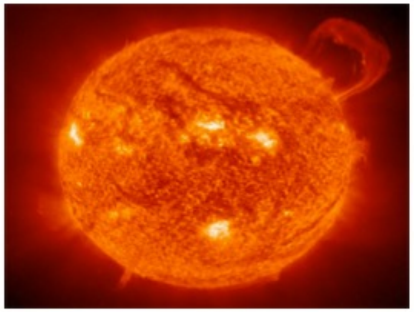
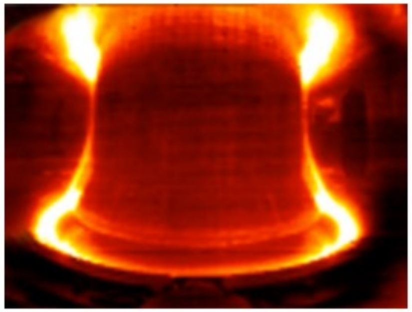
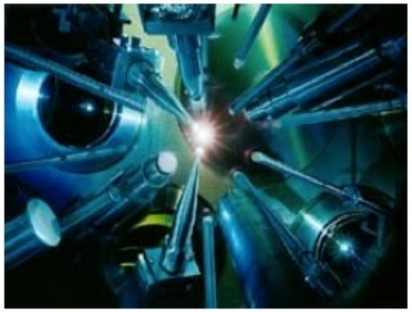
Spectral Line Shapes in Plasmas: state of the art







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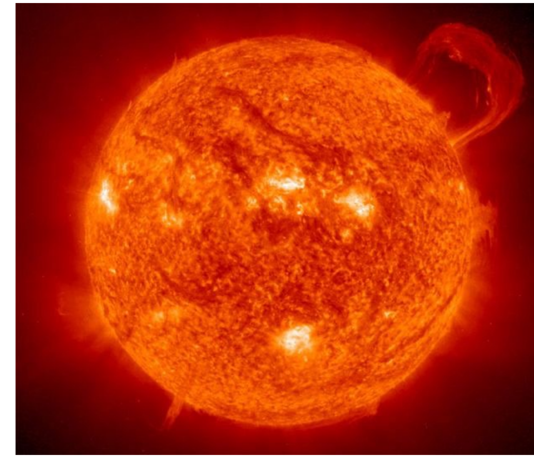
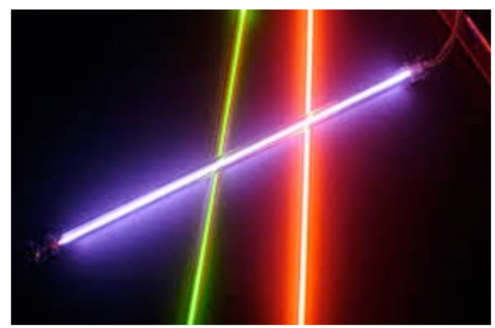
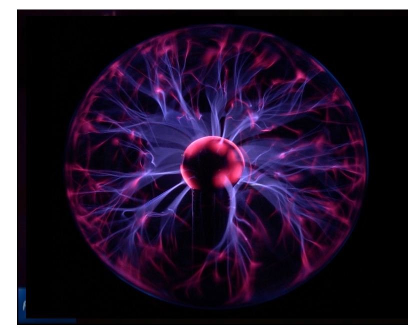
Introduction and Motivations

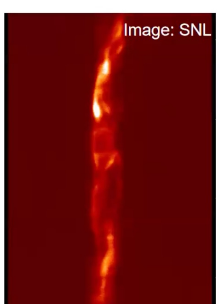
<u>Plasma in the Universe and on Earth :</u>

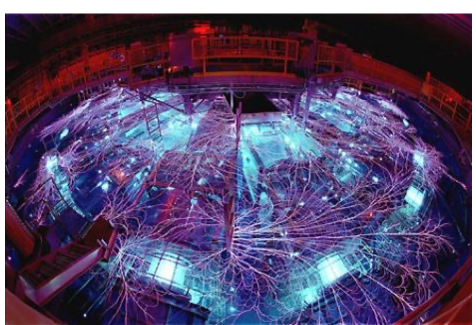


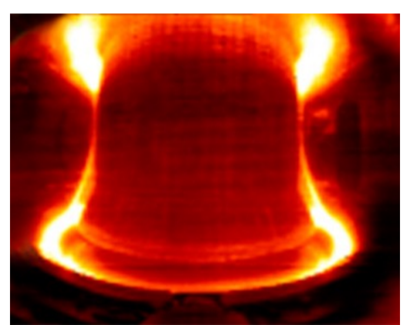
Plasmas emit electromagnetic radiation which contains information on the plasmas.



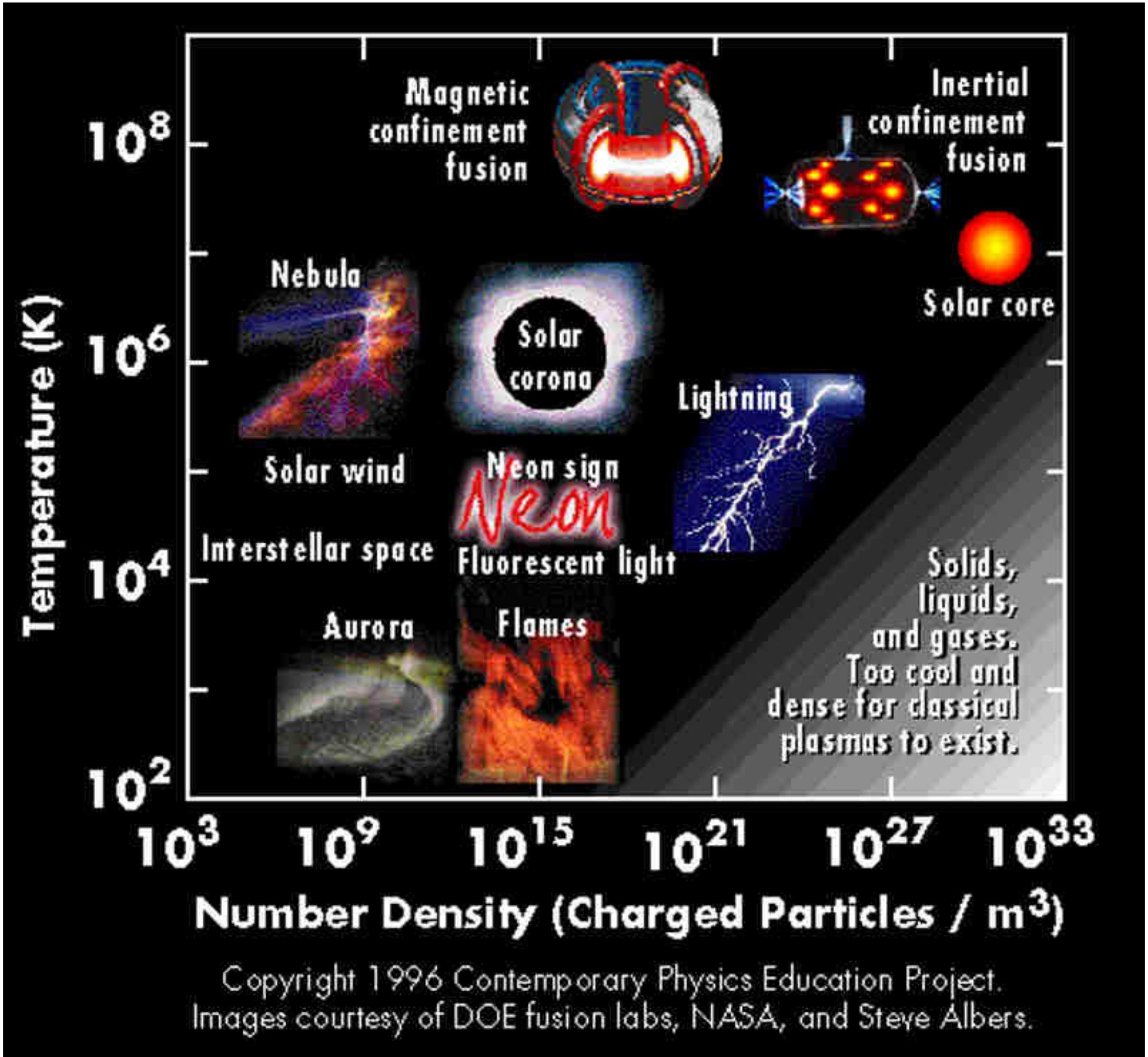


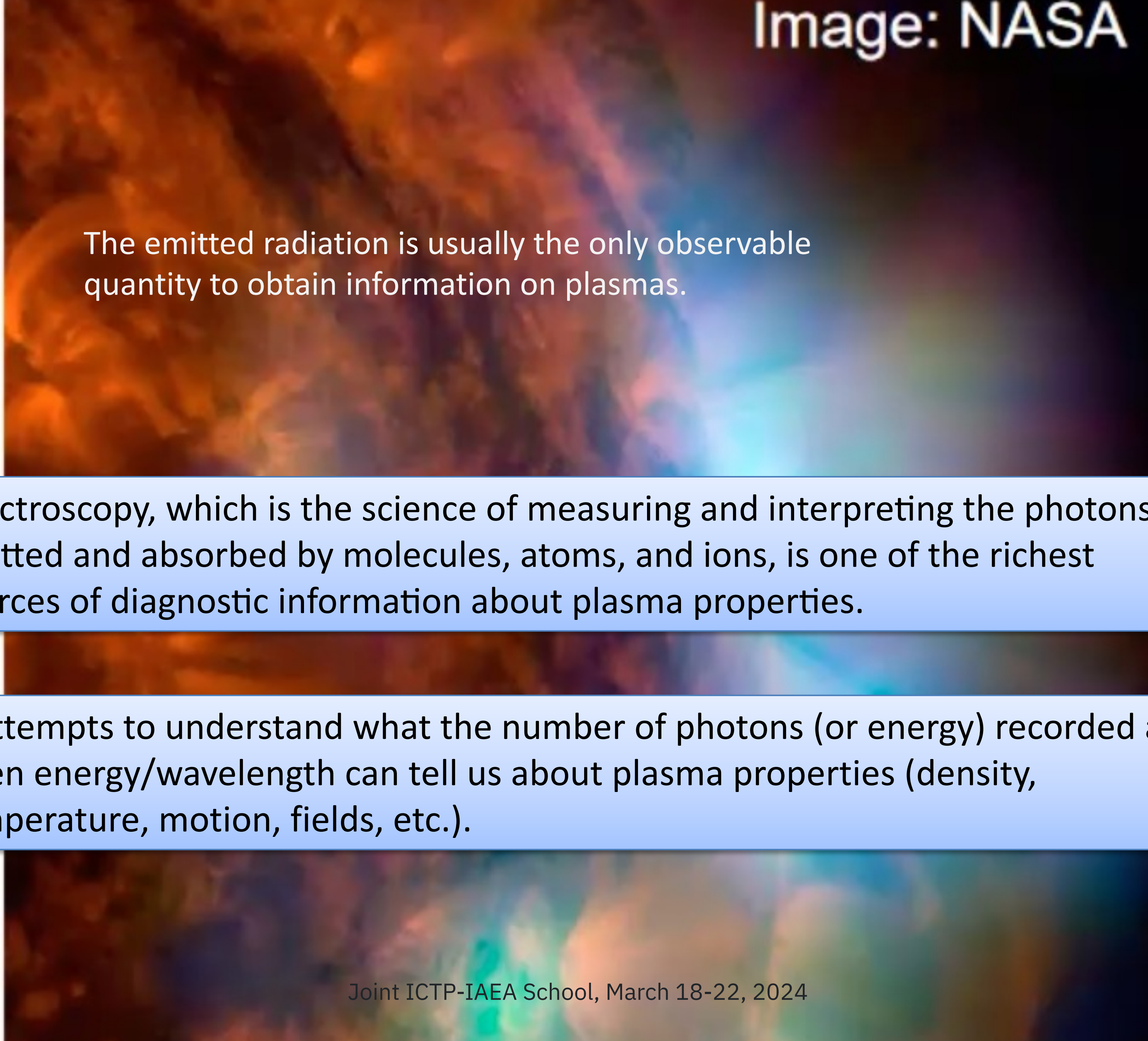






Introduction and Motivations



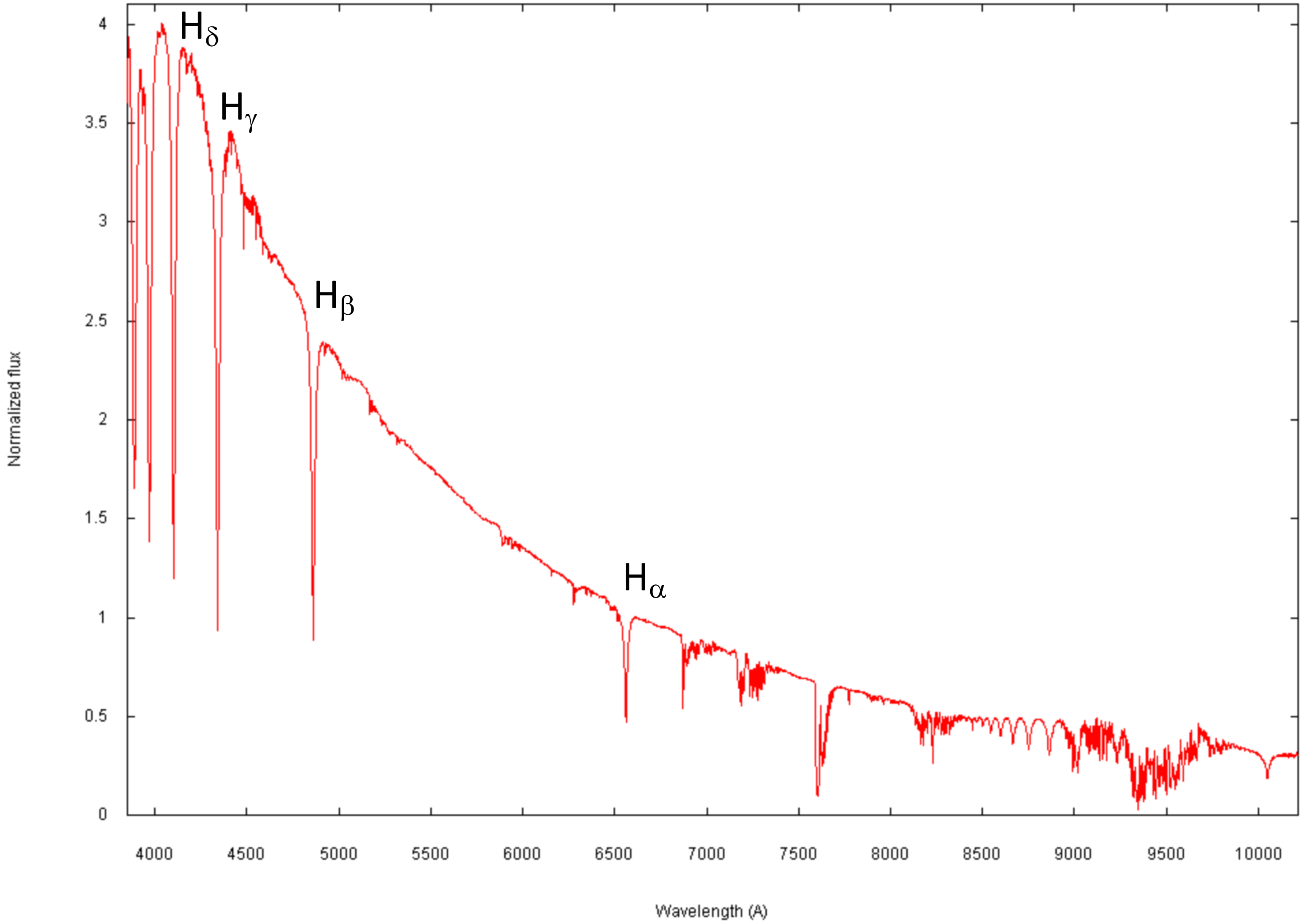


The emitted radiation is usually the only observable quantity to obtain information on plasmas.

Spectroscopy, which is the science of measuring and interpreting the photons emitted and absorbed by molecules, atoms, and ions, is one of the richest sources of diagnostic information about plasma properties.

It attempts to understand what the number of photons (or energy) recorded at a given energy/wavelength can tell us about plasma properties (density, temperature, motion, fields, etc.).

Introduction and Motivations



VEGA - Spectral class A: hot star with a spectrum dominated by hydrogen spectral lines.

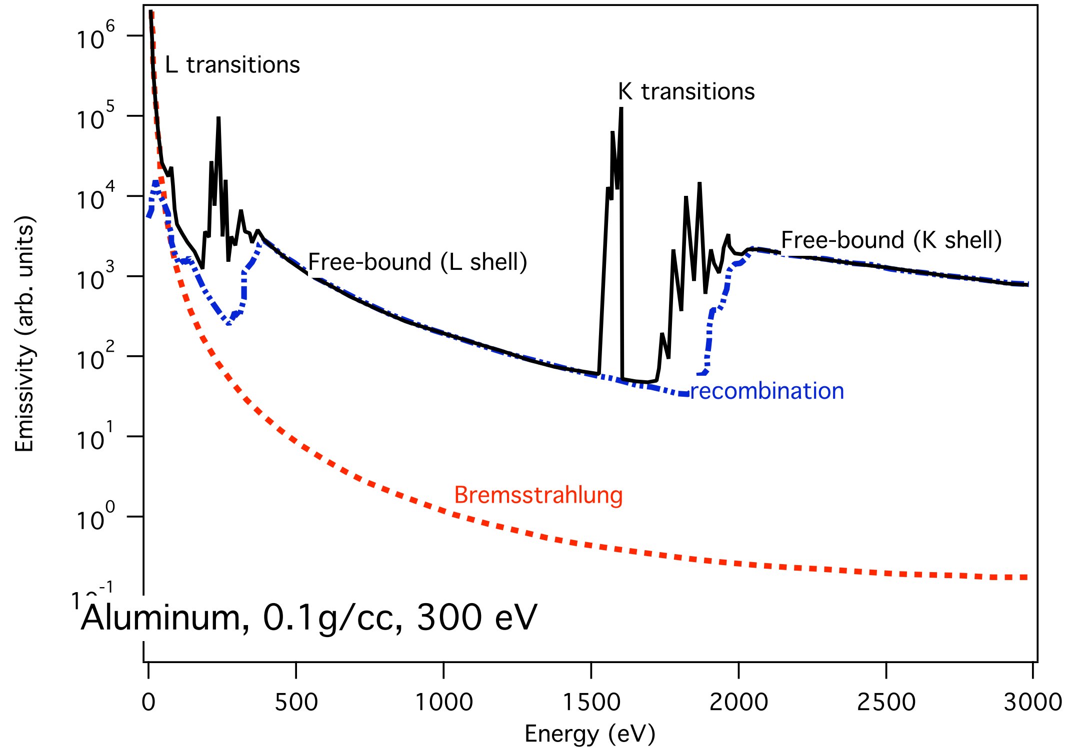
Introduction and Motivations

A hot plasma emits and absorbs radiation depending on its composition and ionization.

3 mechanisms are responsible for the emission of radiation:

- The bremsstrahlung, (free-free) – continuum radiation –
- The radiative recombination (free-bound) – Continuum radiation –

* The spontaneous emission (bound-bound) – line radiation -



Introduction and Motivations

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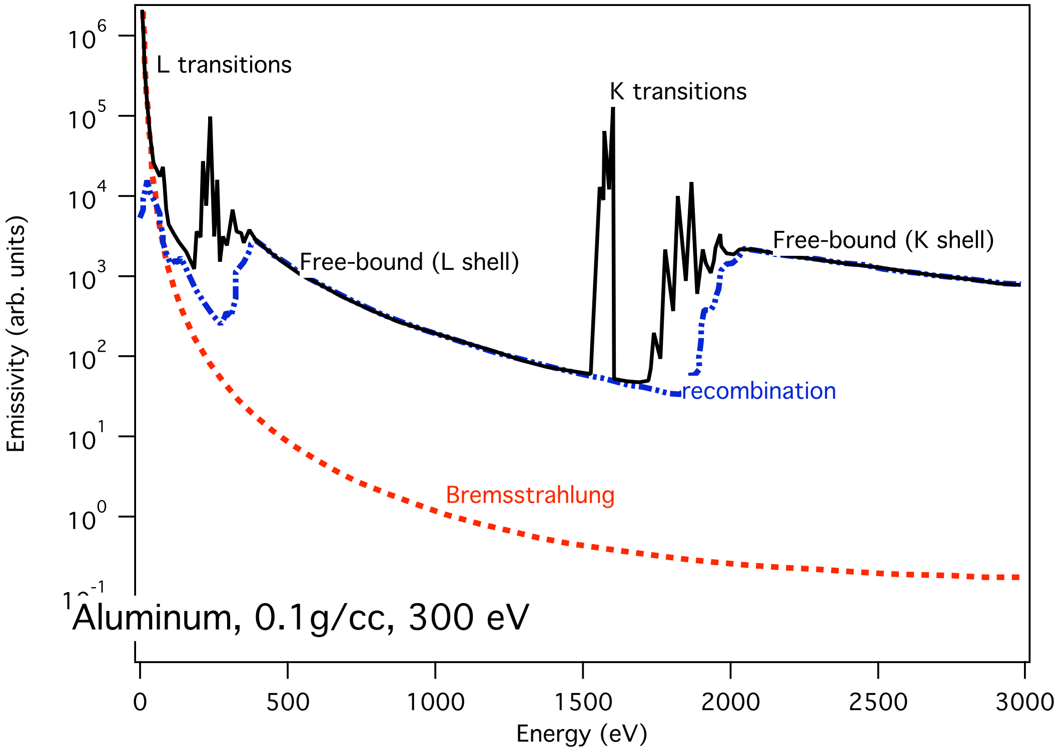
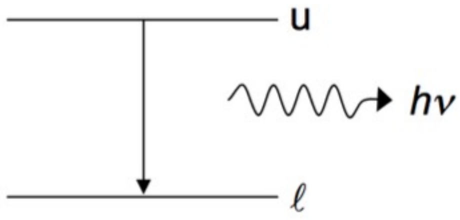


Introduction and Motivations

The line intensity emitted by an ion of charge Z for a transition u-l is given by:

$$N_u^Z A_{ul} h\nu_{ul}$$



N_u^Z, is the upper level population density,
A_{ul}, is the rate of spontaneous radiative decay,
$h\nu_{ul} = E_u - E_l$, is the emitted photon energy,

Absorption and emission lines in spectra are not infinitely narrow. They are broadened by various mechanisms:

$$N_u^Z A_{ul} h\nu_{ul} \phi(\nu)$$

It is necessary to account for the probability to emit (or absorb) photon of a given frequency, $\Phi(\nu)$. **Also called the spectral line shape or spectral line profile.**

Introduction and motivation

• A plasma is a medium containing many charged particles governed by electromagnetic forces.
• The charged particles present collective behavior.

→ The radiation of a plasma depends, not only on the properties of the isolated radiating species, ***but also on the properties of the plasma in the immediate environment of the radiator***.

The emitting atom or ion in a plasma is never isolated from the perturbing effects of other ions and electrons. This

** affects the population densities of bound states,*
**** shifts and broadens energy levels (via the Stark effect),***
** lowers the ionization potentials of atomic species*
** is the cause of continuum radiation emission*
**** is the cause of the emission of normally forbidden lines.***

Introduction and Motivations

Different types of line broadening mechanisms.

• Natural line broadening due to the finite lifetime of levels, homogeneous Lorentzian profile, almost always negligible (except for autoionization broadening of doubly excited states).

• Doppler broadening due to the frequency shift owing to the emitter motion, inhomogeneous gaussian profile, high temperatures and low densities.

• Stark broadening (also pressure broadening) due to the interactions between emitter and charged perturbers, two limit approximations – quasi-static for ions and impact for electrons -, inhomogeneous profile (superposition of homogeneous profiles).

• External field broadening, e.g. Zeeman effect due to magnetic fields…

• re-absorption, linked to absorption probability, affects differently the center and the wings of the line.

• Instrument broadening (usually ~Gaussian but requires measurement)

Any line broadening comes due the emitter experiences the environment as a coherent source only for limited coherence times.

Introduction and Motivations

Homogeneous and Inhomogeneous Broadening

- If a mechanism broadens the lineshape in the same way for each atom, it is homogeneous.

  A single mode laser can excite all the atoms

  Random interruption of the phase evolution → Exponential decay of the coherence

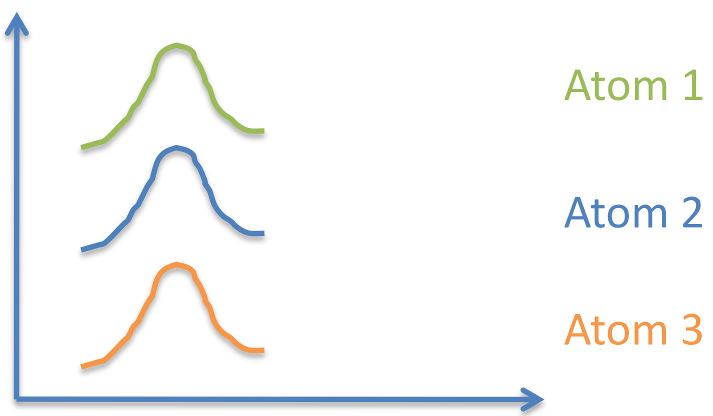
  → Lorentzian profile

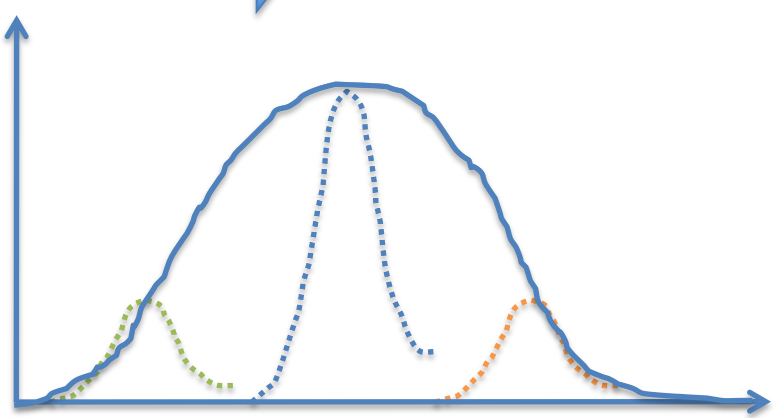
- If the mechanism distributes the resonance frequencies over a spectral range, it is inhomogeneous.

  Random shift to individual atoms and the broadening happens for the ensemble.

  A single mode laser will excite only a class of atoms

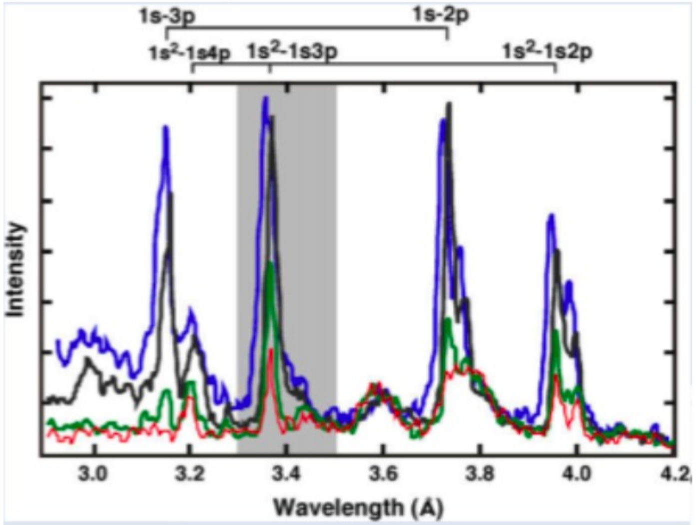
  Random perturbations, normal distribution → Gaussian profile



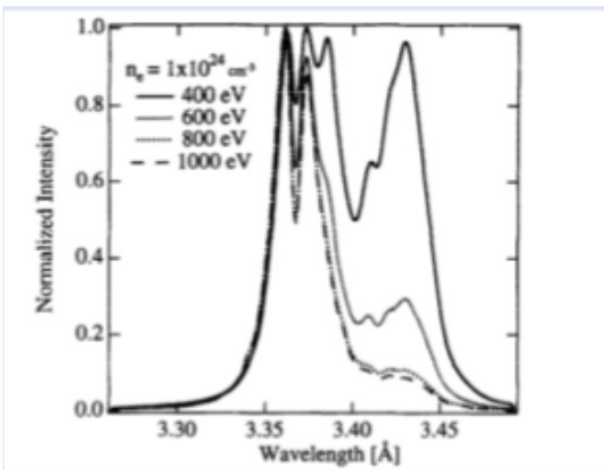


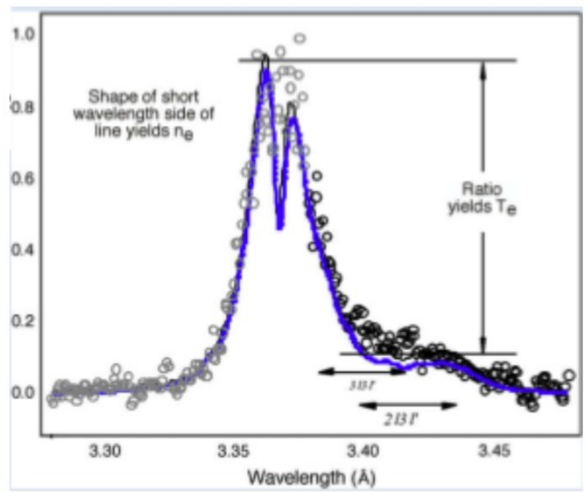
Introduction and Motivations

Ar-doped ICF implosion cores.



The composite spectral feature comprised of the Heβ spectral line and its associated Li-like satellites in argon is used for spectroscopic diagnosis in inertial confinement fusion (ICF) experiments.

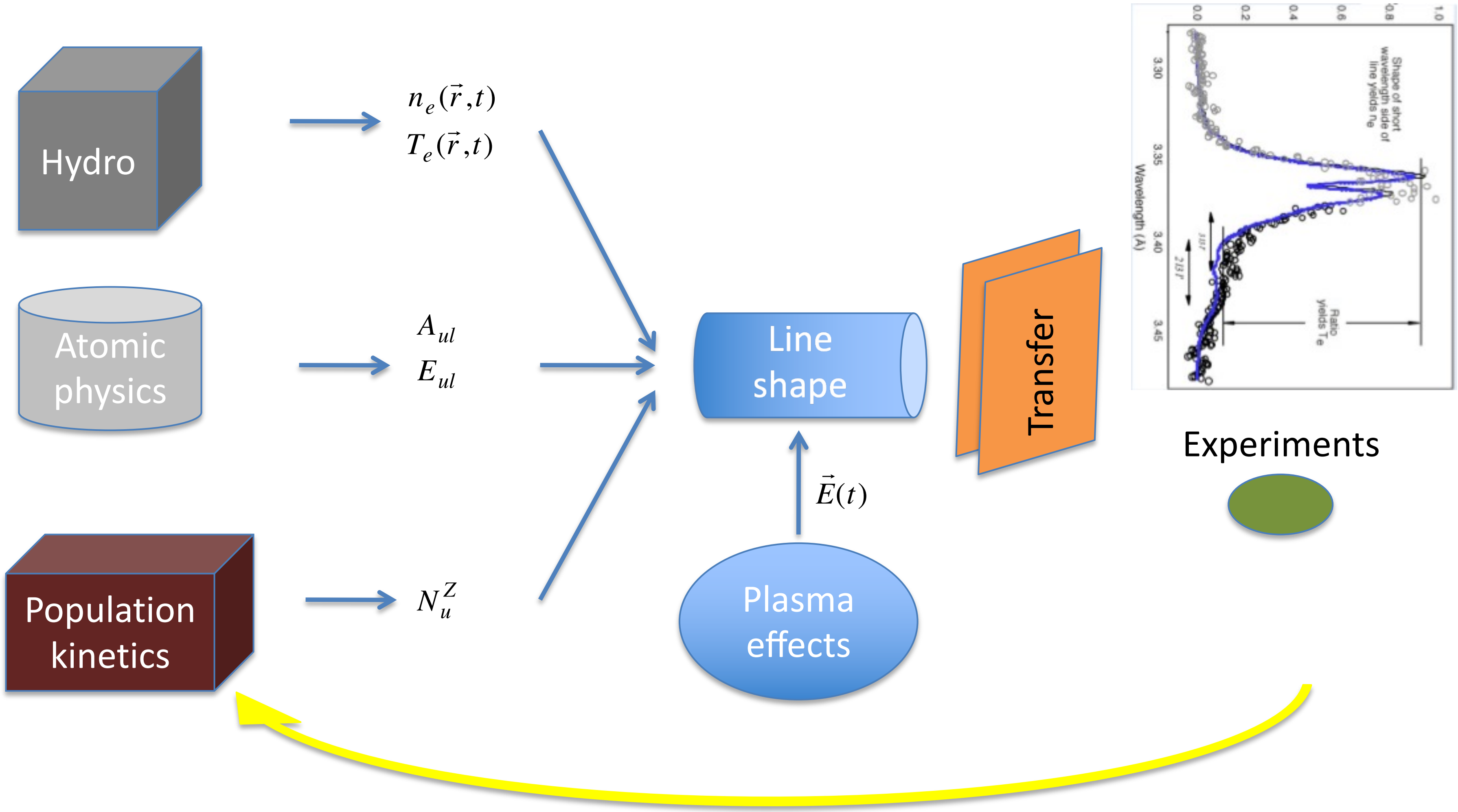




N.C. Woolsey et al., Phys. Rev. E 53, 6396 (1996)

H.K. Chung and R.W. Lee, International J. of Spec., 506346 (2010).

Introduction and Motivations



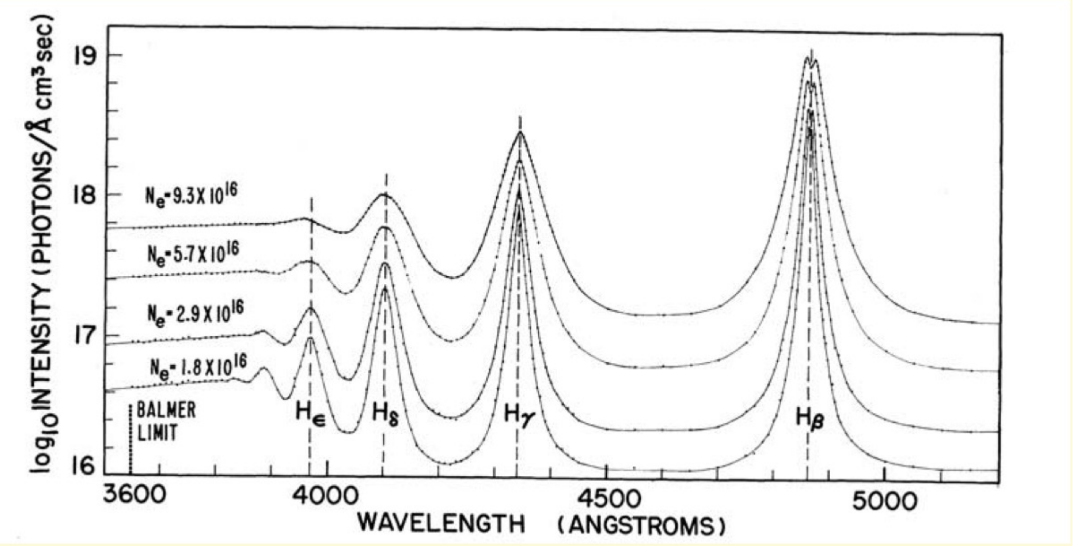
The diagnostic is based on the comparison of observed and modeled data. Evidently, to be reliable, this requires accurate theoretical models of atomic and radiation physics.

Introduction and Motivations

How do we know if our models are reliable?

Test them in careful, "benchmark" experiments with plasma samples that are:

- relatively uniform,
- independently characterized,
- carefully diagnosed



Wiese, Kelleher, and Paquette, Phys. Rev. A 6, 1132 (1972)

Put them to the test by comparing them with other existing models.

The SLSP workshop has been created since 2012 to initiate studies comparing different computational and analytical methods which were almost nonexistent. By detailed comparison of results for a selected set of case problems, it becomes possible to pinpoint sources of disagreements, infer limits of applicability, and assess accuracy.

SLSP

Introduction and Motivations

Line shape modeling in plasmas has a long history

- in the 60s: birth of the theory of spectral line broadening in plasmas [1,2].
- in the 70s: observed discrepancies between experiments and theories are attributed to ion motion → first attempts to include the effects of ion motion in theories [3-6]. Experimental evidence for hydrogen is obtained [7].
- from the 1980s: first N-body simulations [8-13] and sophisticated models for neutral or multi-charged emitters, of varying complexity and applicability [14-24].

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...

https://plasma-gate.weizmann.ac.il/slsp/

Elements of modeling

Consider an atomic oscillator of amplitude *A(t)* emitting radiation without interruptions,

$$A(t) = A_0 e^{i\omega_0 t}$$

The Fourier transform of the amplitude is,

$$\tilde{A}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A(t) e^{-i\omega t} dt = A_0 \delta(\omega - \omega_0)$$

The Fourier spectrum is monochromatic and characterized by a delta function centered at ω_0

The energy spectrum defined as, $E(\omega) = \left|\tilde{A}(\omega)\right|^2$ is a direct measure of the energy in the wave train at frequency ω.

The spectral line is related to the energy delivered per time unit, the power spectrum:

$$I(\omega) \equiv \lim_{T\to\infty} \frac{1}{2\pi T} \left| \int_{-T/2}^{T/2} A(t) e^{-i\omega t} dt \right|^2$$

Or in term of correlation function $I(\omega) = \int_{-\infty}^{+\infty} C(t) e^{-i\omega t} dt$

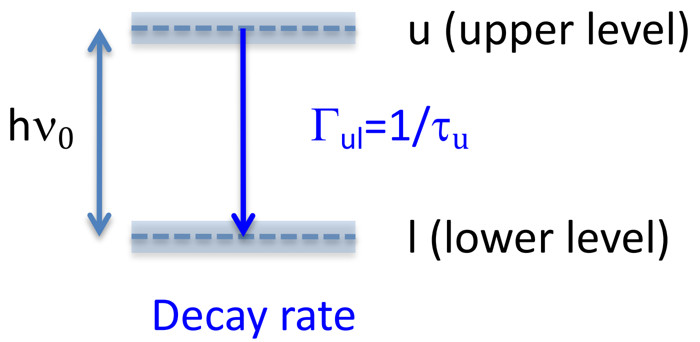
$$\Rightarrow \quad I(\omega) = \lim_{T\to\infty} \frac{A_0^2}{\pi} \frac{\sin^2(\omega - \omega_0)\frac{T}{2}}{(\omega - \omega_0)^2 \frac{T}{2}} = \frac{A_0^2}{\pi} \delta(\omega - \omega_0)$$

The line shape is a delta function

Natural line broadening

Intrinsic to the transition and resulting from the Heisenberg uncertainty principle.

The uncertainty principle relates the lifetime of an excited state (e.g. due to the spontaneous radiative decay) with the uncertainty of its energy.

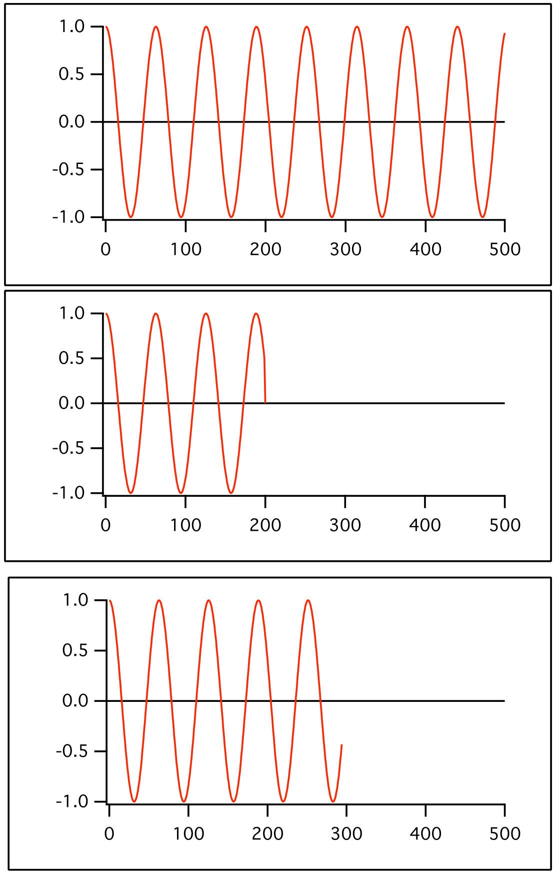


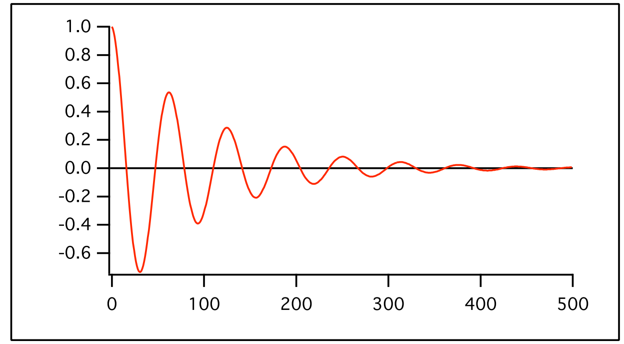
$$\Delta E \Delta t \geq \frac{h}{2\pi}$$

$$\boxed{\Delta \nu = \frac{1}{2\pi\Delta t} \equiv \frac{1}{2\pi\tau_u}}$$

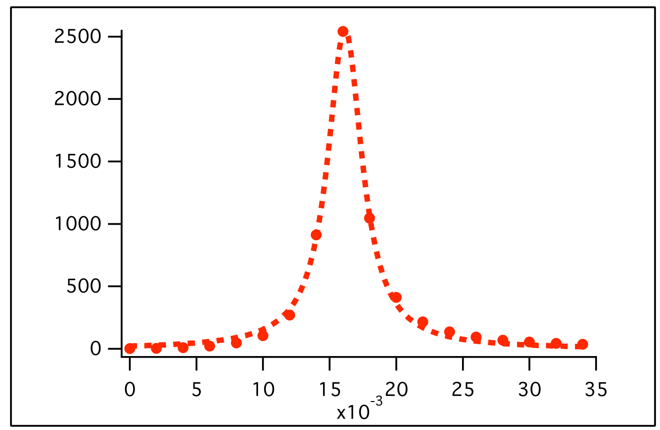
The probability of decay per unit time follows an exponantial law: $P(t) \propto e^{-t/\tau}$

Natural line broadening





Fourier Transform



Lorentzian profile

$$I(\omega) = \frac{1}{\pi} \frac{\gamma/2}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

The broadening of spectral lines by this process is independent of the environment of the atom and is a result primarily of the probabilistic behavior of the atom itself.

Homogeneous

Natural line broadening

Independent of the environment of the radiating atom.

Typical values:

Electronic transitions:
$\Gamma \sim 10^{8}\ \mathrm{s}^{-1} \rightarrow \mathrm{FWHM} \sim 10^{-7}\ \mathrm{eV}$

Vibrational-rotational transitions:
$\Gamma \sim 10^{2}\ \mathrm{s}^{-1} \rightarrow \mathrm{FWHM} \sim 10^{-13}\ \mathrm{eV} = 10^{-10}\ \mathrm{cm}^{-1}$

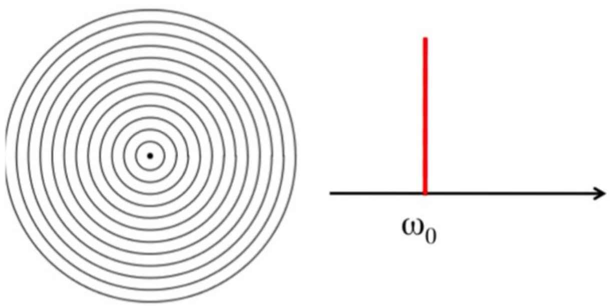
Generally, negligible compared to Doppler and plasma broadening.

Doppler effect

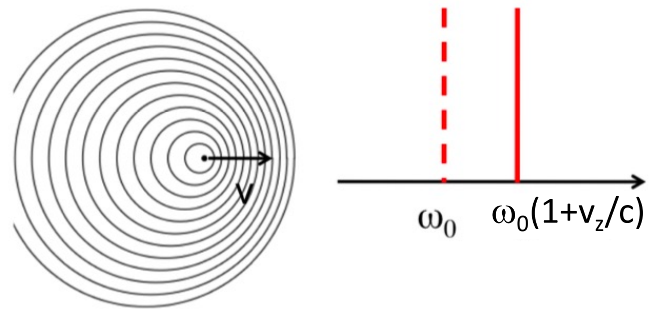
It is the result of the thermal/microscopic motion of the radiators in the plasma.

The Doppler effect tells us that the frequency of waves depends on the motion of source and observer. Doppler-shifted frequency for an atom moving at velocity v_z along the line of sight differs from ν_0 in rest frame of atom:

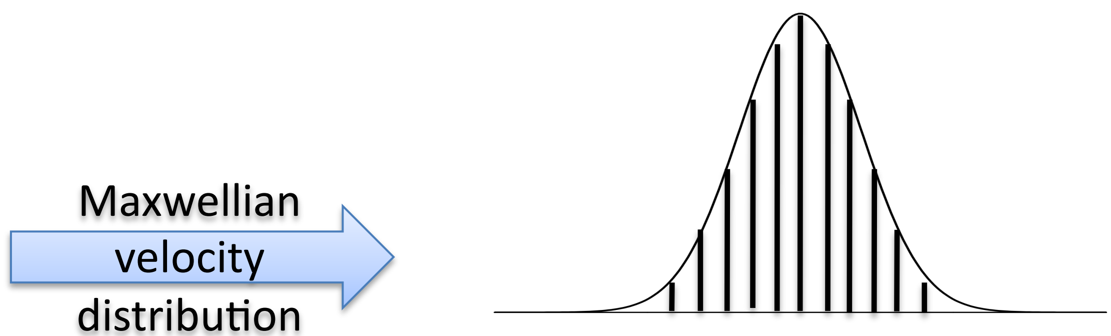
in rest frame of the radiator:



in rest frame of the observer:



$$\nu = \nu_0\left(1 + \frac{v_z}{c}\right)$$



Doppler effect

The spectral line shape of a radiating system is related to the autocorrelation function of its radiated electric field $\vec{E}(t)$ through a Fourier transform.
The electric field emitted from a fixed radiator at position $\vec{r}$ and at time t is:

$$\vec{E} \propto \exp(i\vec{k}_0 \cdot \vec{r} - i\omega_0 t)$$

With k_0 the wave-number vector and ω_0 the oscillation frequency.

For a moving radiator: $\vec{E} \propto \exp(i\vec{k}_0 \cdot \vec{r}(t) - i\omega_0 t)$ with: $\vec{r}(t) = \vec{r}_0 + \int_0^t \vec{v}(t')dt'$

The field autocorrelation function is then:

$$C(t) = \mathrm{Re}\left\langle \exp(-i\vec{k}_0 \cdot \vec{r}(\tau) + i\omega_0 \tau) \right\rangle$$

where $\vec{r}(\tau) = \int_t^{t+\tau} \vec{v}(t')dt'$

and <> an ensemble average

If the oscillators neither collide nor change their velocities, we have: $\vec{r}(\tau) = \vec{v}\tau$

For a Maxwellian velocity distribution within the ensemble: $f(\vec{v}) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(\frac{-m|\vec{v}|^2}{2kT}\right)$

The Fourier transform then yields the area normalized Doppler line profile:

$$\boxed{I(\omega) = \frac{c}{\omega_0}\left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(\frac{-mc^2(\omega - \omega_0)^2}{2kT\omega_0^2}\right)}$$

Gaussian
Inhomogeneous

Doppler effect

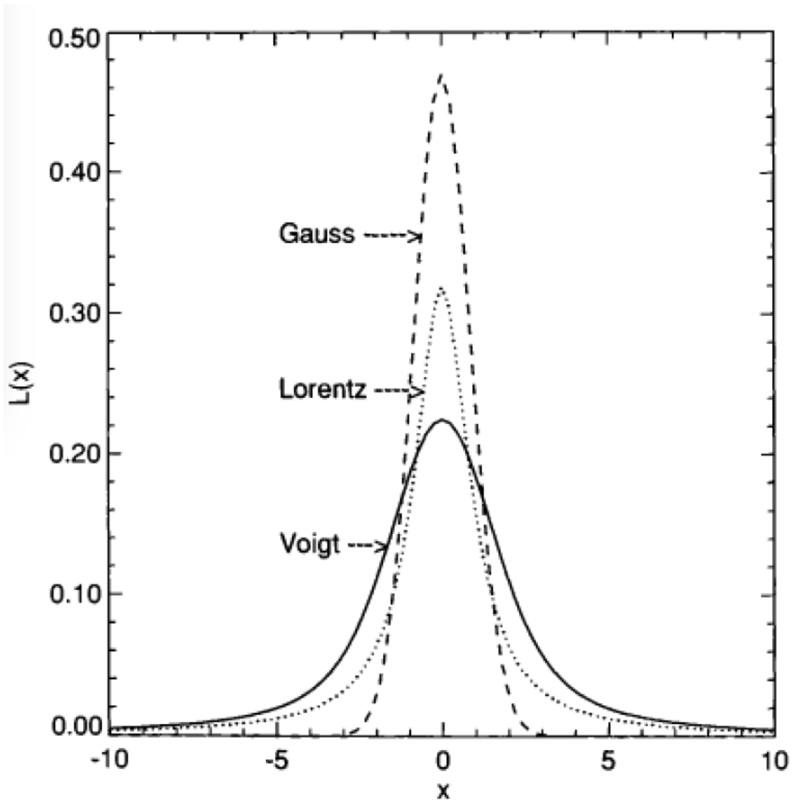
$$FWHM = 2\sqrt{ln2}\,\omega_D = \omega_0 \cdot 7.715 \times 10^{-5}\sqrt{\frac{T_i(eV)}{M_i(u)}}$$

Dominant for H, D, T and He in Tokamak plasmas.

It is of the order of 1 eV in hot plasmas, i.e. for temperatures of the order of 1 keV

Voigt line shape

The combined effect of natural and Doppler broadening is given by convolution of the Lorenztian and Gaussian functions.



©Griem, Principle of Plasma Spectroscopy, (1997)

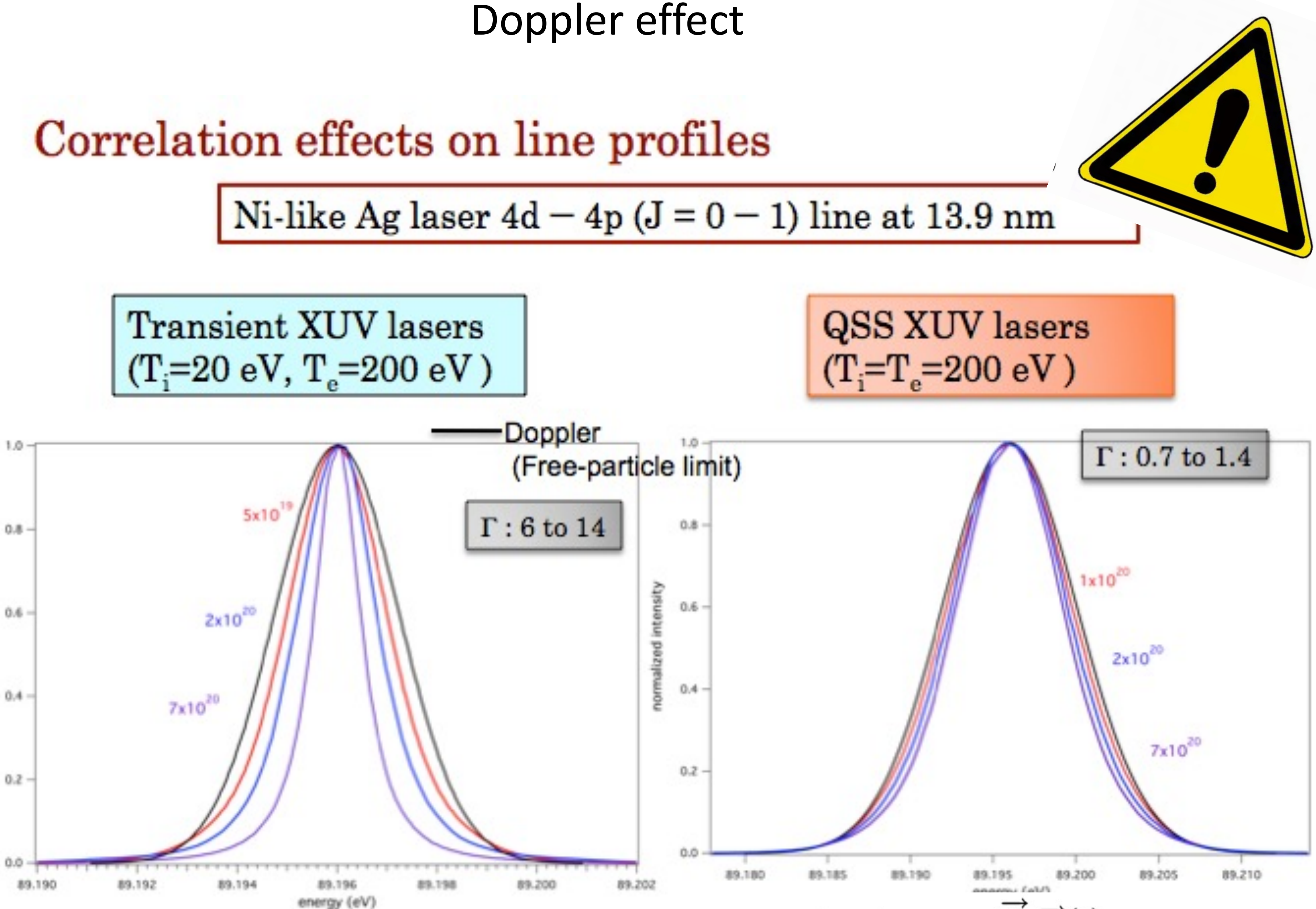
This is the Voigt line shape:

$$L_v(\omega) = H(a, V) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2} dy}{(v-y)^2 + a^2}$$

with

$$V = \frac{\omega - \omega_0}{\Delta\omega_D} \qquad a = \frac{\Gamma}{4\pi\Delta\omega_D}$$

Doppler effect

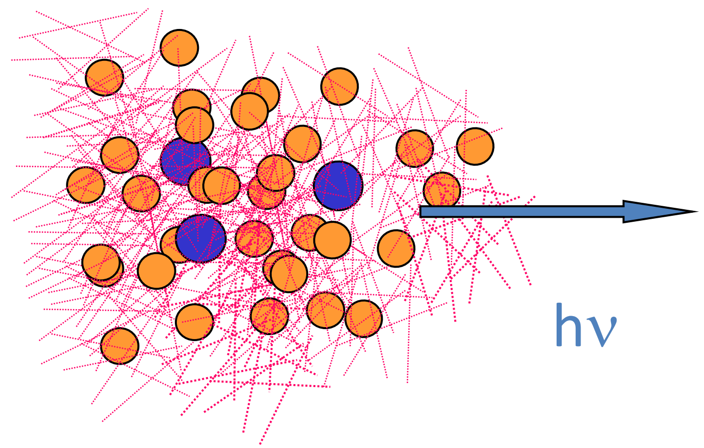


A. Calisti et al., HEDP 9, 516-522 (2013).

$$I(\omega) = S_s(k,t) = \langle e^{i\vec{k}\cdot\vec{r}(t)} \rangle$$

Self-structure factor

Plasma broadening – Stark broadening



A plasma is a medium, containing ions and electrons partially recombined, spanning a very broad area of conditions and involving elements and greatly varying degrees of ionization.

To model the radiation emitted or absorbed by such a medium, it is common to consider that the emitter is embedded in a bath of charged perturbers (ions and electrons).

The radiator is then described quantum-mechanically whereas the bath is treated classically

Plasma broadening – Stark broadening

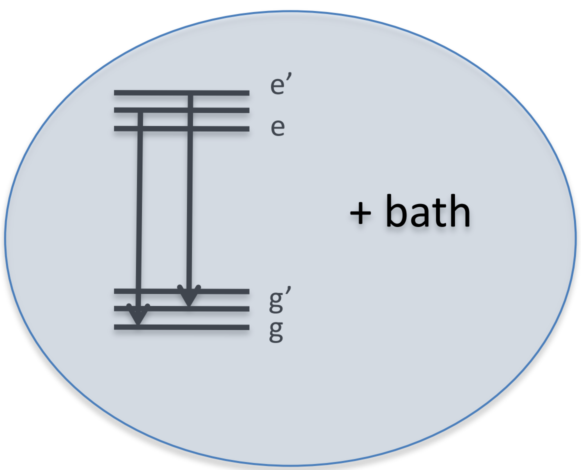
The common starting point for the calculation of spectral line shape :

$$I(\omega) = \frac{1}{\pi} \Re e \int_0^\infty dt\, C(t)\, e^{i\omega t}$$

The autocorrelation function C(t) is given by:

$$C(t) = \left\langle \left\langle \vec{d}^{+} \middle| U(t) \middle| \vec{d} \rho_0 \right\rangle \right\rangle$$

Where U(t) is the evolution operator solution of the stochastic equation :



$$\begin{cases} \dfrac{dU_l(t)}{dt} = -i\left(L_0 + l(t)\right)U_l(t) \\ U_l(0) = 1 \end{cases}$$

$$U(t) = \left\{U_l(t)\right\}_{av}$$

Averaged over the bath of perturbers

Plasma broadening – Stark broadening

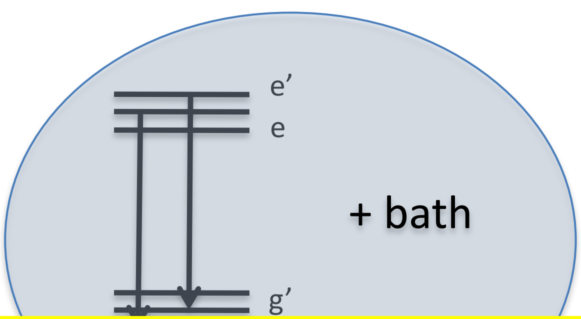
The common starting point for the calculation of spectral line shape :

$$I(\omega) = \frac{1}{\pi} \Re e \int_0^\infty dt\, C(t)\, e^{i\omega t}$$

The dipole autocorrelation function C(t) is given by:

$$C(t) = \left\langle \left\langle \vec{d}^{+} \middle| U(t) \middle| \vec{d} \rho_0 \right\rangle \right\rangle$$

Where U(t) is the evolution operator solution of the stochastic equation :



External fields can also be added, $E_0 \cos(\omega t)\mathbf{z}$ and/or magnetic field $B\mathbf{z}$. ($L_B = \mu_B \mathbf{B}.[g_l \mathbf{L} + g_s \mathbf{S}]$).

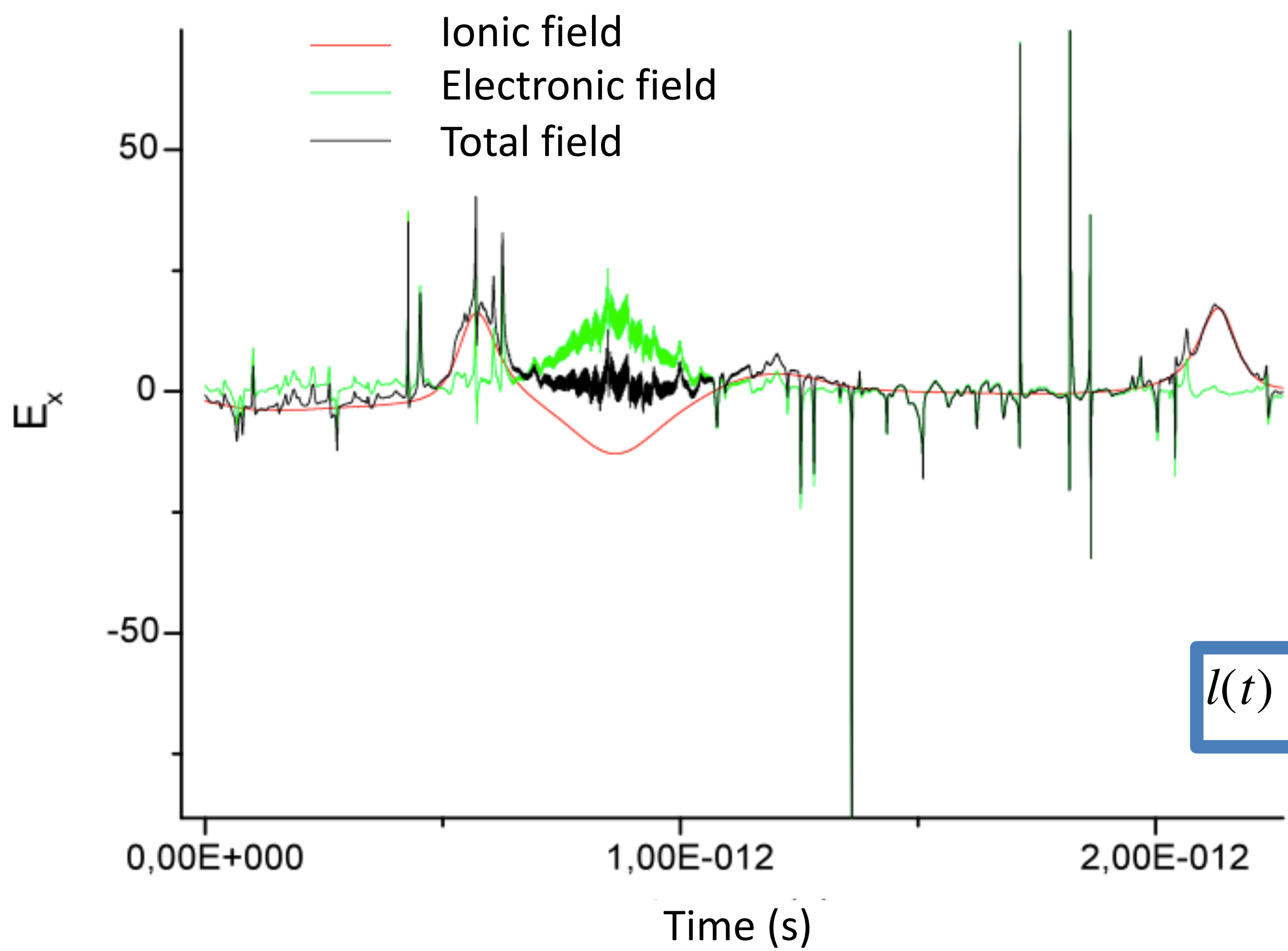
$$\boxed{\begin{cases} \dfrac{dU_l(t)}{dt} = -i\left(L_0 + l(t)\right)U_l(t) \\ U_l(0) = 1 \end{cases}}$$

$$\boxed{U(t) = \left\{U_l(t)\right\}_{av}}$$

Averaged over the bath of perturbers

Plasma broadening – Stark broadening

The charged particles (ions and electrons) of the plasma create fluctuating electric fields which perturb the atomic and ionic emiters.



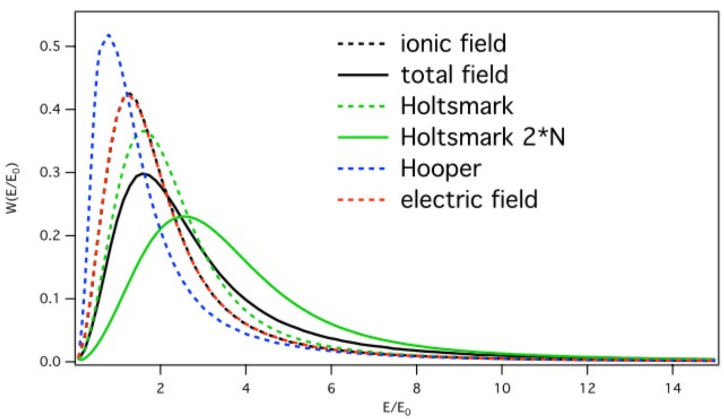
$$l(t) = -\vec{d}\cdot(\vec{E}_l^{\,i}(t) + \vec{E}_l^{\,e}(t))$$

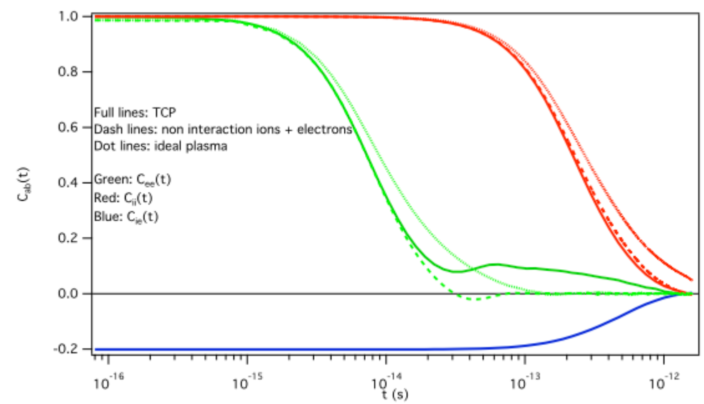
Electric dipole approx.

Plasma broadening – Stark broadening

Numerical simulation has played an increasingly important and unique role.

- Simulate a representative set of electric fields (ionic and electronic) with the correct statistical properties, using particle simulation method intended to provide trajectories in the "phase space" of plasma particles (MD, independent quasi-particles,...):



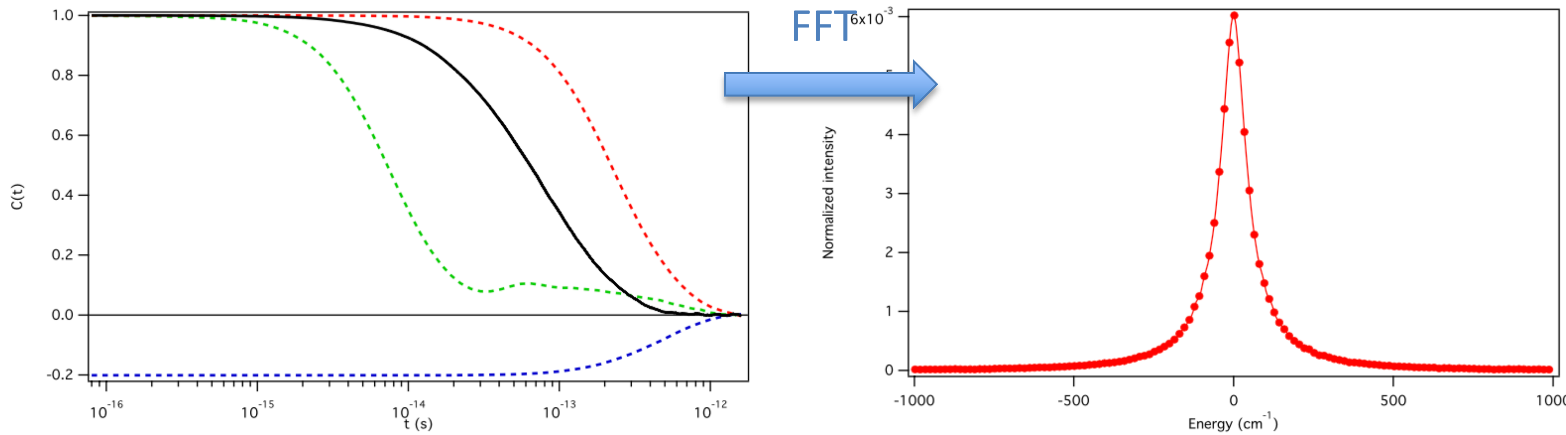


Field measured on hydrogen in proton + electron plasma at N_e = 1x10^{18} cm^{-3} and $T_e = T_i$ = 1 eV.

- Solve the Schrödinger equation describing the time evolution of the emitter's wave functions in the presence of the time-dependent electric field,

Plasma broadening – Stark broadening

- Calculate $C_l(t)$ for several 10^3 different field histories chosen to be statistically independent. $C(t) = \{C_l(t)\}_{av}$ is then a simple algebric average over the number of histories.



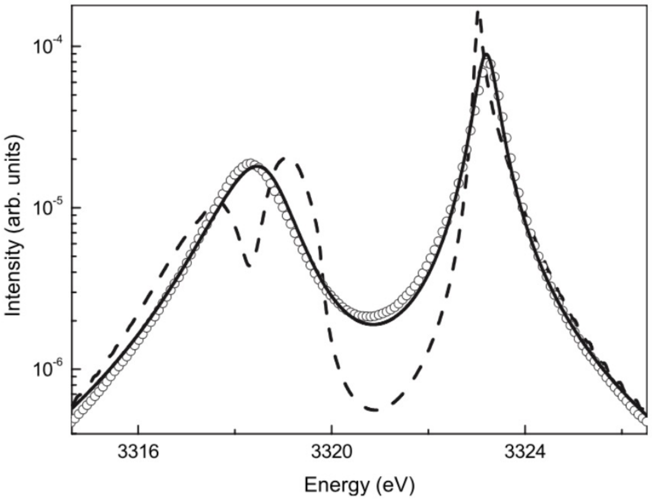
Balmer alpha line ($n = 3 \rightarrow n = 2$) of neutral hydrogen in protons + electrons at $N = 1x\ 10^{18}$ cm^{-3} and $T = 1$eV.

A narrow *C(t)* means a broad line shape and vice versa

C(t) is a measure of ***memory loss***.

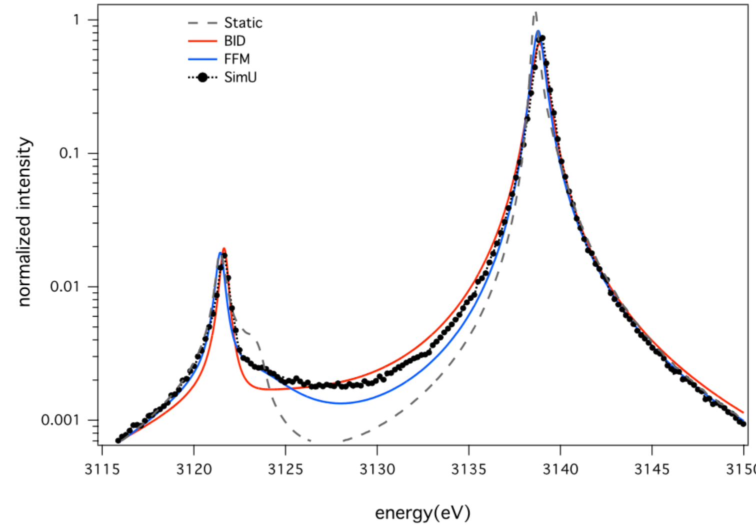
The simulation results are used as data of ideal experiments.

ICF implosion core plasmas applications:
Argon Lyman−α lines for Te =1 keV and Ne=1.5×10^{23} cm^{-3}



Frequency Fluctuations Model (FFM) compared to Molecular Dynamics simulations.
(A.Calisti et al., Phys. Rev. E 81, 016406 (2010))

He-α line for T = 1 keV and N_e=$5\text{x}10^{23}$ cm^{-3}



BID (C. Iglesias et al.) and FFM (A. Calisti et al.) compared to SimU line shape simulations (E. Stambulchik et al.)
(S. Ferri et al., *Atoms 2*, 299-318 (2014))

H-α lines

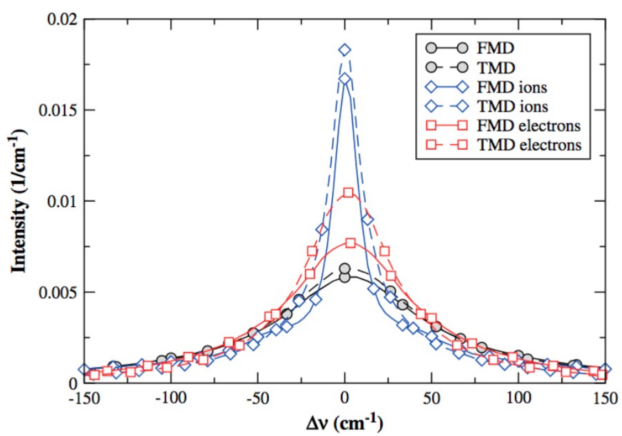


Fig. 1. Comparison of the FMD and TMD results. The contributions of ions and electrons are given separately. The line shapes are area-normalized. Here and in the other figures, $N_e = 10^{18}$ cm^{-3} and $T_e = T_i = 1$ eV are assumed.

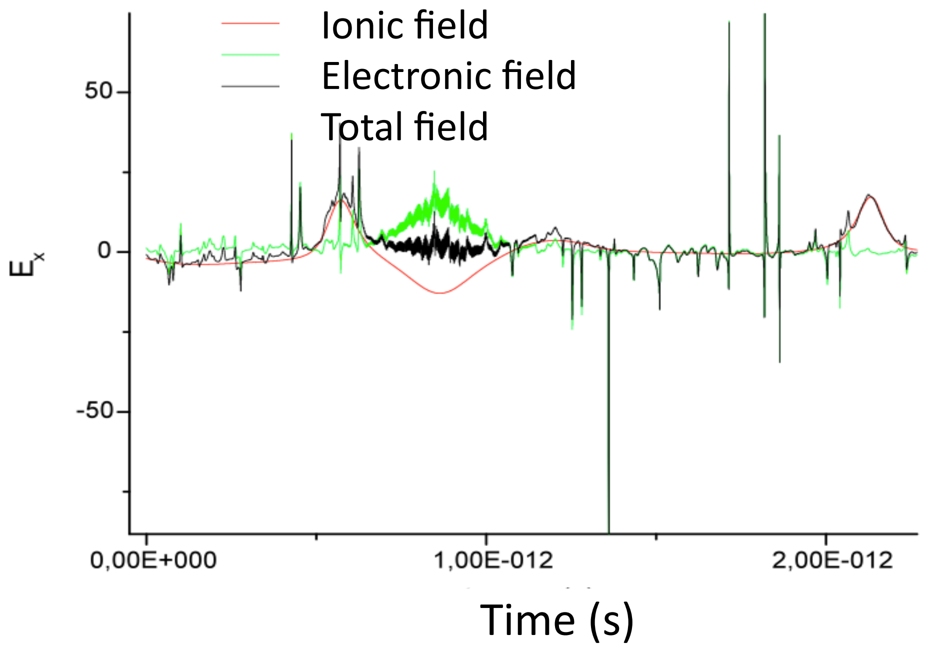
For the investigation on plasma effects, different plasma models can be simulated.
(E. Stambulchik et al., HEDP 3, 272 (2007))

- Interacting ions + electrons simulations: FMD
- Independent ions+ electrons simulations: TMD
- Interacting ions + electrons simulations: FMD-ions
- Interacting electrons + electrons simulations: FMD-electrons
- Independent ions simulations: TMD-ions
- Independent electrons simulations: TMD-electons

Plasma broadening – Stark broadening

But simulation is very time-consuming and therefore limited to small atomic systems.

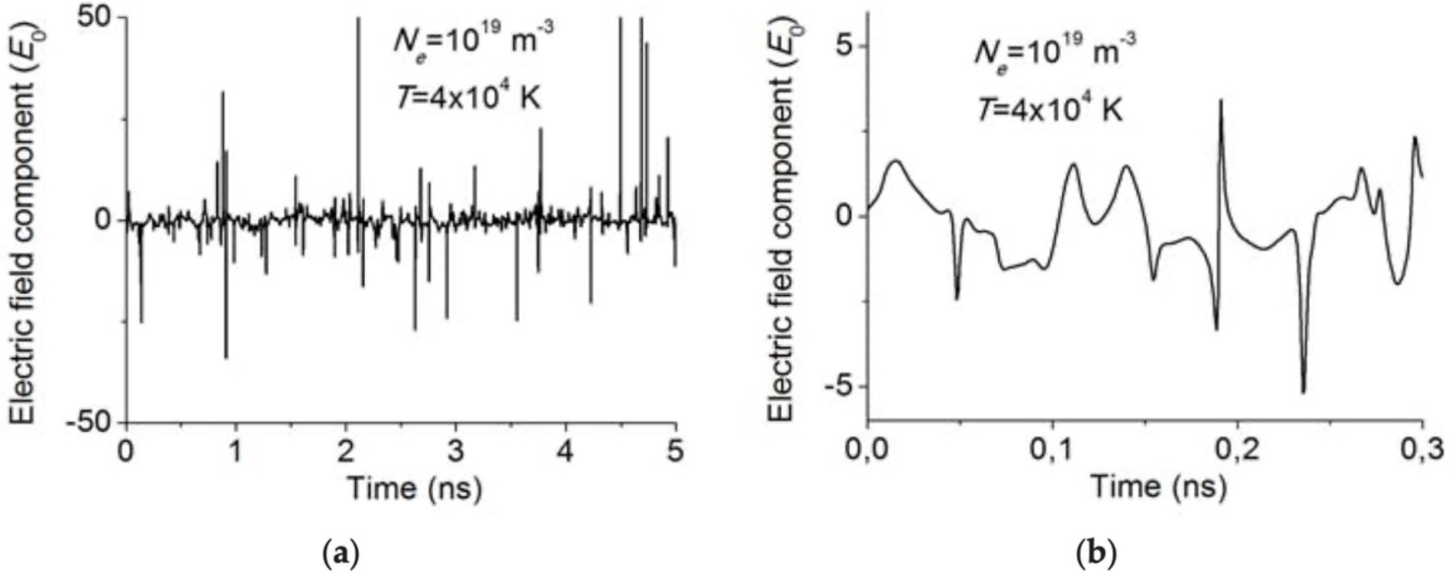
Approximations are then necessary to solve the stochastic equation.



The characteristic times of the fluctuations of the electronic and ionic fields are very different.
Thus the two effects are treated separatly by two different models.

- Impact approximation for electrons
- Quasi static approximation for ions

Plasma broadening – Stark broadening



Electric field component in units of E_0 in a plasma with a density $N_e = 10^{19}$ m^{-3}, and a temperature $T = 40{,}000$ K, during (**a**) a time interval of the order of the time of interest for the L_α line, and (**b**) a time interval of the order of the time of interest for the H_β line.

But beware: an approximation that may be valid for one spectral line may not be valid for another under the same plasma conditions. The study of field fluctuations is not enough.

Plasma broadening – Stark broadening

Impact approximation

Memory loss is produced incrementally each collision contributes its share, which is normally small.

Essentially this approximation works by taking advantage of the fact that e^- collisions are either weak or dominated by a single strong collision, which means there is no many-body problem.

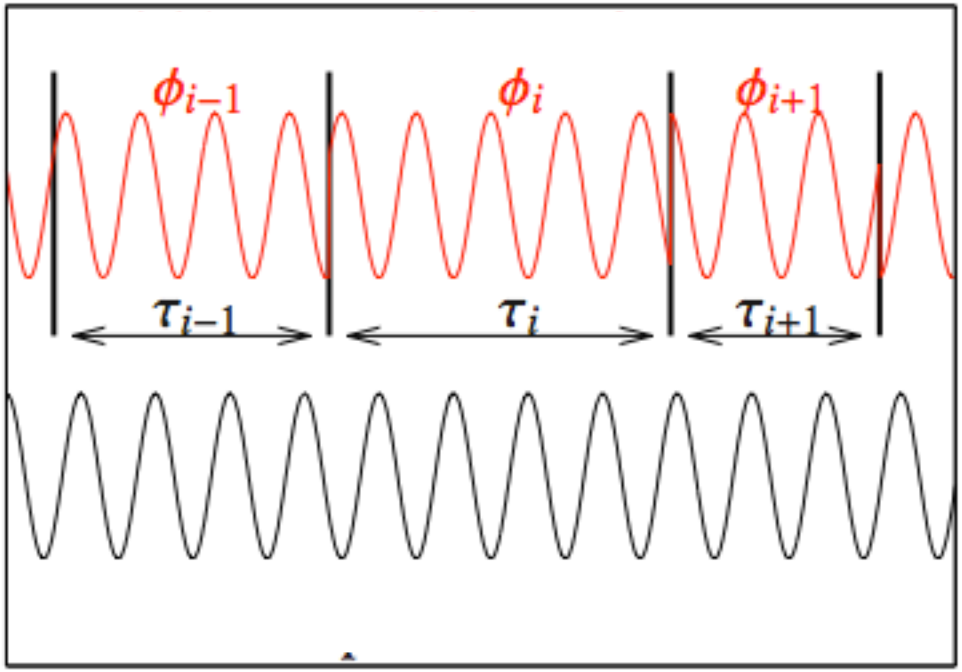
- Strong collision model. They are isolated in time. They completely interrupt the train wave.

- Weak collision model. Individual collisions are not able to break the coherence. The lost of correlation is due to cumulative effect.

Plasma broadening – Stark broadening

Impact approximation

Strong collision model



$$f(t) \propto \exp(-i(\omega_0 t + \phi))$$

The duration of wave trains follows:

$$W(t) = \frac{1}{\tau} e^{-t/\tau}$$

thus

$$C(t) = e^{(i\omega_0 - \frac{1}{\tau})t}$$

and

$$I(\omega) = \frac{1}{\pi} \frac{\gamma}{(\omega - \omega_0)^2 + \gamma^2}$$

with

$$\gamma = \frac{1}{\tau}$$

Similar to the result obtained for natural line broadening.
The profile is lorentzian and homogeneous

Plasma broadening – Stark broadening

Impact approximation

Strong collision model

τ Is the typical time between collisions so γ is the collision frequency. It is given by:

$$\gamma = \frac{1}{\tau} = N\sigma < v >$$

Where N is the perturber density, <v> is the thermal velocity and σ the collisional cross section.

$$\sigma = \pi r_W^2$$

With r_W the Weisskopf radius which determines an effective cross section corresponding to collisions yielding coherence loss of the atomic wavefunction.

$$r_W = \frac{\hbar n^2}{m_e < v >}$$

n is the principal quantum number of the upper level

Plasma broadening – Stark broadening

Impact approximation

Weak collision model

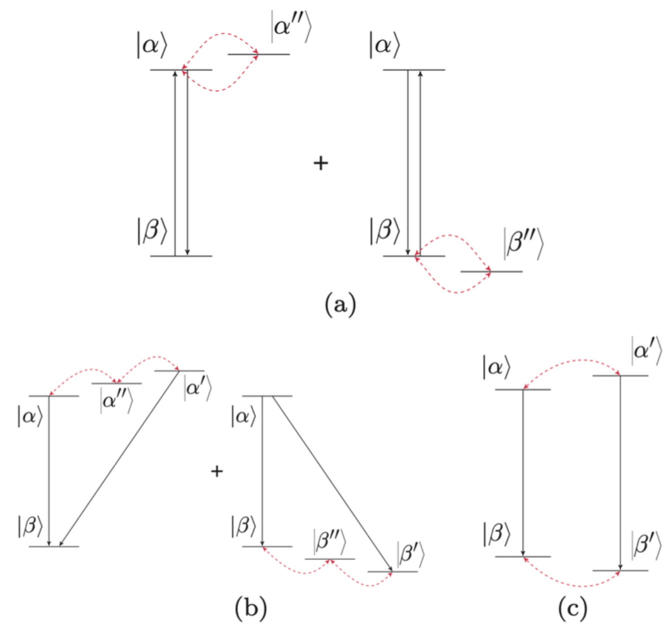
- Collision duration << C(t) time scale
- $\{U(t)\}$ = $\{_0 \Rightarrow\}_t$ Each particle independently collides during one Δt
- Then find an intermediate time scale Δt >> collision duration and << *1/HWHM* (half width at half maximum)
- $\{_0 \Rightarrow\}_t = \{_0 \Rightarrow\}_{\Delta t} \ \{_{\Delta t} \Rightarrow\}_{2\Delta t} \cdots\cdots \{_{t-\Delta t} \Rightarrow\}_t = \{_0 \Rightarrow\}_{\Delta t}{}^{t/\Delta t}$
- Since $\Delta t << t$, $t = N\Delta t$, with $N \rightarrow \infty$. Then $\{_0 \Rightarrow\}_{\Delta t} = 1 - \Phi\Delta t = 1 - \dfrac{\Phi t}{N}$
- and $\{_0 \Rightarrow\}_t = (1 - \dfrac{\Phi t}{N})^N = \exp(-\Phi t)$
- C(t) = exp(-Φt)

Taylor-expand around Δt=0

Plasma broadening – Stark broadening

Electronic phenomenological collision operator

$$\Phi_{\alpha\alpha'\beta\beta'} = \sum_{\alpha''} \delta_{\beta\beta'} \vec{d}_{\alpha\alpha''} \cdot \vec{d}_{\alpha''\alpha'} G(\Delta\omega_{\alpha''\beta})$$
$$+ \sum_{\beta''} \delta_{\alpha\alpha'} \vec{d}_{\beta'\beta''} \cdot \vec{d}_{\beta''\beta} G(-\Delta\omega_{\alpha\beta''})$$
$$- \vec{d}_{\alpha\alpha'} \cdot \vec{d}_{\beta'\beta} \left[G(\Delta\omega_{\alpha\beta'}) + G(-\Delta\omega_{\alpha'\beta}) \right]$$



$$G(\Delta\omega) = -\frac{4\pi}{3}\left(\frac{2m}{\pi k_B T_e}\right)^{1/2} n_e \left(\frac{\hbar}{m}\right)^2 \left(C + \frac{1}{2}\int_y^\infty e^{-x}\frac{dx}{x}\right)$$

$$y = \left(\frac{\hbar n^2}{2z}\right)^2 \frac{\omega^2 + \omega_p^2 + \omega_{\alpha\alpha''}^2}{E_H k_B T}.$$

In the neighborhood of the radiated line center (Δω = 0) the impact limit is reached and G(Δω) tends to the constant value.

Earl W. Smith and C. F. Hooper, Phys. Rev. 157, 126 (1967).
Hans R. Griem, Milan Blaha, and Paul C. Kepple, Phys. Rev. A 19, 2421 (1979).

Plasma broadening – Stark broadening

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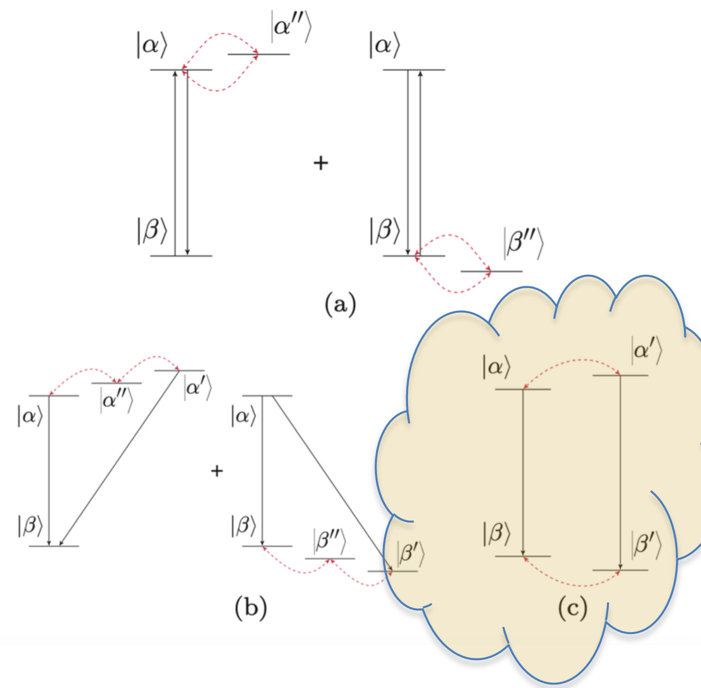
$$\boxed{- \vec{d}_{\alpha\alpha'} \cdot \vec{d}_{\beta'\beta} \left[G(\Delta\omega_{\alpha\beta'}) + G(-\Delta\omega_{\alpha'\beta})\right]}$$



Interference terms

$$G(\Delta\omega) = -\frac{4\pi}{3}\left(\frac{2m}{\pi k_B T_e}\right)^{1/2} n_e \left(\frac{\hbar}{m}\right)^2 \left(C + \frac{1}{2}\int_y^\infty e^{-x}\frac{dx}{x}\right)$$

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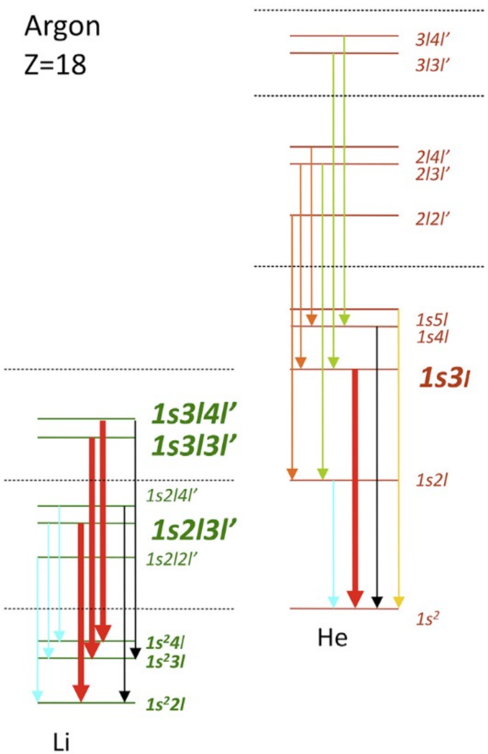
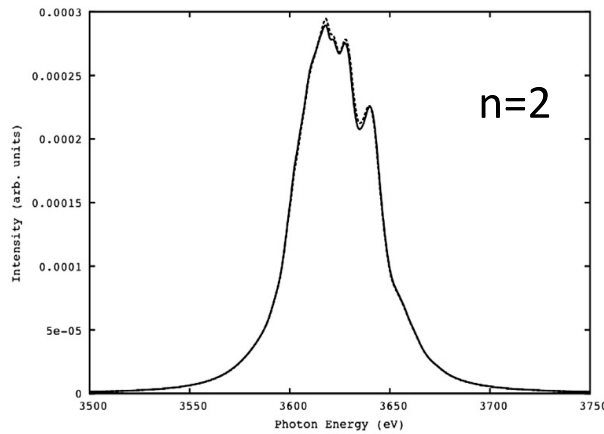
Plasma broadening – Stark broadening

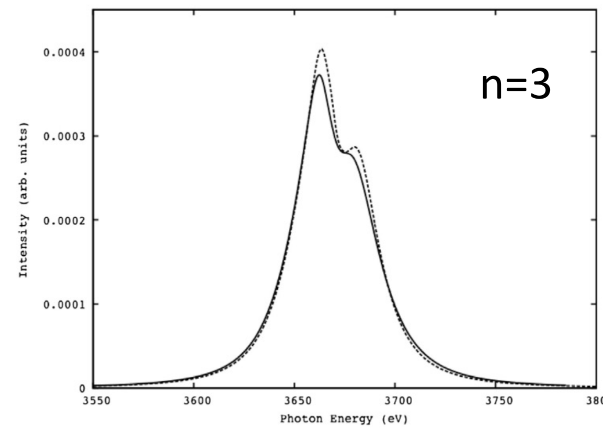
Electronic phenomenological collision operator

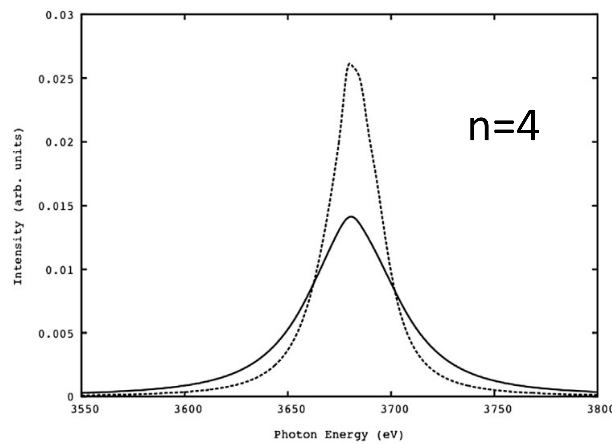
Interference effect

Line with spectator electron







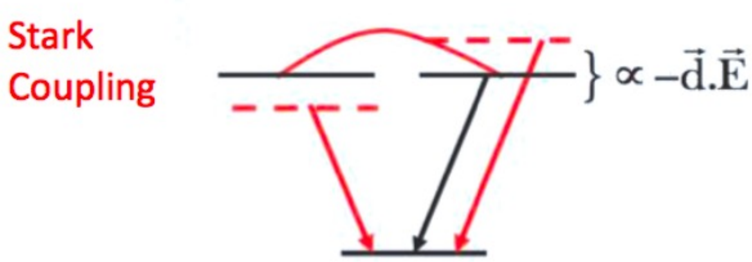


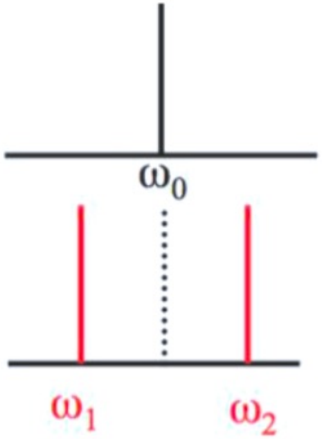
Li-like satellites to the Ar He-β line.
N_e=1x10^{24} cm^{-3} , T_e=1 keV

R.C. Mancini et al, HEDP 9, 731 (2013)

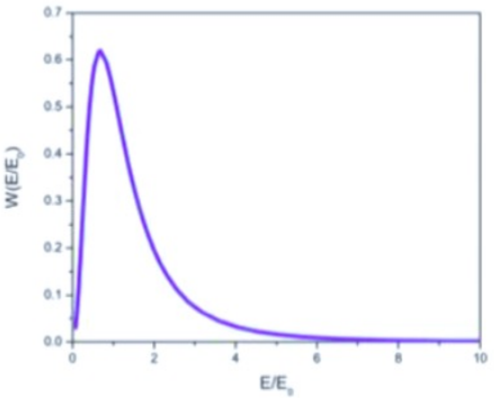
Plasma broadening – Stark broadening

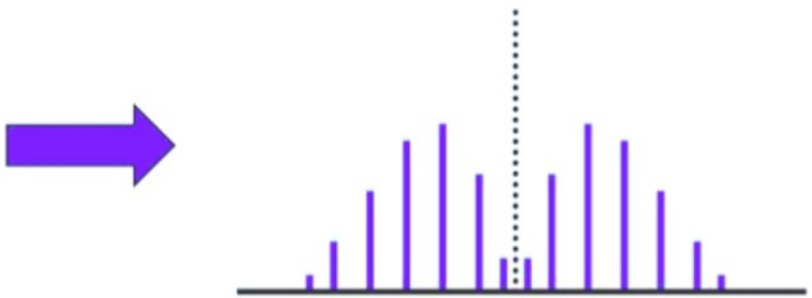
Quasi-static approximation





$$I_S(\omega) = \sum_E W(E) I_E(\omega)$$





Ionic microfield distribution function, $E_0 \propto N_e^{2/3}$

Static profile

Plasma broadening – Stark broadening

Quasi-static approximation

The microfield distribution $Q(\vec{F})$ is defined as the probability density of finding an electric field $\vec{F}$ equal to $\vec{F}_i$ at particle i equal to at particle i.

$$Q(\vec{F}) = \langle \delta(\vec{F} - \vec{F}_i \rangle,$$

For an isotropic plasma, the distribution $W(F)$ of field strengths is

$$W(F) = 4\pi F^2 Q(\vec{F})$$

It is convenient to introduce the dimensionless quantity:

$$\beta = F/F_0$$

with F_0 the normal field strength.
Finally, the distribution $W(\beta)$ is a normalized distribution:

$$\int_0^\infty W(\beta) d\beta = 1$$

Plasma broadening – Stark broadening

Holtsmark model

Quasi-static approximation

- Ensemble of statistically independent pertubers.
- The microfield at the position of the radiators is the superposition of the microfields created by all the perturbers.

$$W(\beta) = \frac{2\beta}{\pi} \int_0^\infty x \cdot sin(\beta x) \cdot e^{-x^{3/2}} dx$$

- The quasi-static line shape is:

$$L_{QS}(\omega) = \int_0^\infty dF \; W(F) L(\omega, F)$$

- Considering $\Delta\omega = \omega - \omega(F_i)$,

$$L_{QS}(\Delta\omega) d(\Delta\omega) \propto W(\beta) \frac{d\beta}{d\Delta\omega} d(\Delta\omega)$$

That leads to line shape with wings $\sim (\Delta\omega)^{-5/2}$.

J. Holtsmark, Ann. d. Phys. 58, 577 (1919)

Plasma broadening – Stark broadening

Quasi-static approximation

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- The quasi-static line shape is:

Beware of the strong approximation!!!

$$\ldots) = \int_0 \quad dF \;\; W(F) L(\omega, F)$$

- Considering $\Delta\omega = \omega - \omega(F_i)$,

$$L_{QS}(\Delta\omega) d(\Delta\omega) \propto W(\beta) \frac{d\beta}{d\Delta\omega} d(\Delta\omega)$$

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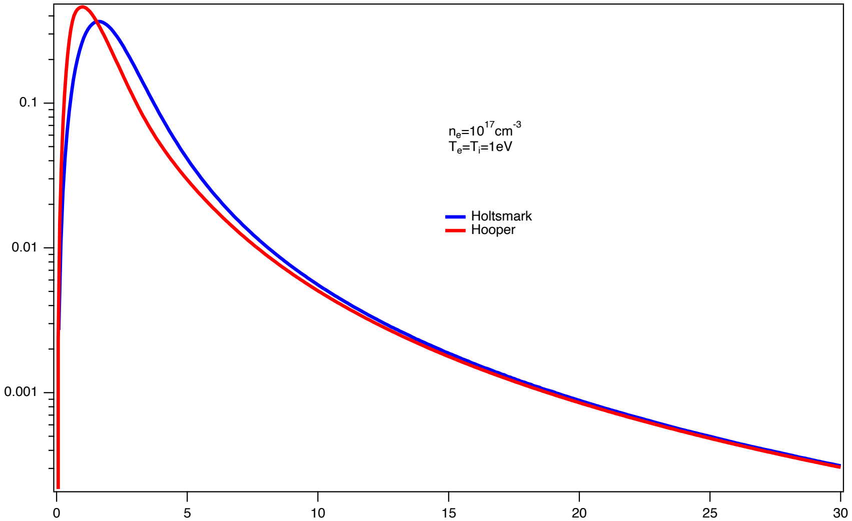
Plasma broadening – Stark broadening

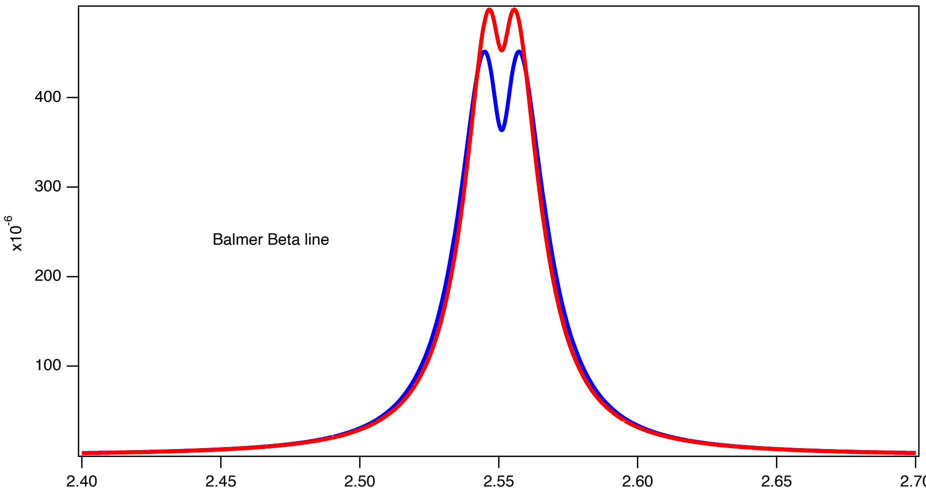
Holtsmark model



Comparisons between Holtsmark and Hooper's distributions

Quasi-static approximation

Hydrogen plasma – $n_e=1x10^{17}cm^{-3}$, $T_e=1eV$



The microfield distribution function can to be calculated by using the APEX method, Hooper or numerical simulations (MD, MC).

C. F. Hooper, Jr., Phys. Rev. 149, 177 (1966); 165, 21 (1968).

C.A. Iglesias, et al., Phys. Rev. A31, 1698 (1985)

M.S. Murillo et al., Phys. Rev. E55, 6289 (1997)

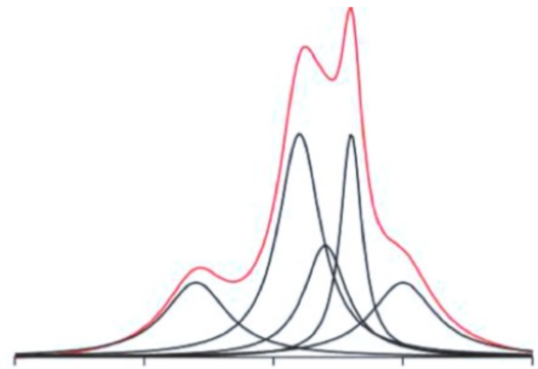
A. Calisti et al., HEDP 50, 101084 (2024)

Plasma broadening – Stark broadening

Quasi-static ions

+ electronic impact broadening:

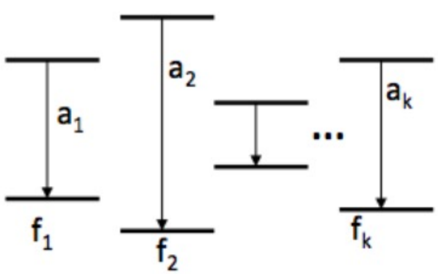
$$\Phi \propto \frac{N_e}{\sqrt{T_e}} \vec{d}.\vec{d}$$



Inhomogeneous profile:
Sum of Lorentzians

$$I_s(\omega) = \frac{1}{\pi} \Re \int_0^{\infty} dE \; W(E) \int_0^{\infty} dt \; e^{i\omega t} \ll \vec{d}^{\dagger} | e^{-i(L_0 - \frac{1}{\hbar} d_z E - i\phi)t} | \vec{d} \rho_0 \gg .$$

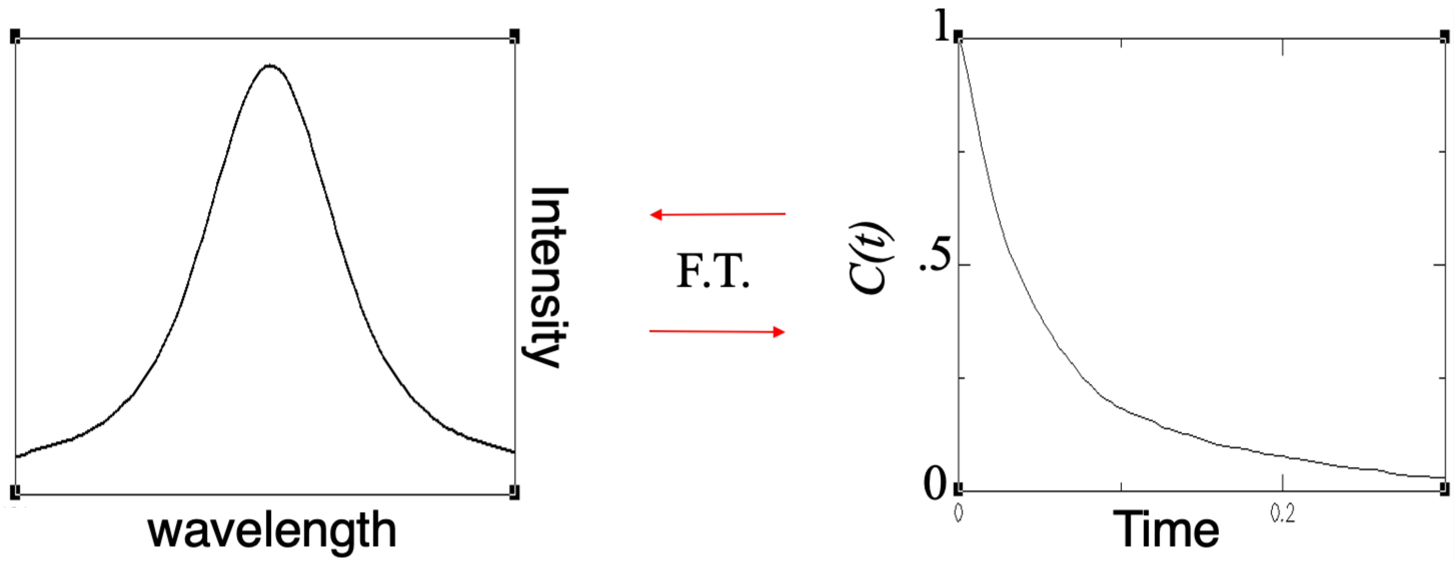
The profile is expressed as a sum of Stark components :



$$I_s(\omega) = \sum_{k=1}^{N} \frac{c_k(\omega - f_k) + a_k \gamma_k}{(\omega - f_k^2) + \gamma_k^2}.$$

Plasma broadening – Stark broadening

Ion dynamics effect



For short times, ions do not have sufficient time to move appreciably, so field is effectively static

Whether static theory is valid or not, depends on whether $C(t)$ decays sufficiently before ions have time to move appreciably.

The decay is determined by all broadening mechanisms:
– ions, electrons, Doppler, etc.

If electrons are not effective *enough*, $C(t)$ can take a long time to decay, long enough that ions can move appreciably.

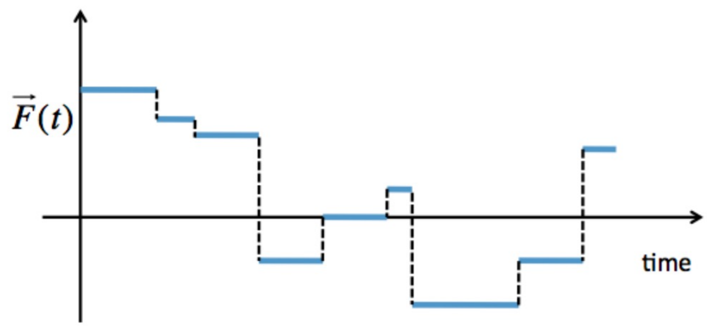
Plasma broadening – Stark broadening

Ion dynamics effect

The main difficulty in introducing the ion dynamics in the Stark line shape calculations is to develop a model that provides a sufficiently accurate solution of the evolution Equation in the intermediate, nonstatic, nonimpact cases.

The model microfield method (MMM) is representative:

This method, developed for neutral emitters in plasmas, is purely analytical.
It requires the history functions for the ion field to belong to a well-defined measurable stair-function space or, equivalently, it requires the time-dependent field fluctuations to obey a particular Markov process, the kangaroo process, that enables an exact resolution of the SLE.



$$\langle U(\omega)\rangle_{\mathrm{MMM}} = \langle U_{\mathrm{St}}(\omega + \mathrm{i}\nu)\rangle + \langle \nu U_{\mathrm{St}}(\omega + \mathrm{i}\nu)\rangle \langle \nu I - \nu^2 U_{\mathrm{St}}(\omega + \mathrm{i}\nu)\rangle^{-1} \langle \nu U_{\mathrm{St}}(\omega + \mathrm{i}\nu)\rangle$$

U. Frisch and A. Brissaud, JQSRT 11, 1753(1971)

Plasma broadening – Stark broadening

Ion dynamics effect

The Boercker, Iglesias, Dufty model (BID) is representative too:

Can be viewed as a general formulation of the MMM. An advantage of this general formulation is that it is easily extended to charged radiators, and approximation methods from transport theory can be applied.

$$I(\omega) = -\frac{1}{\pi}\mathrm{Im}\left\langle d^* \left| \frac{\int dFQ(F_i)G_{BID}(\omega,F_i)}{1+i\nu(\omega)\int dFQ(F_i)G_{BID}(\omega,F_i)} \right| d\rho_0 \right\rangle$$

$$G_{BID} = (\omega - H_0 + d\cdot F_i - i\nu(\omega))^{-1}$$

$\nu(\omega) = \nu/(1+i\omega\tau)$ is the "jump frequency" for the microfield, where ν and τ are the low- and high-frequency limits of the momentum autocorrelation function.

$$C_{FF}(t) = < \vec{F} \cdot \vec{F}(t) > = < F^2 > \left\{ \frac{\omega_+ e^{-\omega_+ t} - \omega_- e^{-\omega_- t}}{\omega_+ - \omega_-} \right\}$$

$$< F^2 > = \gamma < F^2 >_{OCP} = 4\pi n T \gamma$$

where:

$$\omega_\pm = \frac{\nu}{2}\left[1 \pm \sqrt{1 - \frac{4\gamma\omega_p^2}{3\nu^2}}\right]$$

D. Boercker, C. Iglesias and J. Dufty, PRA 36, 2254 (1987)

Plasma broadening – Stark broadening

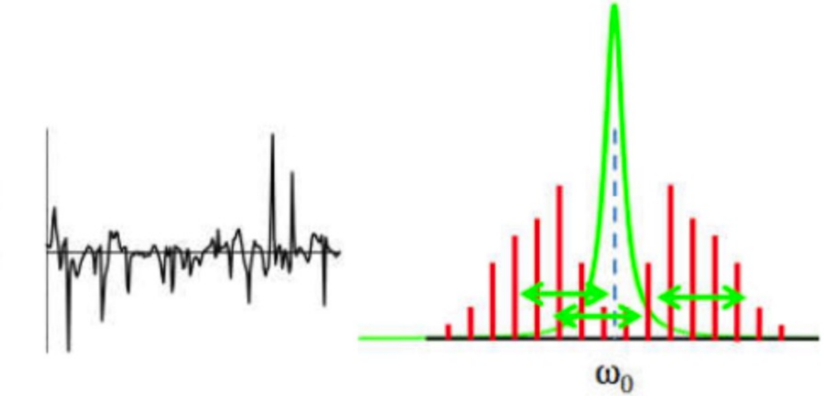
Ion dynamics effect

Another approach is the frequency fluctuation model (FFM), on which the PPP code and, recently, the QC-FFM code rely.

The FFM is based on the premise that a quantum system perturbed by an electric microfield behaves like a set of field dressed two-level transitions, the Stark dressed transitions (SDT).

If the microfield is time varying, the transitions are subject to a collision-type mixing process induced by the field fluctuations.

A Markov process is used to mix the static frequencies.



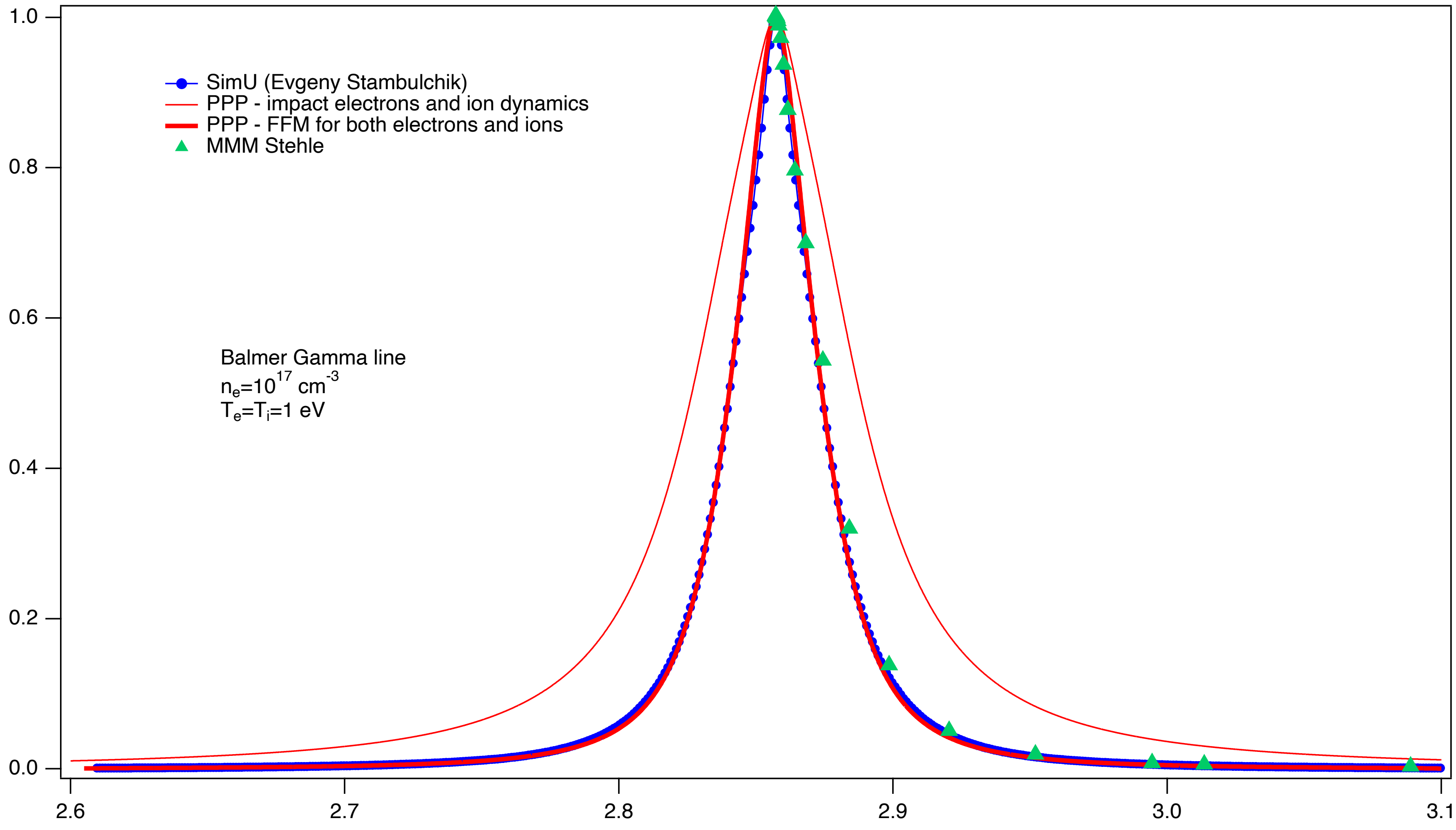
$$I_d(\omega) = \frac{r^2}{\pi} Re \frac{\sum_k \frac{(a_k + ic_k)/r^2}{\nu + \gamma_k + i(\omega - \omega_k)}}{1 - \nu \sum_k \frac{a_k/r^2}{\nu + \gamma_k + i(\omega - \omega_k)}}.$$

Here, the mixing rate ν is related to the characteristic time of the field fluctuations, $\nu = v/r_0$

B. Talin et al., PRA 51, 1918 (1995)
A. Calisti et al., PRE 81, 016406 (2010)

Plasma broadening – Stark broadening

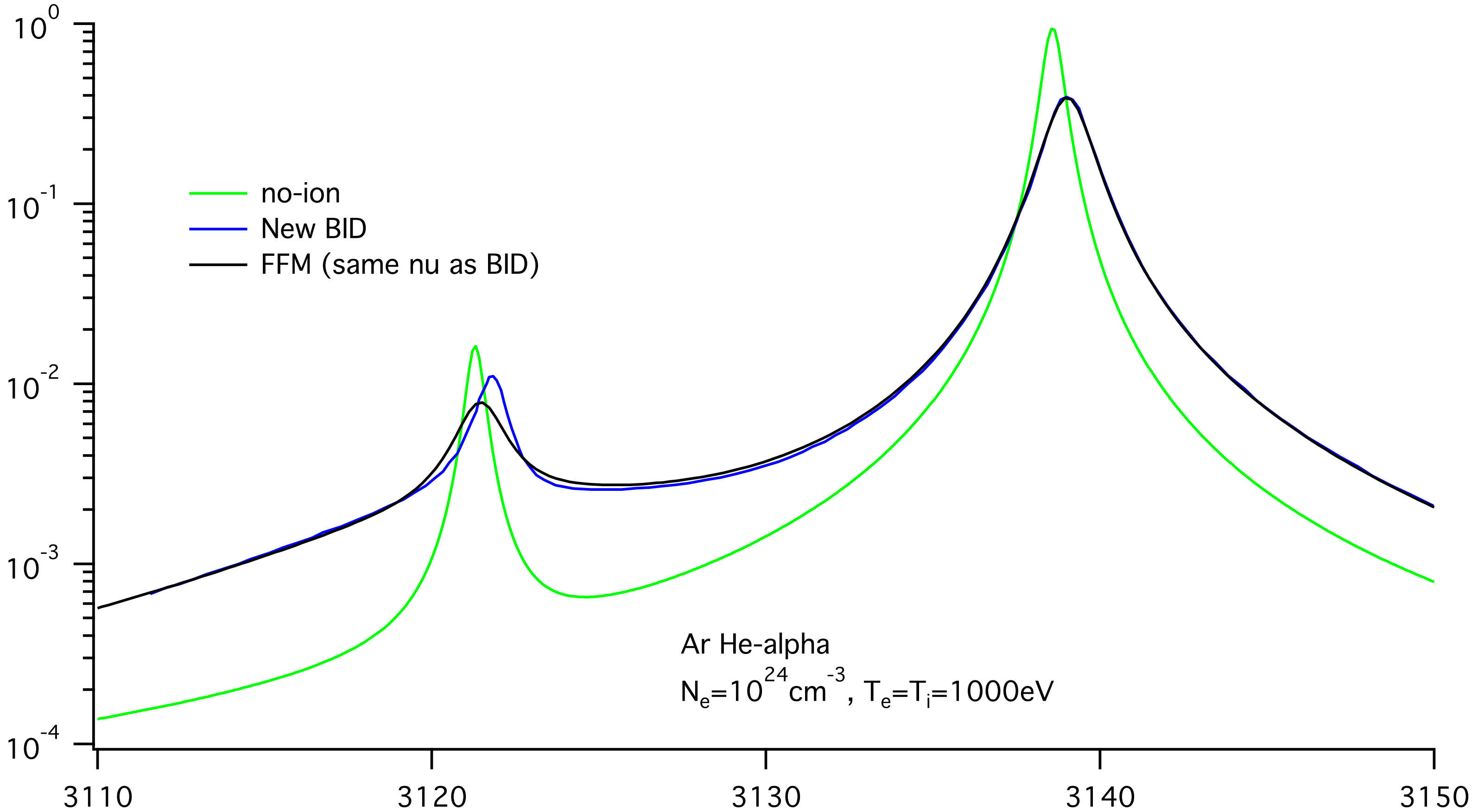
Ion dynamics effect



In this case, the full impact approximation for electrons is not valid.
It is necessary to take into account the dependence of Φ in ω.

Plasma broadening – Stark broadening

Ion dynamics effect



If they use the same ν they compare very well

Plasma broadening – Stark broadening

Ion dynamics effect

Models to solve the ion dynamics:

MMM

tabulated Stark-broadening profiles for H lines:

C. Stehlé and R. Hutcheon, Astron. Astrophys. Suppl. Series 140, 93 (1999).

B.W. Acon et al., Spectrochimica Acta Part B: Atomic Spectroscopy 56, 527 (2001).

QuantST.MMM S. Lorenzen, Plasmas. Contrib. Plasma Phys., 53, 368 (2013).

BID

MERL R. C. Mancini et al., Plasmas. Comput. Phys. Commun, 63, 314322 (1991).

MELS C.A. Iglesias, High Energy Density Phys. 6, 399 (2010).

FFM

PPP: A. Calisti, Phys. Rev. A 42, 5433 (1990).

PPP_B: S. Ferri, Phys. Rev. E 84, 026407 (2011).

QC-FFM: E. Stambulchik et al., AIP Conf Proc 1438, 203 (2012).

FST: S. Alexiou, HEDP 9, 375, (2013).

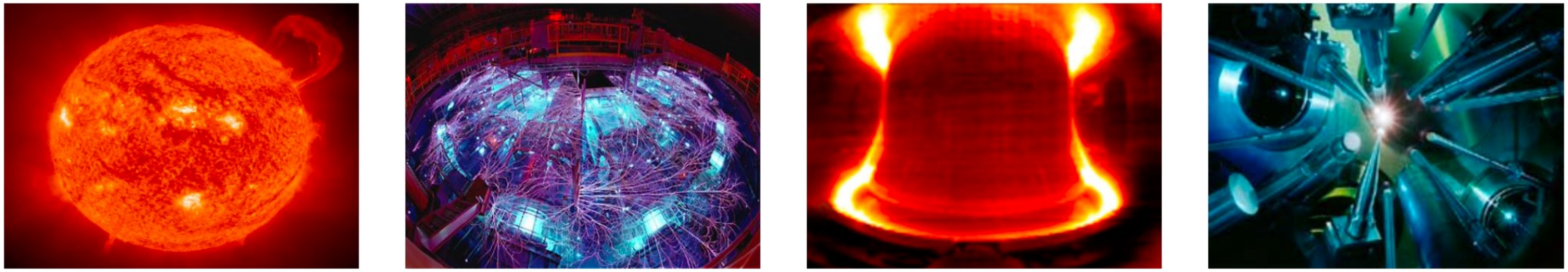
QuantST.FFM S. Lorenzen, Plasmas. Contrib. Plasma Phys., 53, 368 (2013).

ZEST: F. Gilleron et al., Atoms 6, 11 (2018).

ALICE: E.G. Hill et al., HEDP 26, 56 (2018).

Plasma broadening – Stark-Zeeman broadening

Generalities



The presence of static magnetic field is common for many types of plasmas and revives the interest for modeling the line shapes affected simultaneously by Stark and Zeeman effects.

A magnetic field has three essential effects on Stark-broadened spectral lines :

- partial polarization of the emitted light : $I(\omega, \alpha) = I_{//}(\omega) cos^2\alpha + I_{\perp}(\omega) sin^2\alpha$,
- additional splitting due to the coupling of the magnetic field to the magnetic moment of the atom : $V_M = -\vec{\mu} \cdot \vec{B}$,
- bending of the electron trajectories into a helical path around magnetic lines of forces.

Plasma broadening – Stark-Zeeman broadening

Generalities

Different methods have been developed or extended to magnetic plasmas since the initial work of **Nguyen Hoe et al.**,(*JQSRT,* **7**, *429 (1967)*).

based on the Standard / Unified / Advanced theories :

- **G. Mathys**, *A&A,* **141**, *248 (1984)*.
- **L. D'yanchkov et al.**, *PSFC/RR-99-9. (1999)*.
- **A. Derivianko and E. Oks**, *PRL,* **73**, *2059 (1994)*.
- **M.L Adams et al.**, *PRE,* **66**, *06613 (2002)*.
- **X. Li et al.**, *JQSRT,* **76**, *31 (2003)*.

based on models accounting for ion dynamics :

- **S. Günter and A. Könies**, *JQSRT,* **62**, *425 (1999)*.
- **C. Stehlé**, *EPJD,* **11**, *491 (2000)*.
- **L. Godbert-Mouret et al.**, *JQSRT,* **71**, *365 (2001)*.
- **S. Ferri et al.**, *PRE,* **84**, *026407 (2011)*.
- **S. Ferri et al**., Matter Radiat. Extremes 7, 015901 (2022)

based on numerical simulations :

- **E. Stambulchik et al.**, *JQSRT,* **99**, *730 (2006)*.
- **M. Gigosos and M. González**, *JQSRT,* **105**, *533 (2007)*.
- **J. Rosato et al.**, *PRE,* **79**, *046408 (2009)*.

Plasma broadening – Stark-Zeeman broadening

Generalities

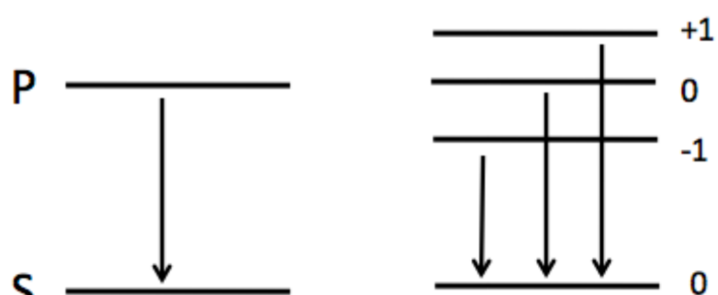
Hamiltonian corresponding to the Stark and Zeeman effect :

$$H(t) = H_0 - \vec{d} \cdot \vec{F}(t) + \mu_B \vec{B} \cdot \ [\vec{L} + g_s \vec{S}]$$

the perturbations are treated in the following approximations :

Strong-field approximation

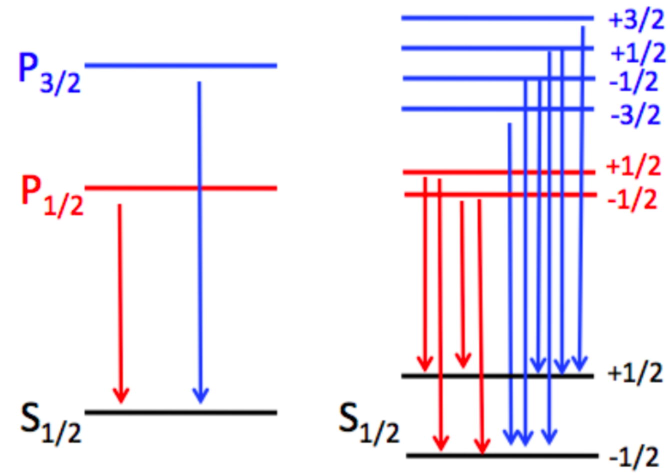
$$H_B = \mu_B B_z (m_l + 2m_s) + \xi m_l m_s$$



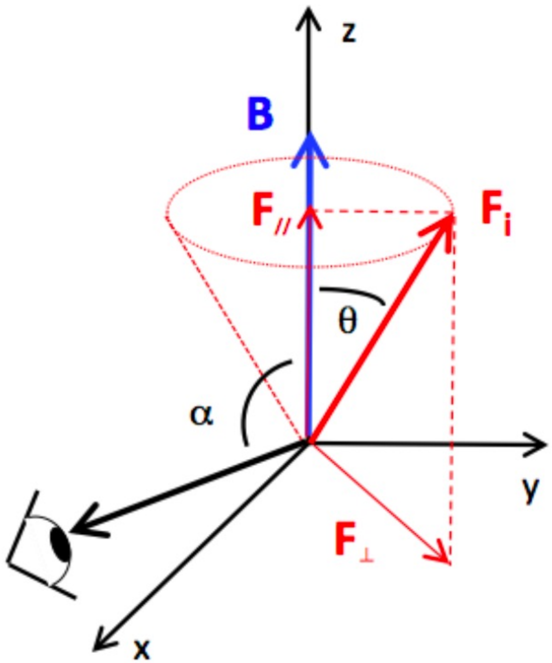
Weak-field approximation

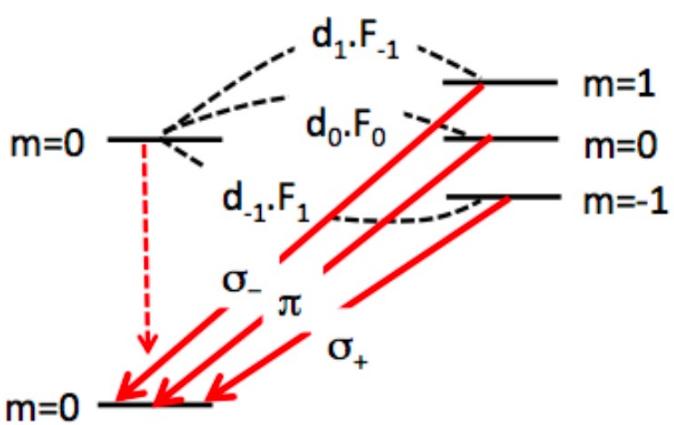
$$H_B^{diag} = \mu_B B_z \ g_{LS} \ m_J$$

$$H_B^{off} = \mu_B B_z \ < nlsjm|...|nlsj{-}1m >$$



Geometry imposed by the external magnetic field





- The 3 directions of space have to be considered for the electric field :

$$F_{//} = F_i \times \mu \text{ and } F_\perp = F_i \times \sqrt{(1-\mu^2)},$$

with $\mu = cos\theta$

- The selection rules for electric dipole radiation are :

$$\begin{aligned} \Delta m &= \pm 1, \sigma \text{ components} \\ \Delta m &= 0, \pi \text{ components} \end{aligned}$$

- The static line intensity associated to each polarization state is :

$$I_{q,s}(\omega) = \int_0^\infty W(F_i) \int_{-1}^{+1} J_q(F_i, \mu; \omega) d\mu dF_i,$$

with $q = 0, \pm 1$

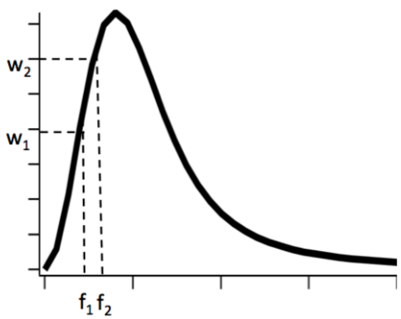
Plasma broadening – Stark-Zeeman broadening

Generalities

Integration over the electric field

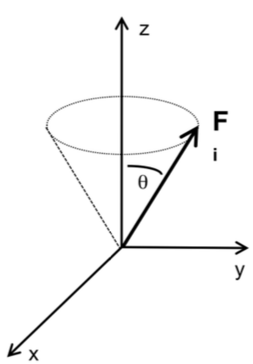
$$I_{q,s}(\omega) = \sum_{f}^{n_f} W_f^{(2)} \sum_{\mu}^{n_{GL}} W_{\mu}^{(G)} J_q(f, \mu; \omega),$$

- two-point integration weights, $W_f^{(2)}$:



$$dw = \frac{1}{2}(w_1 + w_2)(f_2 - f_1)$$

- Gauss-Legendre quadrature weights, $W_{\mu}^{(G)}$: $\int_a^b f(x)\overline{w}(x)dx$



if $[a, b] = [-1, 1]$ then $\overline{w}(x) = 1$ and

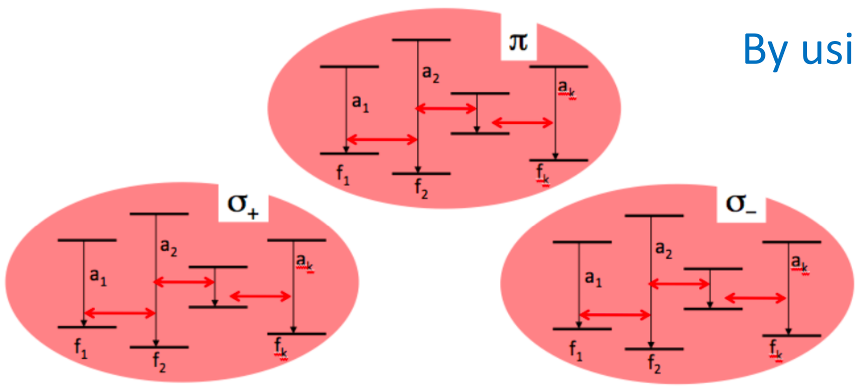
$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i f(x_i) \quad \text{with} \quad w_i = \frac{-2}{(n+1)P_n'(x_i)P_{n+1}(x_i)}$$

Plasma broadening – Stark-Zeeman broadening

Generalities

For each radiative transition :

By using the FFM for example.



- Static line profiles :

$$I_{s,q}(\omega) = \sum_{k=1}^{n_k} \frac{c_k(\omega - f_{q,k}) + a_{q,k}\gamma_{q,k}}{(\omega - f_{q,k})^2 + \gamma_{q,k}^2} \text{ with } n_{q,k} = n_f \times n_e \times n_g \times n_{GL}$$

- Dynamic line profiles :

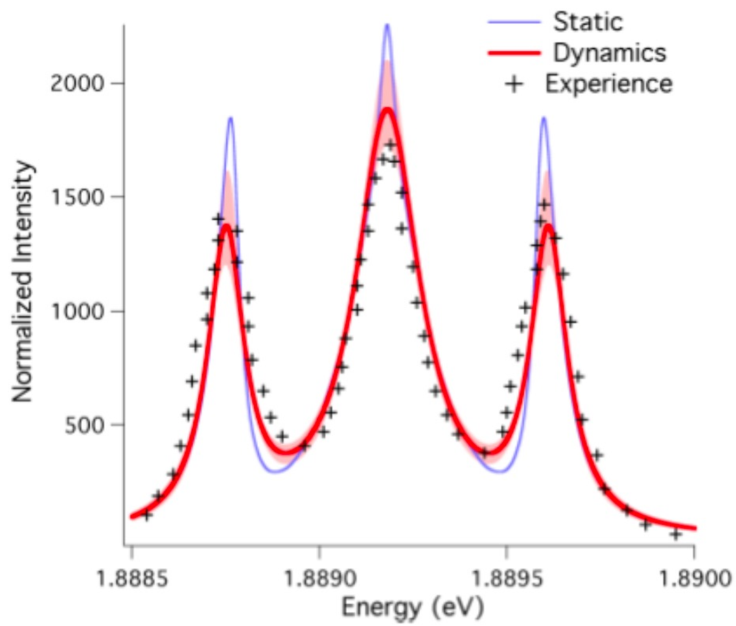
$$I_{d,q}(\omega) = \frac{r_q^2}{\pi} Re \frac{\sum_k \frac{(a_{q,k}+ic_{q,k})/r_q^2}{\nu+\gamma_{q,k}+i(\omega-\omega_{q,k})}}{1-\nu\sum_k \frac{a_{q,k}/r_q^2}{\nu+\gamma_{q,k}+i(\omega-\omega_{q,k})}}$$

Plasma broadening – Stark-Zeeman broadening

Generalities

Magnetic Fusion Plasma.

Comparison with Alcator C-Mod MARFE D-α experimental line.



$$N_e = 1.2 \times 10^{15} cm^{-3}, kT_e = 1\text{eV and } B = 7T$$

S. Ferri et al. PRE 84, 026407 (2011).

Plasma broadening – Stark-Zeeman broadening

Generalities

The Zeeman effect in intermediate coupling is accounted for by the atomic-physics code MASCB that generates B-field-dependent atomic-physics quantities.

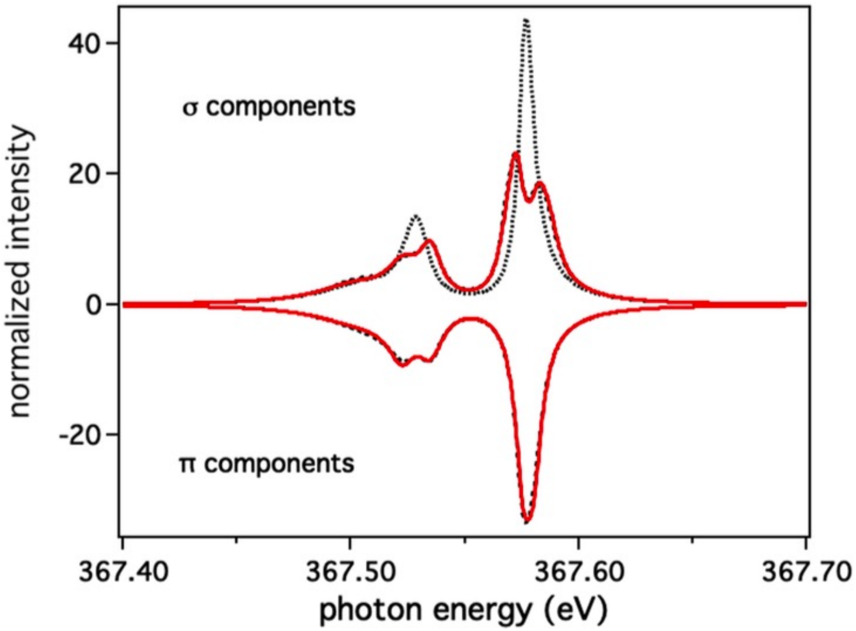


FIG. 3. SZ Lyman-α line profiles of C VI, using the weak-field (dashed) and intermediate-field (solid) approximations for $B = 100$ T, $N_e = 5 \times 10^{19}$ cm^{-3}, $T_e = 100$ eV. The short-dashed line corresponds to the pure Stark profile.

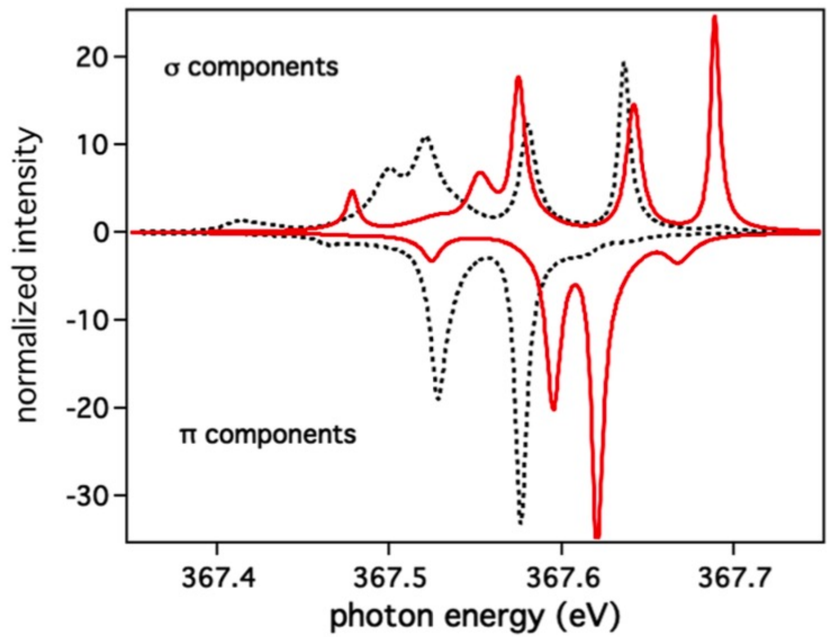


FIG. 5. As Fig. 3 but for $B = 10^3$ T.

S. Ferri et al. Matter Radiat. Extremes 7, 015901 (2022)

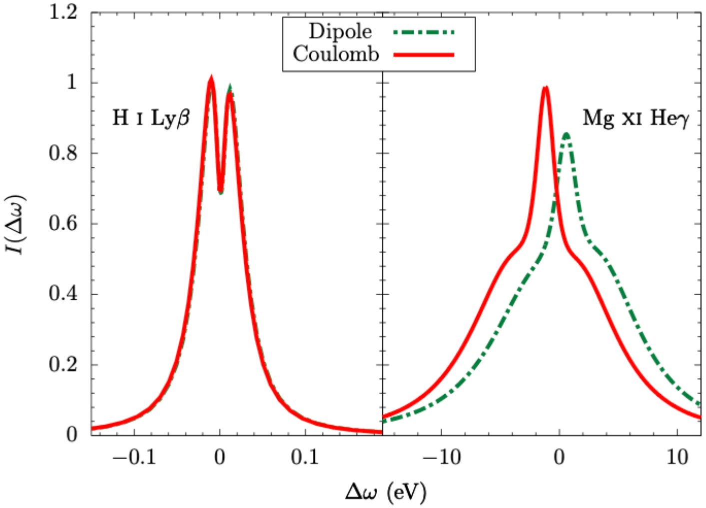
Plasma broadening – Conclusion

The idea that codes can provide exact profiles should be given up.

Besides the numerical traps, any lineshape calculation involves a series of necessary approximations.

Numerous approximations:

1. The Electric Dipole Approximation
2. Factorization of the Density Matrix
3. Screening Approximations
4. Classical Approximation
5. Static-Ion Approximation
6. Second-Order Approximation
7. Binary-Collision Approximation
8. Impact Approximation ......



T. Gomez et al.
Introduction to Spectral Line Shape Theory

More work is needed

Who are the line broadeners

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Evgeny Stambulchik: Faculty of Physics, Weizmann Institute of Science, Rehovot, Israel

And many others!

Spectral Line Shapes in Plasmas Workshops

http://plasma-gate.weizmann.ac.il/slsp/

Except for limiting cases, line-shape calculations imply a usage of computer codes of varying complexity and requirements of computational resources. However, studies comparing different computational and analytical methods are almost nonexistent. This workshop purports to fill this gap. By detailed comparison of results for a selected set of case problems, it becomes possible to pinpoint sources of disagreements, infer limits of applicability, and assess accuracy.

Scientific committee

- A. Calisti (CNRS, France)
- H.-K. Chung (IAEA, Austria) / C. Hill (IAEA, Austria)
- M. Á. González (U. of Valladolid, Spain) / M.A. Gigosos (U. of Valladolid, Spain)
- E. Stambulchik (WIS, Israel)

A forum has been created for discussions: http://plasma-gate.weizmann.ac.il/slsp/phpbb/

SLSP7 in Gran Canaria in October 2024.

Spectral Line Shapes in Plasmas Workshops

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M.A. Gigosos (U. of Valladolid, Spain)
E. Stambulchik (WIS, Israel)

The choice of themes and cases is currently being discussed on the forum. Some suggestions:

- Neutral perturbers – resonance and/or van der Waals broadening.
- Motional Stark effect – for tokamak and/or magnetized WD conditions.
- Penetration effects in the presence of magnetic field.
- QM vs SC calculations of the Stark broadening in the presence of B –
- QM vs SC calculations for isolated lines, with detailed data to be submitted on partial wave contributions, etc.
- two-photon lineshapes.
- Comparisons with recent experimental data.

http://plasma-gate.weizmann.ac.il/slsp/phpbb/

This lecture has been prepared with the help of various lectures given by others.
In particular:

- « An overview of spectral line broadening », Dick Lee, University of Berkeley (California, USA),
- « HED plasma spectroscopy », Roberto Mancini, University of Reno (Nevada, USA)
- « Atomic and Optical Physics », Wolfgang Ketterle, MITOPENCOURSEWARE,

Massachusetts Institute of Technology (Massachusetts, USA)

- « Spectral Line Broadening », Sandrine Ferri, Aix Marseille University (France)

Special thanks to them