rotation of the collisional (z') frame on the angle θ to match z frame
  Edmonds A R 1957 *Angular Momentum in Quantum Mechanics* (Princeton, NJ: Princeton University Press)

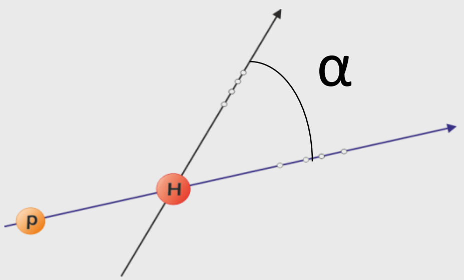
- Transformation between the spherical and parabolic states in the same frame z
  Landau L D and Lifshitz E M 1976 *Quantum Mechanics: Non-Relativistic Theory*

Transformation between the spherical and parabolic states

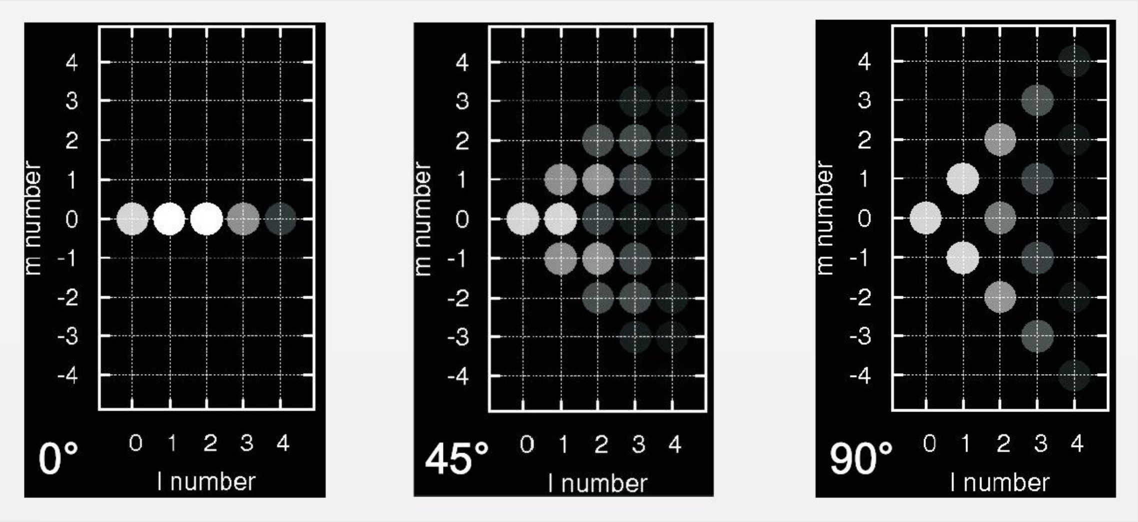
a)

$$\varphi_{a'} \to \varphi_a : \varphi_{nlm} = \sum_{m'=-l}^{l} D_{lm}^{lm'}(\alpha)\varphi_{nlm'}$$

$$\varphi_a \to \psi_a : \psi_{nkm} = \sum_{l=|m|}^{n-1} C_{nk}^{lm}\varphi_{nlm}$$



b) Example for the state: n=5, k=4, m=0



Calculation of the cross sections and the density matrix

$$\sigma = \left| < n_i k_i m_i \,|\, \hat{O} \,|\, n_j k_j m_j > \right|^2 = \left| \sum_{\Delta m'=2-n_a-n_b} c_i c_j F_{a_i}^{b_j}(\vec{q}) \right|^2 + \left| \sum_{\Delta m'=3-n_a-n_b} c_i c_j F_{a_i}^{b_j}(\vec{q}) \right|^2 + \ldots$$

$$+ \left| \sum_{\Delta m'=n_a+n_b-3} c_i c_j F_{a_i}^{b_j}(\vec{q}) \right|^2 + \left| \sum_{\Delta m'=n_a+n_b-2} c_i c_j F_{a_i}^{b_j}(\vec{q}) \right|^2$$

- ❑ The coefficients c_i and finally the cross section depend on the angle between the field and direction of the projectile

- ❑ Presence of coherence terms in the expansion

- ❑ Calculation of the cross section is equivalent to the calculation of the **density matrix**

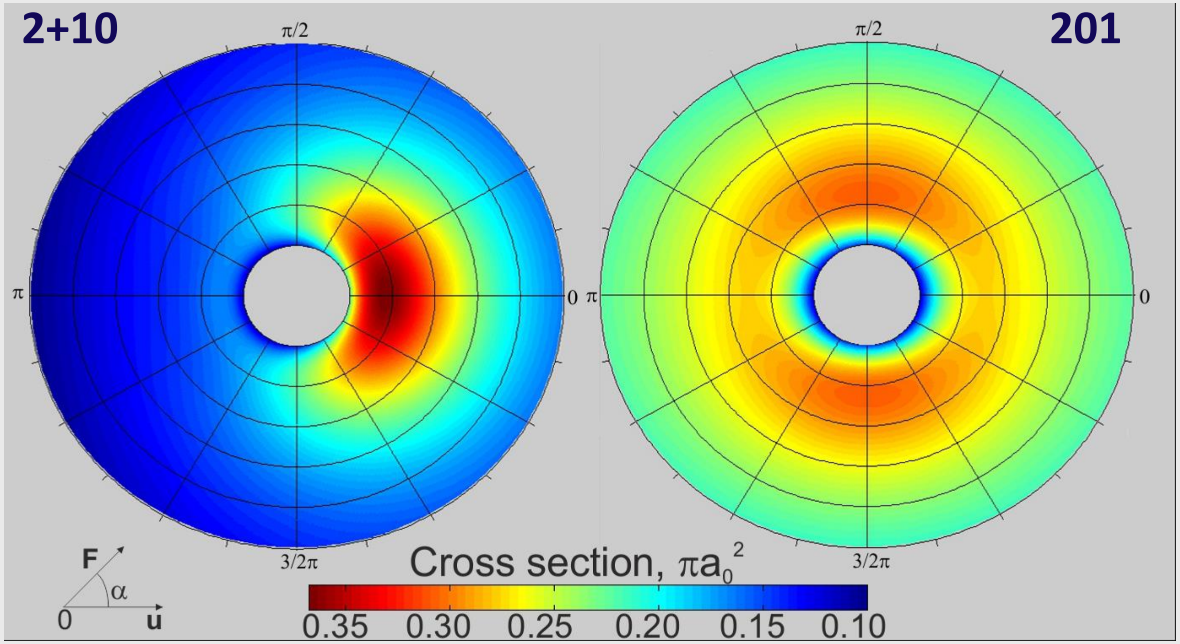
$$\sigma_{2\pm10} = \frac{1}{2}\sigma_{2s0} + \frac{1}{2}\cos^2(\theta)\sigma_{2p0} + \frac{1}{2}\sin^2(\theta)\sigma_{2p1} \mp \cos(\theta) Re(\rho_{2s0}^{2p0})$$

$$\sigma_{20\pm1} = \frac{1}{2}\sin^2(\theta)\sigma_{2p0} + \sigma_{2p1}\left(1 - \frac{1}{2}\sin^2(\theta)\right)$$

$\rho(n=2) =$

$2s_0$		s-p	
	$2p_{-1}$		
s-p*		$2p_0$	
			$2p_1$

Influence of the orientation on the cross sections.
AOCC calculations.



Marchuk O *et al.* 2013 *AIP Conf. Proc.* 1545 153
Marchuk O *et al.* 2011 *AIP Conf. Proc.* 1438 169

- Energy is varied in radial direction : 20…200 keV/u
- Polar angle is the angle between the field direction and the projectile

MSE : polar angle α = π/2

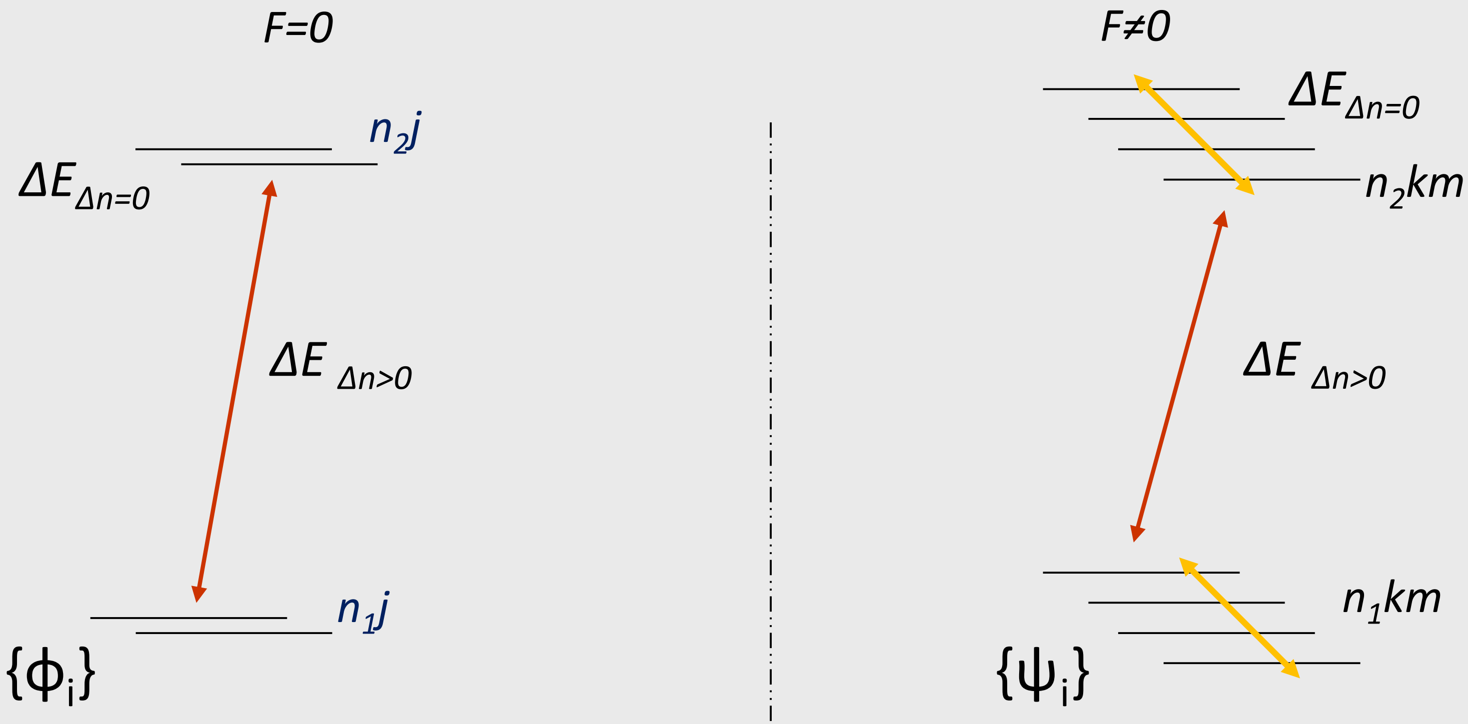
Example of the expression for the cross-sections:

$$\sigma_{2\pm10} = \frac{1}{2}\sigma_{2s0} + \frac{1}{2}cos^2(\alpha)\,\sigma_{2p0} + \frac{1}{2}sin^2(\alpha)\,\sigma_{2p1} \mp \cos(\alpha)Re(\rho^{2p0}_{2s0})$$

$$\sigma_{20\pm1} = \frac{1}{2}sin^2(\alpha)\,\sigma_{2p0} + \sigma_{2p1}\left(1 - \frac{1}{2}sin^2(\alpha)\right)$$

- Statistical models are based on the atomic data in spherical representation
- The beam *eigenstates* are close to the parabolic ones

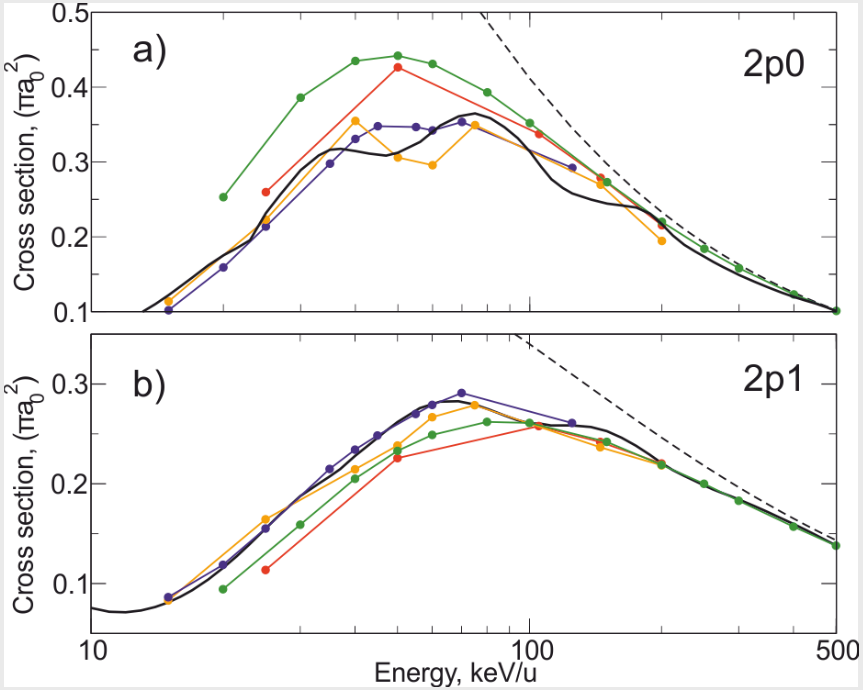
$$\Delta E_{\Delta n=0, F=0} \ll \Delta E_{\Delta n=0, F\neq 0} \ll \Delta E_{\Delta n>0} \qquad (*)$$

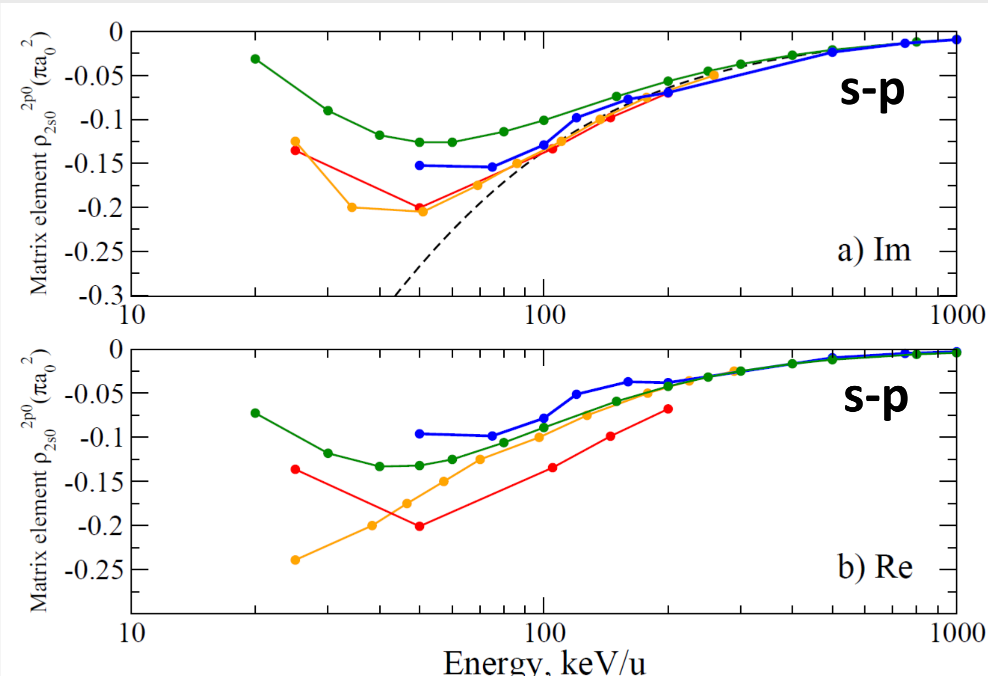


$$\sum\nolimits_{spherical} \sigma = \sum\nolimits_{parabolic} \sigma \qquad \text{at } (*)$$

$$\sum\nolimits_{spherical} A = \sum\nolimits_{parabolic} A \qquad \text{at } (*)$$

Calculation of the cross sections in parabolic states





black – AOCC calculation

blue - SAOCC Winter TG, Phys. Rev. A 2009 **80** 032701

green – Glauber approximation

dashed - Born approximation

orange - SAOCC Shakeshaft R Phys. Rev. A 1976 **18** 1930

red - EA Rodriguez VD and Miraglia JE J. Phys. B: At. Mol. Opt. Phys. 1992 **25** 2037

blue - AOCC calculation

green - Glauber approximation

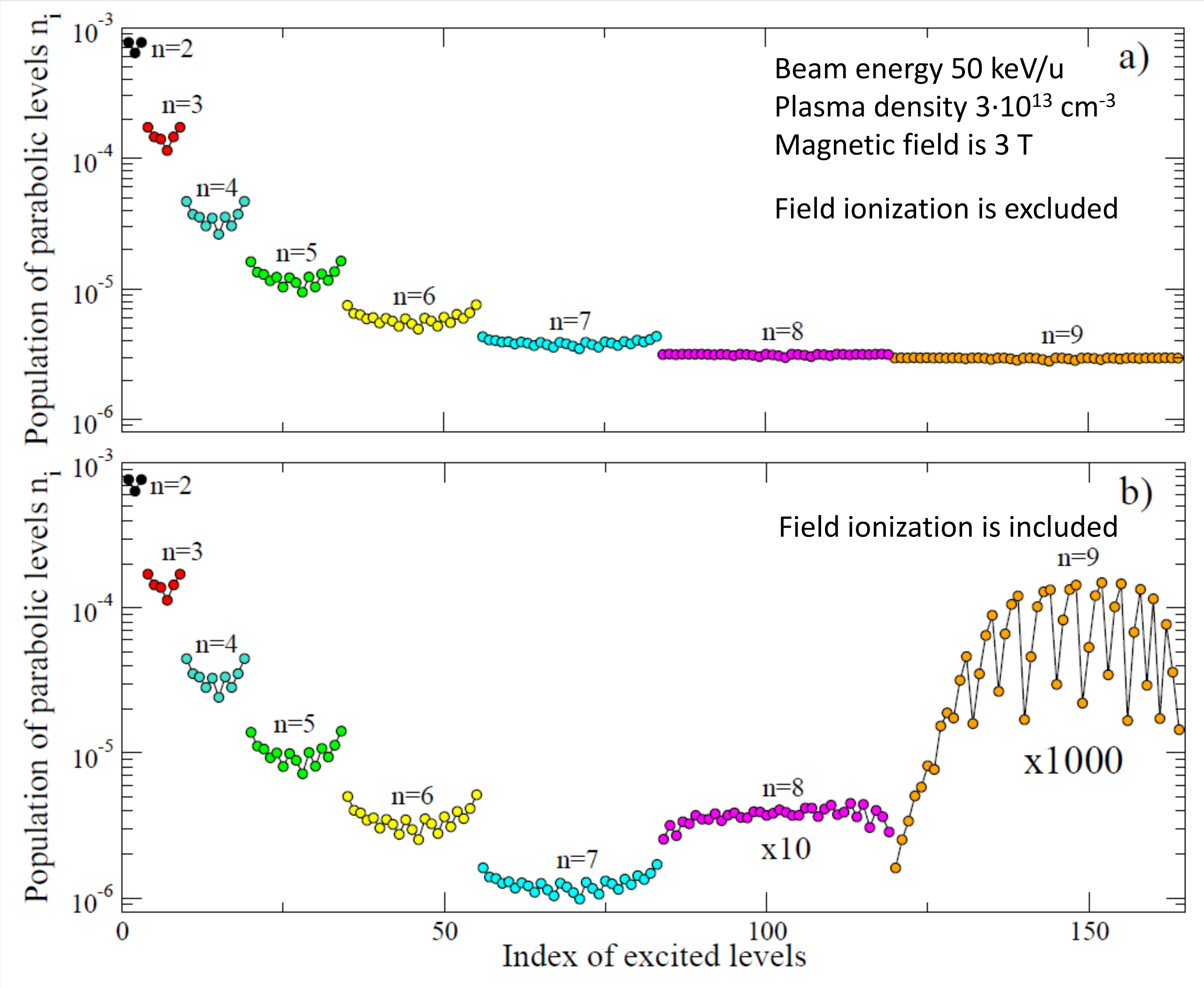
dashed - Born approximation

orange - CC method, Schöller O et al. J. Phys B.: At. Mol. Opt. Phys. **19** 2505 (1986)

red - EA Rodriguez VD and Miraglia JE J. Phys. B: At. Mol. Opt. Phys. 1992 **25** 2037

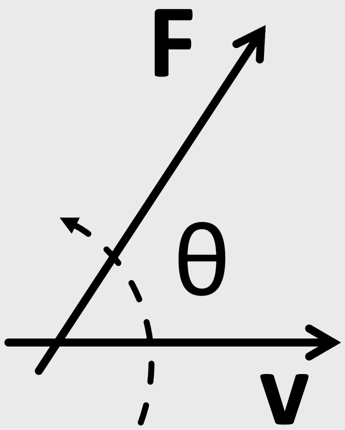
O. Marchuk, Yu. Ralchenko and DR Schultz Plasma Phys. Control. Fusion **54** (2012)

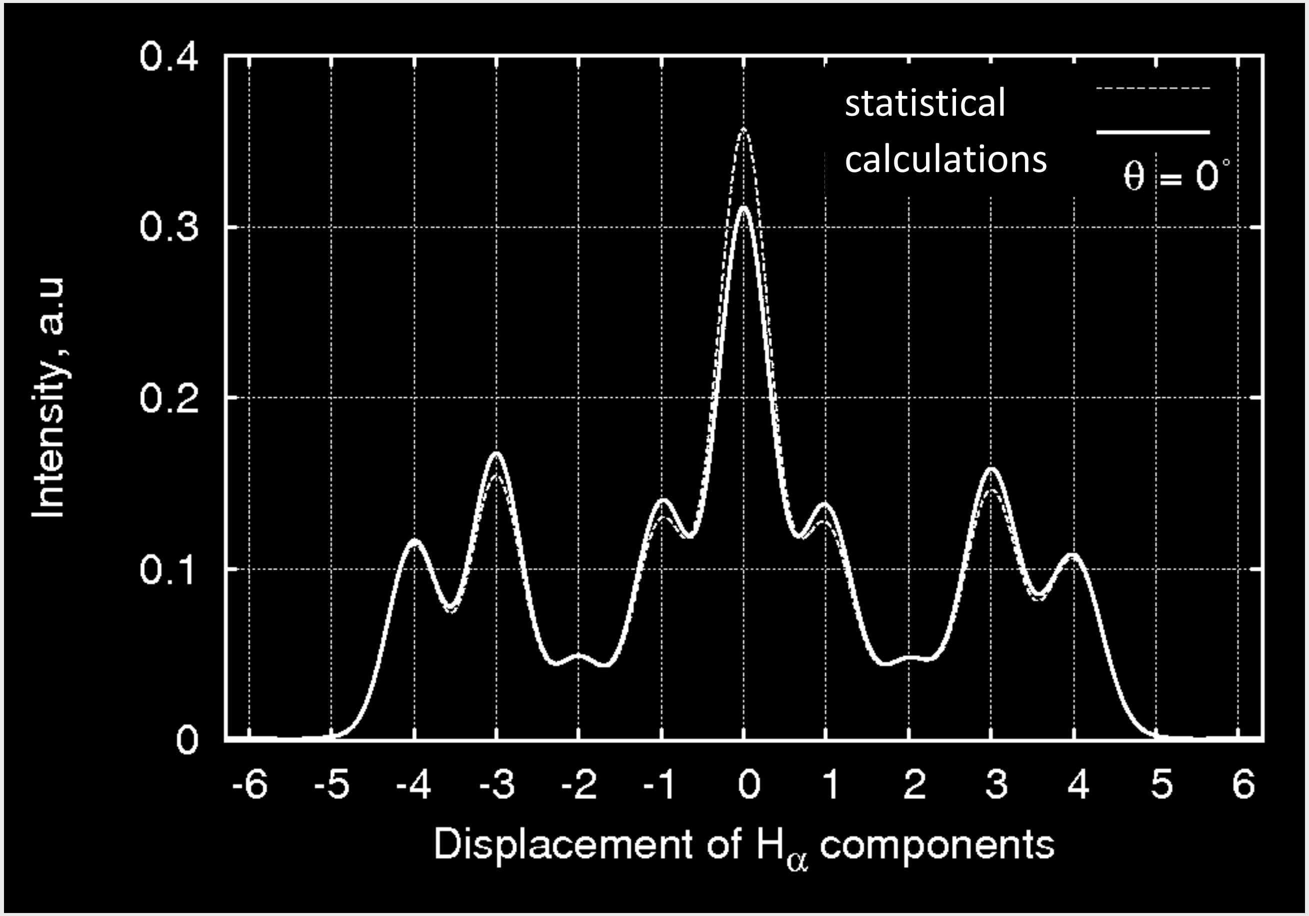
Populations of parabolic Stark levels



O. Marchuk, Yu. Ralchenko and DR Schultz Plasma Phys. Control. Fusion **54** (2012)

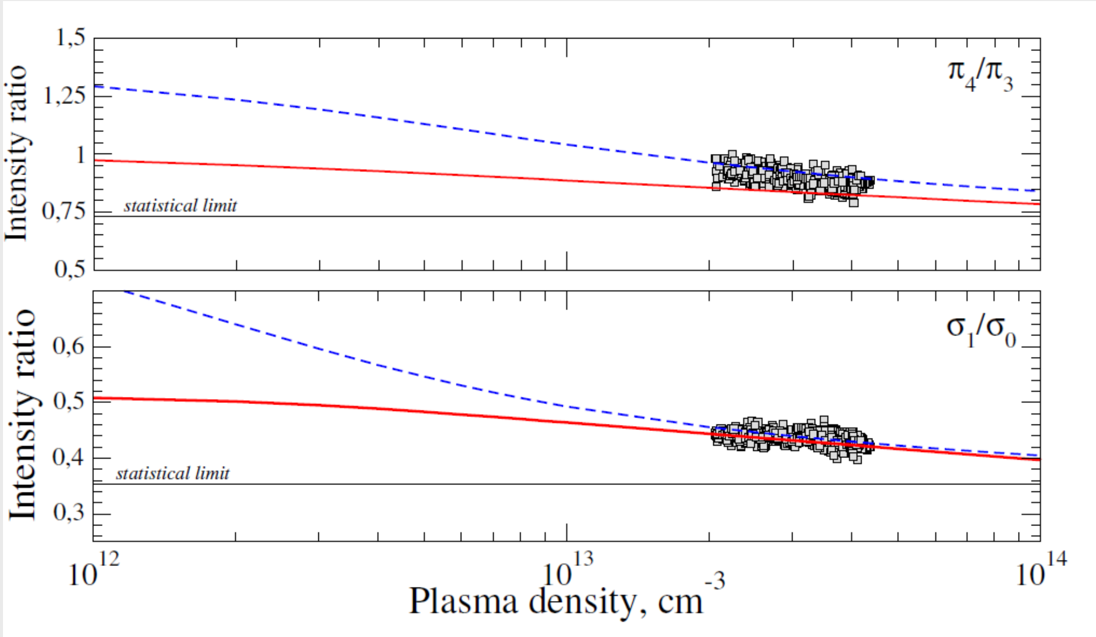
Influence of the orientation on the Stark multiplet emission





O. Marchuk, Phys. Scr. **89** 114010 (2014)

Comparison with JET data



„statistical"- is the standard atomic model up to 2010

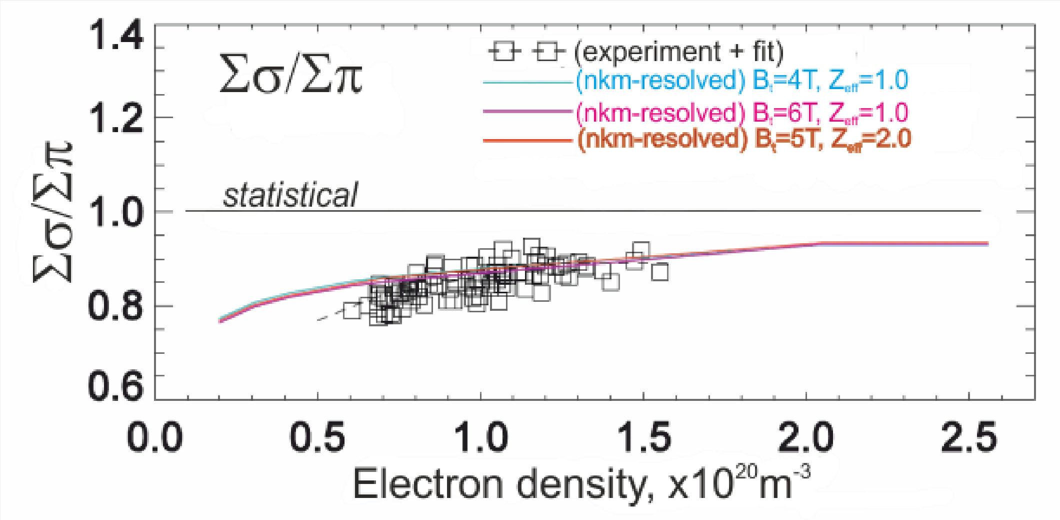
O. Marchuk et al. J. Phys B. : At. Mol. Opt. Phys (2010)

O. Marchuk et al. PPCF (2012)

E. Delabie et al. PPCF (2010)

- ❑ Significant deviations of the measurements to the standard statistical models

Comparison with ALCATOR-C Mod data



- ❑ Only at low densities some deviations to the new CRM results are observed
- ❑ The net emission of σ component is reduced relative to π one

I. Bespamyatnov et al. Nuclear Fusion ***53*** *123010 (2013)*

Summary

- The m-resolved model in parabolic state up to n=10 was developed..
  - arbitrary orientation between the direction of the field and the atoms relative velocity
- The collisional redistribution among the parabolic states was taken into account in the CRM NOMAD
- The experimental data on non-statistical populations of σ- and π – components in fusion plasma were explained …
- Impact of atomic models on the measurements of the q-profile is still ongoing…

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