Lineshape modeling for collisional-radiative calculations

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Introduction

- Collisional-radiative (CR) modeling is widely used to diagnose laboratory and astrophysical plasmas through interpreting measured spectra.
- Lineshape analysis is an invaluable tool for plasma diagnostics. It allows for nonintrusively inferring plasma properties.
- In addition, line broadening affects the radiation transfer and, hence, the level populations in non-optically-thin plasmas.
- Therefore, failure to include line broadening in CR calculations may result in severe degradation of their diagnostics power.
- However, accurate lineshape calculations are rather time-consuming; inlcuding them directly in CR calculations is unrealistic.

Computationally effective approximate methods of lineshape modeling—that retain a reasonably good accuracy—are required.

Introduction (cont.)

What is a “reasonably good accuracy”?

Factor $\times 2$ or better in FWHM.

It should usually be sufficient for level population dynamics and qualitative overall spectra. However, FWHM alone is not always sufficient.

Opacity: Line wings are important, especially in astrophysics; radiation energy flow.

Outline of the talk

1. Spectral line broadening by plasmas
   - Line broadening processes
   - Stark effect: Isolated and hydrogenlike lines
2. Isolated lines
   - Baranger formalism
   - ... and a bit beyond
3. Hydrogenlike transitions and intermediate cases
   - “Standard theory”
   - Computer simulations
   - Quasi-contiguous approximation
4. Examples
   - He spectrum
   - $K\alpha$ in WDM
   - Continuum lowering
5. Conclusions

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Processes that affect lineshapes

- Natural broadening (spontaneous radiative decay, autoionization, including the Auger effect):

  $$w_{u\ell} \sim \sum_{\text{relevant phenomena}} (\text{time of life of } |\text{u}\rangle)^{-1} + (\text{time of life of } |\ell\rangle)^{-1};$$

  Lorentzian shape
- Doppler broadening associated with thermal or non-thermal radiator motion:

  $$w_{u\ell} \sim \frac{v}{c}\omega^0_{u\ell}; \text{Gaussian shape for thermal}$$

- Electromagnetic fields
  - Microfields due to the motion of electrons and ions (including impact processes like excitation etc)
  - Macroscopic fields (external or due to collective plasma phenomena, e.g. waves)

This is the complex one... and focus of this talk.

Stark effect :: Isolated and hydrogenlike lines

ΔE_{ij} – distance between dipole-"talking" levels;
$V_{ij} = -d_{ij}F$ – perturbation due to electric field F.
Simple estimates assuming quasistatic picture is valid for perturber at a distance r; binary approximation:

$$w_{st} \simeq \langle \delta E \rangle = \int_{V_1} \delta E(r)\, P(r) dr; \quad P(r)dr = \frac{1}{V_1} 4\pi r^2 dr \equiv 4\pi N_p r^2 dr$$

Quadratic effect ($V_{ij} \ll \Delta E_{ij}$):

$$\delta E(r) = |V|^2/\Delta E \propto |F(r)|^2 \propto 1/r^4$$

$$w_{st} \propto N_p \int \frac{r^2}{r^4} dr \propto N_p r_{min}^{-1} \propto N_p;$$

⇒Short-range (impact) collisions

Linear effect ($V_{ij} \gg \Delta E_{ij}$):

$$\delta E(r) = V_{ij} \propto F(r) \propto 1/r^2$$

$$w_{st} \propto N_p \int \frac{r^2}{r^2} dr \propto N_p r_{max} \propto N_p^{2/3};$$

⇒Long-range "collisions"

Outline of the talk

Broadening of isolated lines

According to [Baranger, 1958], a $u \to \ell$ transition assumes Lorentzian shape with FWHM defined by

$$w = N_e \int_0^\infty vF(v)\mathrm{d}v \left(\sum_{u' \neq u} \sigma_{uu'}(v) + \sum_{\ell' \neq \ell} \sigma_{\ell\ell'}(v) + |f_u(v) - f_\ell(v)|^2 \right),$$

where $F(v)$ is the (Maxwellian) electron velocity distribution, $\sigma_{ik}(v)$ is impact cross section from i to k, and $f_k(v)$ is elastic scattering amplitude.

$$w \equiv w_{\mathrm{in}} + w_{\mathrm{el}}$$

The inelastic part:

$$w_{\mathrm{in}} \equiv N_e \int_0^\infty vF(v)\mathrm{d}v \left(\sum_{u' \neq u} \sigma_{uu'}(v) + \sum_{\ell' \neq \ell} \sigma_{\ell\ell'}(v) \right)$$

or

$$w_{\mathrm{in}} = \sum_{u' \neq u} \langle \sigma_{uu'} N_e v \rangle_v + \sum_{\ell' \neq \ell} \langle \sigma_{\ell\ell'} N_e v \rangle_v$$

Broadening of isolated lines (cont.)

Typically (except for near-threshold energies), $w_{\mathrm{el}} < (\mathrm{or} \ll) w_{\mathrm{in}}$.

$$w \approx w_{\mathrm{in}} = \sum_{u' \neq u} \langle \sigma_{uu'} N_e v \rangle_v + \sum_{\ell' \neq \ell} \langle \sigma_{\ell\ell'} N_e v \rangle_v$$

Compare to the natural broadening:

$$w = \sum_{\text{relevant phenomena}} (\text{time of life of } |\mathrm{u}\rangle)^{-1} + (\text{time of life of } |\ell\rangle)^{-1}$$

Generalizing to other impact mechanisms (ionization, recombination of any kind),

$$w \approx \sum_{\text{all mechanisms}} \text{depop. rate of } |\mathrm{u}\rangle + \sum_{\text{all mechanisms}} \text{depop. rate of } |\ell\rangle$$

N.B.:

All these rates are calculated anyway in CR models.

Broadening of isolated lines (cont.)

One caveat

If the partial width w_{ik} of level i due to level k becomes comparable to ΔE_{ik}

$$\langle \sigma_{ik} N_e v \rangle_v \simeq \Delta E_{ik},$$

the isolated line assumption is no longer valid.

Continuing using the Baranger formalism will bring unphysical results (overestimated broadening).

A simple solution: $w_{ik} = \min\{\langle \sigma_{ik} N_e v \rangle_v, \Delta E_{ik}\}$

(A better approach will be discussed below).

Outline of the talk

“Standard theory” of line broadening

In the “standard theory” (ST), the ions are usually given a [quasi]static role, while electrons are dynamic (impact):

$$I(\omega) = \frac{1}{\pi} \mathrm{Re}\, Tr \int_0^\infty dF_i W(F_i) \{d^\dagger [i\omega - iH_s(F_i) + \phi_e(F_i)]^{-1} d\}_{av}$$

Alternatively, if applicable, ions may be treated in the impact approximation, like electrons ($\phi_e \to \phi_e + \phi_i$):

$$I(\omega) = \frac{1}{\pi} \mathrm{Re}\, Tr\{\Delta_d [i\omega - iH_0 + \phi_e + \phi_i]^{-1}\}_{av}$$

Intermediate cases?

Ion dynamics

Significant disagreements between theory and experiments in shapes of Lyman and Balmer α and β. Hints for ion motion.

H_β [Kelleher and Wiese, 1973]

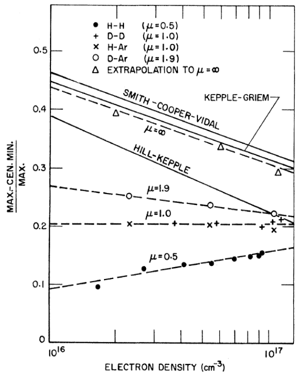
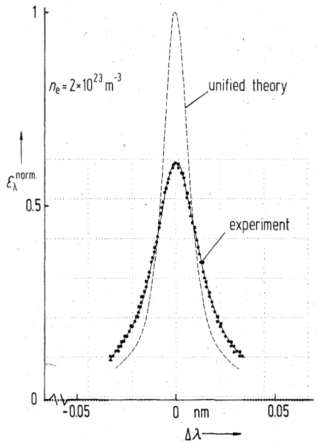


FIG. 3. Relative dip versus electron density for the Smith-Cooper-Vidal (Ref. 2), Kepple-Griem (Ref. 3), and Hill-Kepple (Ref. 10) calculations, as well as the indicated experimental values.

Ly_α [Grutzmacher and Wende, 1977]



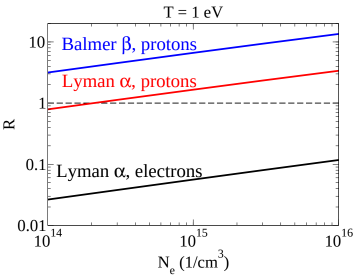
Ion dynamics (cont.)

Ratio between the quasi-static Stark width and the typical frequency of the microfield fluctuations:

$$R = \frac{w_{st}}{w_{dyn}}.$$

$$w_{st} \simeq (\langle d_u - d_\ell \rangle) F_0/\hbar,$$

$$w_{dyn} \simeq \frac{\langle v \rangle}{\langle r \rangle} = \frac{(kT/m_p)^{1/2}}{\left(\frac{4\pi}{3} N_p\right)^{-1/3}}$$



Computer simulations :: description

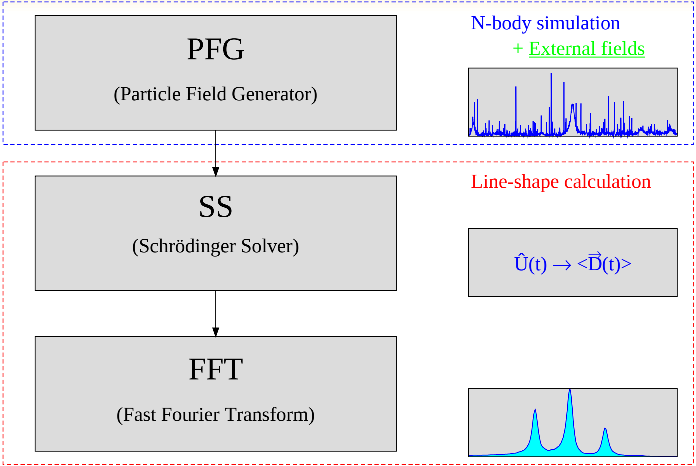
The closest to *ab initio* calculations; since [Stamm and Voslamber, 1979].

The shape of a spectral line is calculated in three steps:

- The perturbing fields are simulated using the Particle Field Generator (PFG), by calculating the motion of a finite number of interacting electrons and ions (of a few types).
- Using this field as a perturbation, the emitter oscillating function is calculated by the Schrödinger Solver (SS).
- The power spectrum of the emitter oscillating function is evaluated using the Fast Fourier Transformation (FFT) method, giving the spectral line profile.

We use a specific implementation [Stambulchik and Maron, 2006].

Computer simulations :: Scheme



Computer simulations :: Method

The Hamiltonian of the atomic system:

$$H = H_\circ + V(t).$$

The perturbation $V(t)$ is due to the plasma electric field (simulated by the PFG) and external electric and magnetic fields. We solve the Schrödinger equation

$$id\Psi(t)/dt = H\Psi(t)$$

using the time-development operator U in the interaction representation:

$$id\bar{U}(t)/dt = V(t)\bar{U}(t).$$

Computer simulations :: Method (cont.)

The evolution of the dipole operator $D(t)$ is then obtained:

$$\vec{D}(t) = U(t)^{\dagger}\vec{D}(0)U(t).$$

The Fourier transform of the dipole operator $\vec{D}(\omega)$ is further used to calculate the line spectrum:

$$I^{\lambda}(\omega) \propto \sum_{i}\sum_{f}\omega_{fi}^{4}|\vec{e}_{\lambda}\cdot\langle\vec{D}_{fi}(\omega)\rangle|^{2}.$$

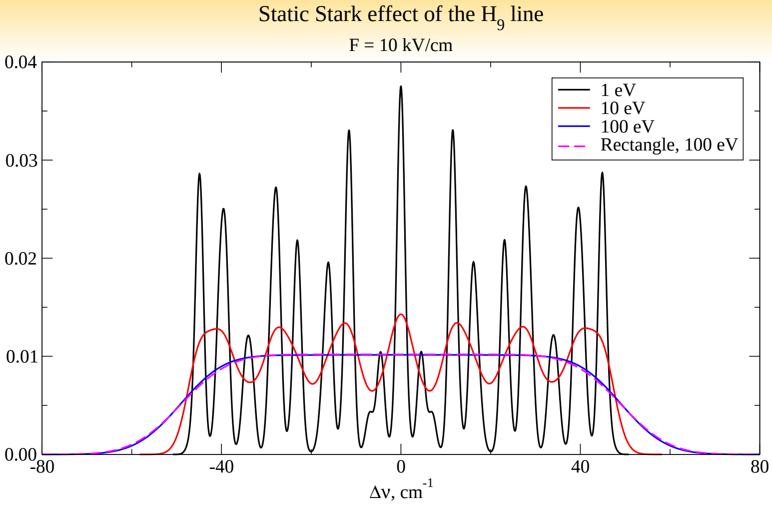
The angle brackets denote an averaging over several runs of the code (which corresponds to the averaging over an ensemble of emitters).

Computer simulations :: Features

- Interactions between plasma particles are included.
- Degenerate and non-degenerate cases are treated correctly within the same framework.
- Ion-dynamical effects are taken into account naturally.
- Addition of external magnetic and electric fields is possible.

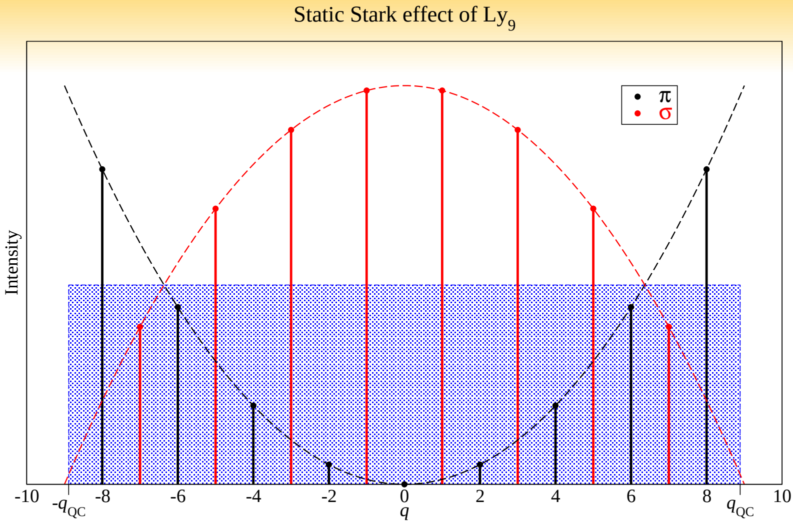
Very powerful but also very computation-resource intensive. Alternatives?

Quasi-contiguous (QC) approximation



What seems to be a rather complex pattern gradually becomes a simple rectangle.

Quasi-contiguous (QC) approximation



Intensities of the π and σ components form two parabolae, which, on average, can be substituted with a simple rectangular shape.

Quasi-contiguous (QC) approximation

Therefore:

$$I_n(\omega) = \begin{cases} \frac{I_n^{(0)}}{2\alpha_n F/\hbar} & \text{for } |\hbar\omega| \le \alpha_n F \\ 0 & \text{for } |\hbar\omega| > \alpha_n F, \end{cases}$$

where $I_n^{(0)}$ is the total line intensity, and α_n is the linear-Stark-effect coefficient:

$$\alpha_n = \frac{3}{2}(n^2 - 1)\frac{ea_0}{Z}.$$

Generalization for $n' > 1$:

$$\alpha_{nn'} = \frac{3}{2}(n^2 - n'^2)\frac{ea_0}{Z}.$$

QC approximation: quasistatic shape

Convolution with a microfield distribution $W(F)$:

$$I(\omega) = I_{nn'}^{(0)} \int_{\hbar\omega/\alpha_n}^{\infty} \frac{W(F)dF}{2\alpha_{nn'}F/\hbar} \equiv I_{nn'}^{(0)} L_{\mathrm{qs}}(\omega),$$

or, with the reduced field strength $\beta = F/F_0$ and detuning $\bar{\omega} = \omega/\Delta_0$,

$$L_{\mathrm{qs}}(\bar{\omega}) = \frac{1}{2} \int_{\beta}^{\infty} \frac{H(\beta)}{\beta} \mathrm{d}\beta,$$

where

$$H(\beta) = W(F)/F_0\ ,$$

$$\Delta_0 = \frac{\alpha_{nn'}F_0}{\hbar}\ \text{, and}$$

$$F_0 = 2\pi \left(\frac{4}{15}\right)^{2/3} Z_p e N_p^{2/3}\ \text{(the Holtsmark field).}$$

QC approximation: quasistatic shape

Ideal plasma ⇒ Holtsmark distribution:

$$H(\beta) = \frac{2}{\pi}\beta \int_0^\infty x \sin(\beta x) \exp(-x^{3/2}) \mathrm{d}x.$$

$$L_{\mathrm{qs}}(\bar{\omega}) = S(\bar{\omega}),$$

where the S function is defined as

$$S(\bar{\omega}) = \frac{1}{\pi} \int_0^\infty \cos(\bar{\omega} x) \exp(-x^{3/2}) \mathrm{d}x.$$

[Stambulchik and Maron, 2008]; also corrections due to moderate plasma coupling.

QC approximation: dynamical effects

Quasi-static width:

$$w_{\rm qs} = 2\bar{\omega}^0_{1/2}\Delta_0 \ .$$

Typical field frequency:

$$w_{\rm dyn} = \frac{\langle v \rangle}{\langle r \rangle} = \sqrt{\frac{kT}{m_p^*}}\left(\frac{4\pi N_p}{3}\right)^{1/3} \ .$$

Introduce a “quasistaticity” factor f:

$$f = \frac{R}{R + R_0},$$

where

$$R = \frac{w_{\rm qs}}{w_{\rm dyn}}$$

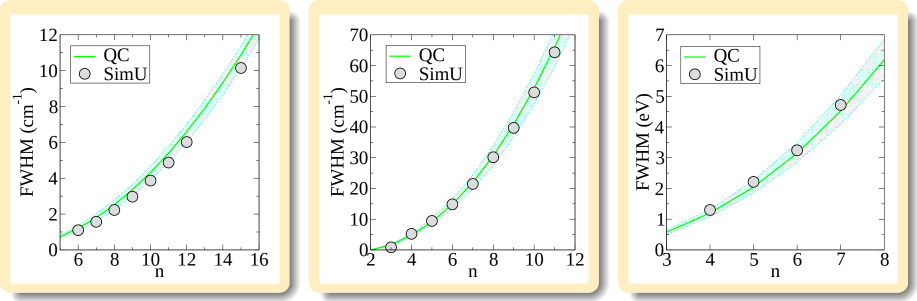
and R_0 is a constant of the order of unity. The full Stark width then

$$w = f\, w_{\rm qs} \to \begin{cases} w_{\rm qs} & \text{for } R \gg 1, \\ \propto w_{\rm qs}^2/w_{\rm dyn} \propto N_p/\sqrt{T} & \text{for } R \ll 1. \end{cases}$$

QC approximation: examples

We compare QC results with results of a computer simulation modeling (SimU) [Stambulchik and Maron, 2006], applied to

- H Balmer lines, $N_e = 1.2 \times 10^{13}$ cm^{-3}, $kT = 0.16$ eV
- D Balmer lines, $N_e = 5 \times 10^{14}$ cm^{-3}, $kT = 4$ eV
- Ne Lyman lines in a D plasma with $N_e = 10^{21}$ cm^{-3}, $kT = 1000$ eV



QC-FFM :: When FWHM is not enough

Applying frequency-fluctuation model (FFM) [Calisti et al., 2010]:

$$L(\bar{\nu};\bar{\omega}) = \frac{1}{\pi}\,\mathrm{Re}\,\frac{J(\bar{\nu};\bar{\omega})}{1-\bar{\nu}J(\bar{\nu};\bar{\omega})}\ ,$$

where

$$J(\bar{\nu};\bar{\omega}) = \int \frac{L_{\mathrm{qs}}(\bar{\omega'})\mathrm{d}\bar{\omega'}}{\bar{\nu}+i(\bar{\omega}-\bar{\omega'})}$$

$$\bar{\nu} \sim w_{\mathrm{dyn}}/\Delta_0$$

For ideal one-component plasma:

$$J(\bar{\nu};\bar{\omega}) = \int_0^\infty \mathrm{d}\tau \exp\left(-\tau^{3/2} - i(\bar{\omega}-i\bar{\nu})\tau\right)\ .$$

[Stambulchik and Maron, 2013].

Non-ideal OCP:

$$J(\bar{\nu};\bar{\omega}) = \int_0^\infty \mathrm{d}\tau\, e^{-i(\bar{\omega}-i\bar{\nu})\tau} C_{\mathrm{qs}}(\tau)\,,$$

where

$$C_{\mathrm{qs}}(\tau) \equiv \mathcal{F}\left\{L_{\mathrm{qs}}(\bar{\omega})\right\}(\tau) = -\,\mathrm{Im}\,\tau^{-1}\mathcal{F}\left\{\beta^{-1}W(\beta)\right\}(\tau).$$

$W(\beta)$ can be provided by computer simulations or a model, e.g., APEX [Iglesias et al., 2000]. Or from an analytical model:

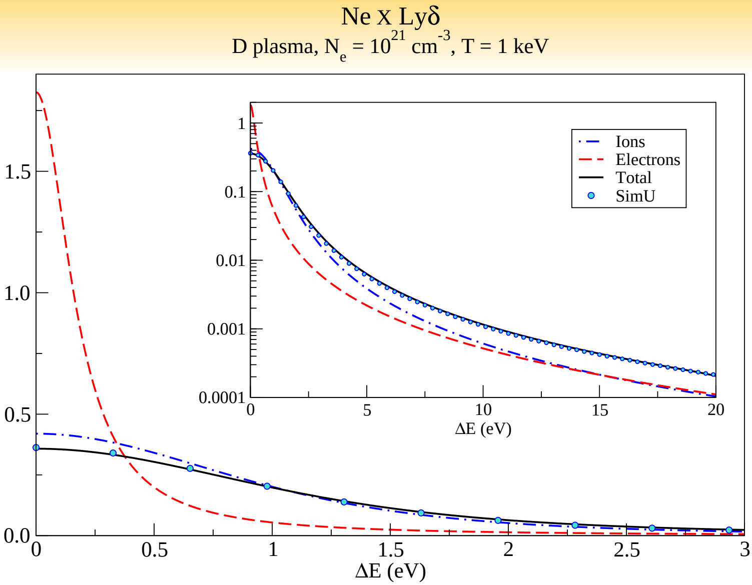
$$W(\beta) = \frac{2}{\pi}\beta \int_0^\infty x\sin(\beta x)\exp\left[-f(x)\right]\mathrm{d}x$$

(ideal plasma ⇒ Holtsmark distribution ⇒ $f(x) \to x^{3/2}$). Then,

$$J(\bar{\nu};\bar{\omega}) = \int_0^\infty \mathrm{d}\tau \exp\left[-f(\tau) - i(\bar{\omega} - i\bar{\nu})\tau\right].$$

A simple 1D integral!

QC + FFM: An example



Application: z-pinch diagnostics, talk of Yitzhak Maron tomorrow.

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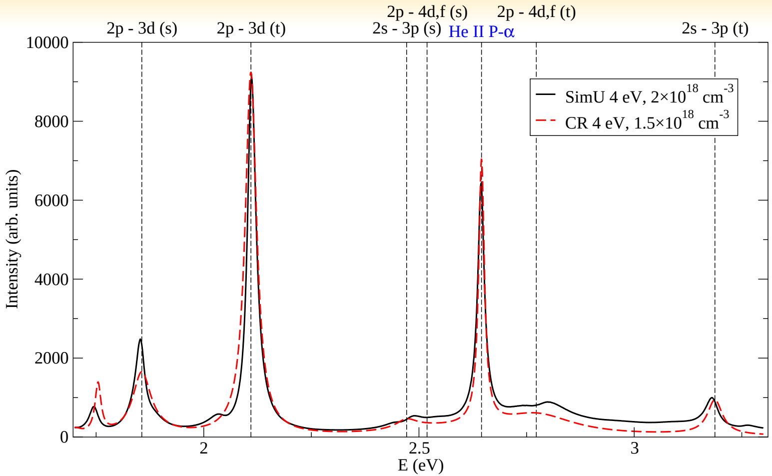
He I/II $n = 3, 4 \rightarrow 2, 3$ transitions

Fitting “ab initio” computer simulation spectrum with CR modeling.

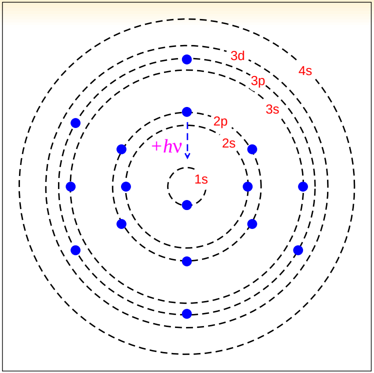


N_e is determined with a 20–30% accuracy.

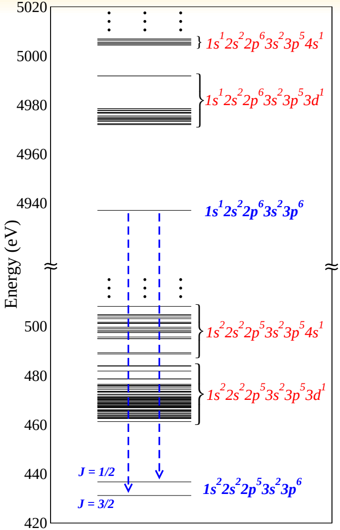
SimU CPU time: 1 week. Lineshapes in CR: $\sim 1\,\mathrm{ms}$.

$K\alpha$ radiation + satellites

Electron shells of Ti

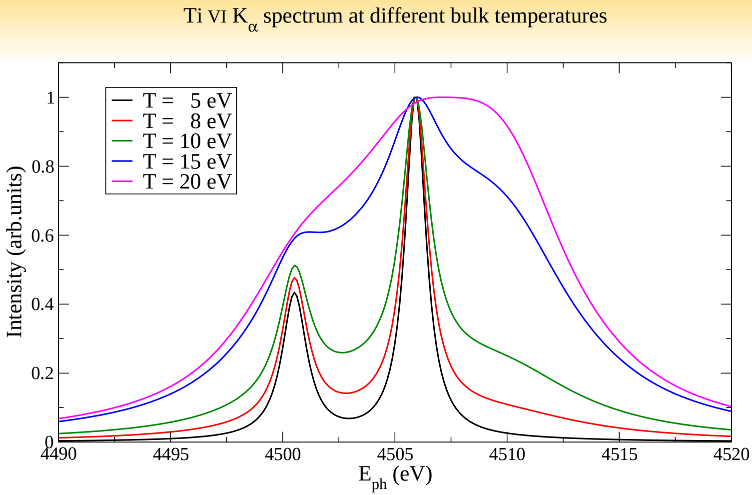


Ti VI inner-shell Grotrian diagram
(using the FAC code of M.F. Gu)



Outer electrons stripped; Ti I → Ti V.
Inner shell ionization → Ti VI.
Finite T → a $3p$ electron excited.

Ti VI $K\alpha$ spectrum



[Stambulchik et al., 2009]. Thousands of unresolved satellites.
Application to diagnostics of WDM: talk of Ulf Zastrau on Thursday.

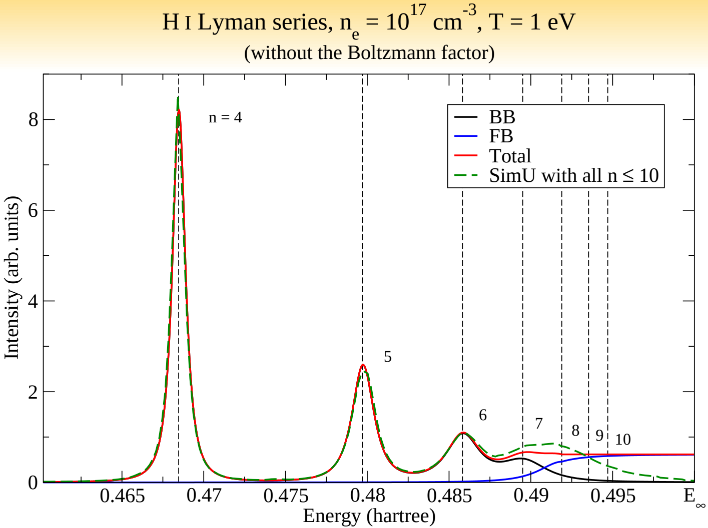
QC-FFM :: High-n series & continuum lowering

The approach (closely following [Griem, 1997]):

- Calculate bound-bound (BB) $n_\ell \to n_u$ shapes for a series of n_u until FWHM exceeds $|E_{n_u} - E_{n_u+1}|$ (the "Inglis-Teller" reasoning).
- (Optional) continue for a few more n_u with the same width.
- Assume the free-bound (FB) edge at the E_{n_u+1} energy.
- Convolve the FB continuum with the last ($n_\ell \to n_u$) BB lineshape.
- Sum up.

No sharp-FB-edge artifacts. No ionization potential depression assumed.

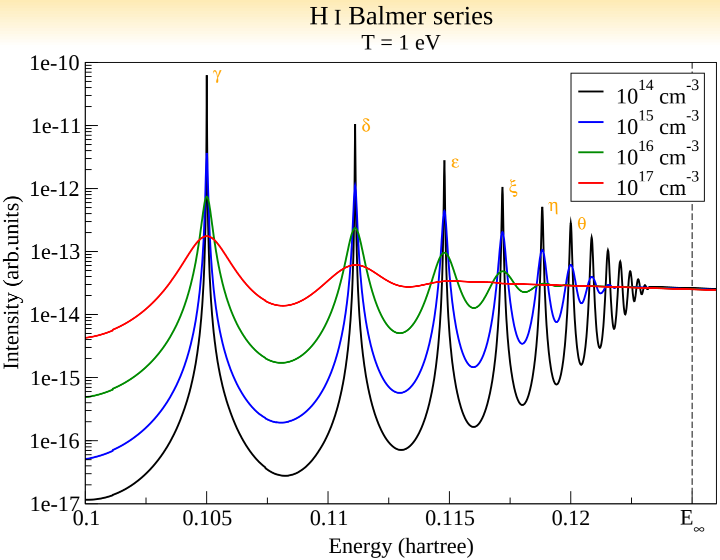
QC-FFM :: High-*n* series & continuum lowering (cont.)



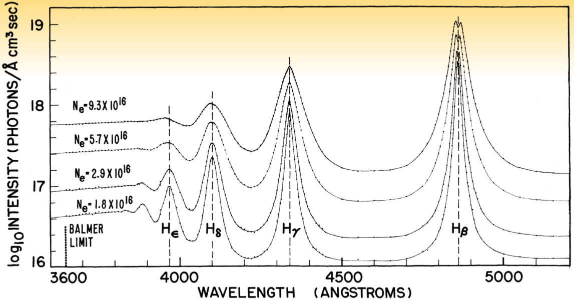
SimU: Hamiltonian with 385 fully interacting states.

SimU CPU time: > 1 month. QC-FFM: $\sim$ 1 sec ($\sim \times 3,000,000$).

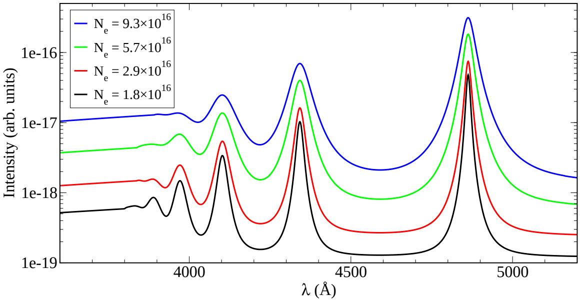
QC-FFM :: High-*n* series & continuum lowering (cont.)



QC-FFM :: High-*n* series & continuum lowering (cont.)



[Wiese et al., 1972]



Outline of the talk

Conclusions

- Lineshape analysis is a very important tool for plasma diagnostics. Lineshapes affect the radiation transfer and level populations.
- Accurate detailed lineshape modeling requires substantial computational resources; but this should not be an excuse to abandon it in CR calculations altogether: Reasonably accurate and very fast approximate methods do exist.
- Use simplified Baranger formalism for isolated lines, quasi-contiguous approximation with frequency-fluctuation model for hydrogenlike transitions, and simple interpolations between the two for intermediate cases.

Thank you!

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