Stellar/Planetary Atmospheres

Part 12: line opacities

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24. Juni 2018

Topics

- line opacities
  - natural line profile, oscillator strength
  - thermal line broadening, Gauss profiles
  - Voigt profile
  - pressure broadening
  - impact approximation
  - statistical theory
  - quasi-static ion broadening (H I)

natural line profile

- classical harmonic oscillator:
- scattering of photons
- equation of motion:

$$m(\ddot{x} + \omega_0^2 x) = eE_0 \exp(i\omega t) - m\gamma\dot{x}$$

- m, e: mass and charge
- E_0: amplitude of driving field
- ω_0: harmonic oscillator frequency
- $\gamma = 2e^2\omega_0^2/3mc^2$: *classical damping constant*

natural line profile

- steady state solution

$$x = \Re\left[\frac{(e/m)E_0 \exp(i\omega t)}{(\omega^2 - \omega_0^2) + i\omega t}\right]$$

and

$$\ddot{x} = \Re\left[\frac{-(e\omega^2/m)E_0 \exp(i\omega t)}{(\omega^2 - \omega_0^2) + i\omega t}\right]$$

natural line profile

- total scattered energy out of the beam

$$< P(\omega) >= \left(\frac{e^4\omega^4}{3m^2c^2} \right) \frac{E_0^2}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}$$

- convert to specific intensities:

$$< P(\omega) >= \sigma(\omega) \int I \, d\Omega = \frac{cE_0^2}{8\pi}\sigma(\omega)$$

if scattering cross-section $\sigma(\omega)$ is isotropic

$$\sigma(\omega) = \frac{8\pi e^4\omega^4}{3m^2c^4} \frac{1}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}$$

natural line profile

- optical wavelengths $\gamma \ll \omega \rightarrow$
- $\sigma(\omega)$ sharply peaked around $\omega = \omega_0$
- $\rightarrow$

$$(\omega^2 - \omega_0^2) = (\omega + \omega_0)(\omega - \omega_0) \approx 2\omega_0(\omega - \omega_0)$$

so that

$$\sigma(\omega) = \frac{\pi e^2}{mc} \frac{\gamma}{(\omega - \omega_0)^2 + (\gamma/2)^2}$$

- $\rightarrow$ *Lorentz profile*

natural line profile

- total cross section:

$$\sigma_{\rm tot} = \frac{\pi e^2}{mc}\int_0^\infty \frac{(\gamma/4\pi)^2\,d\nu}{(\nu-\nu_0)^2+(\gamma/4\pi)^2} = \frac{\pi e^2}{mc}\int_{-\infty}^{\infty}\frac{dx}{1+x^2} = \frac{\pi e^2}{mc}$$

- QM $\rightarrow$ same form for $\sigma(\omega)$ but (vastly) different $\sigma_{\rm tot}$
- $\rightarrow$ write QM results as

$$\sigma_{\rm tot} = \frac{\pi e^2}{mc} f_{ij}$$

- f_{ij}: *oscillator strength*

natural line profile

- classical damping constant (λ in cm)

$$\gamma = \frac{2e^2\omega^2}{3mc^2} = \frac{0.2}{\lambda^2}$$

- for most lines: too small by orders of magnitude!
- $\rightarrow$ needs QM calculation
- classical dipole approximation $\rightarrow$ emission $\rightarrow$ energy dissipation

$$\frac{dW}{dt} = -\frac{2}{3}\frac{e^2\omega^2}{mc^2}W = -\gamma W$$

natural line profile

- QM $\rightarrow W = N_u h\nu$ where N_u is the upper level's population
- $\rightarrow$
$$\frac{dN_u}{dt} = -\gamma N_u$$
- for a transition $u \rightarrow l$ we have a rate
$$\frac{dN_l}{dt} = 4\pi A_{ul} N_u$$

so that

$$\frac{dN_u}{dt} = -\sum_l \frac{dN_l}{dt} = -4\pi \sum_l A_{ul} N_u$$

natural line profile

- this gives a total damping constant

$$\gamma_u = 4\pi \sum A_{ul}$$

- γ_u is related to the lifetime of the level u

$$\Delta t = \frac{1}{4\pi \sum A_{ul}}$$

  is the average time interval an electron will stay in level u
- similar for the lower level (if not ground state!)

natural line profile

- $\rightarrow$ probability for a electron having an energy within the 'band' of the level u is

$$\sigma(\Delta\omega) = \frac{2\pi e^2}{mc} \frac{\gamma/2}{\Delta\omega^2 + (\gamma/2)^2}$$

- same for the lower level l
- $\rightarrow$ a transition can occur anywhere within the combined energy band!
- total absorption coefficient by convolution of 2 Lorentz profiles
- $\rightarrow$ another Lorentz profile with

$$\gamma_{ul} = \gamma_u + \gamma_l$$

natural line profile

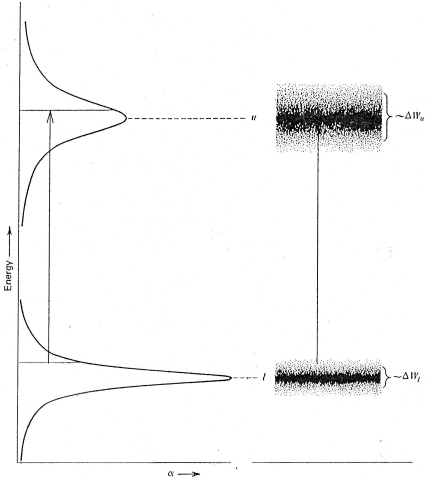


Fig. 11.1. This schematic energy-level diagram illustrates the width of the atomic levels. An absorption line transition starts somewhere in the lower level with a probability of a specified energy given by the α for the lower level. The transition ends in the upper level with a terminal energy given by the α for the upper level.

thermal broadening

- thermal motions in the gas $\rightarrow$
- absorption & emission shifted

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta\nu}{\nu} = \frac{v_r}{c}$$

- distribution of $\Delta\lambda$ $\rightarrow$ profile of thermally broadened line

thermal broadening

- thermal velocity distribution

$$\frac{dN}{N} = \frac{1}{v_0\sqrt{\pi}} \exp\left[-\left(\frac{v_r}{v_0}\right)^2\right] dv_r$$

with

$$v_0^2 = \frac{2kT}{m}$$

- $\rightarrow$ wavelength shift

$$\Delta\lambda_D = \frac{v_0}{c}\lambda = \frac{\lambda}{c}\left(\frac{2kT}{m}\right)^{1/2}$$

thermal broadening

- distribution in $\Delta\lambda \rightarrow$
$$\frac{dN}{N} = \frac{1}{\sqrt{\pi}} \exp\left[-\left(\frac{\Delta\lambda}{\Delta\lambda_D}\right)^2\right] d\left(\frac{\Delta\lambda}{\Delta\lambda_D}\right)$$
- the thermal line profile is
$$\sigma(\lambda)d\lambda = \frac{\pi e^2}{mc} f_{ij} \frac{\lambda^2}{c} \frac{1}{\sqrt{\pi}} \exp\left[-\left(\frac{\Delta\lambda}{\Delta\lambda_D}\right)^2\right] \frac{d\lambda}{\Delta\lambda_D}$$
- $\rightarrow$ *Doppler profile, Gauss profile*

Voigt profile

- overall line profile $\rightarrow$
- convolution of the intrinsic line profile(s) with thermal profile

$$\varphi(\nu) = \int_{-\infty}^{\infty} \varphi_L(\nu - \xi \frac{v}{c}) \varphi_D(\xi) \, d\xi$$

Voigt profile

- inserting the profiles and using

$$
\begin{aligned}
v &= \frac{(\nu - \nu_0)}{\Delta\nu_D} \\
y &= \frac{\Delta\nu}{\Delta\nu_D} \\
\alpha &= \frac{\gamma}{4\pi\Delta\nu_D}
\end{aligned}
$$

$\rightarrow$ *Voigt function*

$$H(\alpha, v) = \frac{\alpha}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-y^2)\, dy}{(v - y)^2 + \alpha^2}$$

Voigt profile

- schematic picture

$$H(\alpha, v) \propto \exp(-v^2) + \frac{\alpha}{\sqrt{\pi} v^2}$$

- 1. term: Doppler 'core'
- 2. term: Lorentz (damping) 'wing'

Voigt profile

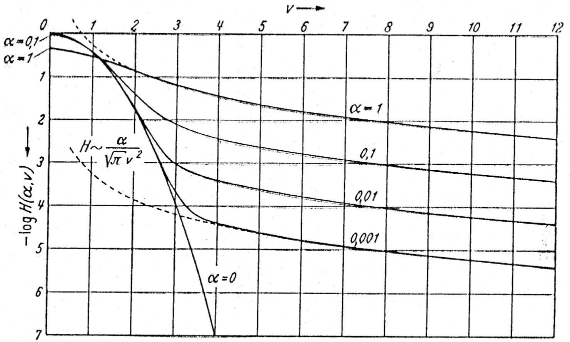


Abb. 107. Logarithmische Darstellung der VOIGT-*Funktionen* $H(\alpha, v)$ mit $\alpha = \frac{\beta_1}{\beta_2}$ als Parameter. Bei den Kurven für $\alpha = 1$ und 0,001 ist gestrichelt die reine Dispersions-(Dämpfungs-)verteilung $H(\alpha, v) = \frac{\alpha}{\sqrt{\pi}\, v^2}$ eingezeichnet; für große v ist sie von der exakten Kurve nicht zu unterscheiden. $\alpha = 0$ entspricht der reinen GAUSS-(Doppler-)Verteilung.

pressure broadening

- broadening due to collisional interactions
- typical perturbers: atoms, ions, molecules
- interaction disturbs energy levels of radiating particle
- depends on separation absorber — perturber

pressure broadening

- net effect depends on
  - distribution of encounters
  - shape of interaction energy curves
- can be
  - line shift
  - asymmetry
  - broadening

pressure broadening

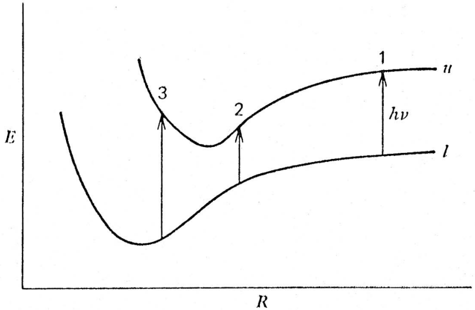


Fig. 11.2. The energies associated with the upper and lower atomic levels on a transition depend on the distance R to the perturber. The transition energy can be either greater or less than the unperturbed value.

pressure broadening

- important case:
- energy change due to collision follows power law

$$\Delta E \propto r^{-n}$$

- r: separation absorber — perturber
- n depends on the interaction type:

pressure broadening

Table 11.1. *Types of pressure broadening.*

n	Type	Lines Affected	Typical Perturber
2	Linear Stark	Hydrogen	Protons, electrons
4	Quadratic Stark	Most lines, especially in hot stars	Electrons
6	Van der Waals	Most lines, especially in cool stars	Neutral hydrogen

pressure broadening

- energy change → frequency shift

$$\Delta E_u - \Delta E_l = h\Delta\nu$$

- written as

$$\Delta\nu = \frac{C_n}{r^n}$$

- C_n: interaction constant, measured or calculated
- for each transition!
- → known only for few lines

impact approximation

- high temperature atmospheres
- $\rightarrow$ high velocities for radiating particles
- (in particular for H, He, electrons)
- $\rightarrow$ relatively short duration of perturbation
- (small compared to time between collisions)
- impact approximation (Lorentz, 1906!)
  - EM wave of radiating particle terminated by impact
  - later: phase shift of EM wave leads to broadening

impact approximation

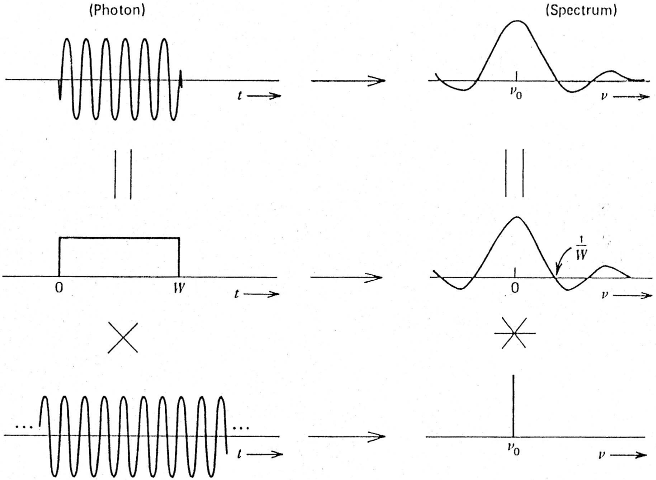


Fig. 11.3. Any real photon has a finite length of a few centimeters or $\approx 10^{-9}$ s, and a simplified way to view this is shown here. Specifically, the duration of the photon determines the width of the spectral line it produces.

impact approximation

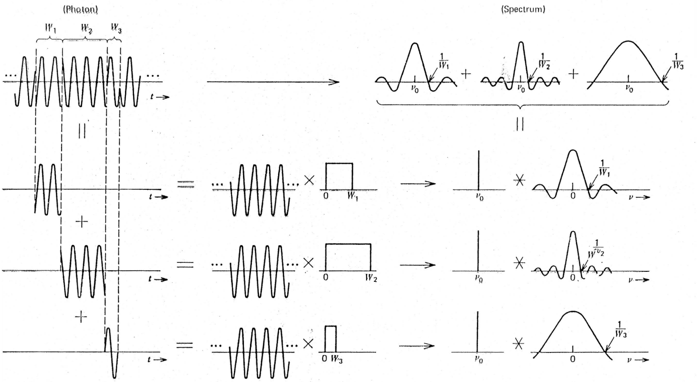


Fig. 11.4. The photon wave at the upper left is disturbed by collisions that produce phase shifts. Each segment between phase shifts can be thought of as a product of an infinite sinusoidal with a box (center section). In the transform domain (right), the sinc functions corresponding to the segments sum together to give the spectrum. Each box is necessarily shorter than the original photon, making the spectral line broader as a result of collisions.

impact approximation

- W_0: average time to radiate undisturbed
- $\rightarrow$ distribution of several segments

$$dP(W_j) = \exp(-W_j/W_0)dW_j/W_0$$

- $\rightarrow$ line absorption coefficient

$$\propto \int_0^\infty W^2 \left(\frac{\sin(\pi(\nu-\nu_0)W)}{\pi(\nu-\nu_0)W}\right)^2 \exp\left(\frac{W}{W_0}\right)\frac{dW}{W_0}$$

impact approximation

- which gives

$$\varphi(\nu) \propto \frac{\gamma_n/4\pi}{(\nu-\nu_0)^2 + (\gamma_n/4\pi)^2}$$

  where

$$\gamma_n = \frac{2}{W_{0,n}}$$

  collisional damping constant

- $\rightarrow$ impact approximation gives same line shape as natural broadening
- line *shape* does not depend on interaction type!

calculation of γ_n

- consider only large phase shifts ($> 1\,\text{rad}$)
  - *Weisskopf approximation*
- ignore all others
- single phase shift

$$\Delta\nu = \frac{C_n}{r^n}$$

- cumulative change $\rightarrow$

$$\Phi = 2\pi \int \Delta\nu \, dt = \int 2\pi \frac{C_n}{r^n} \, dt$$

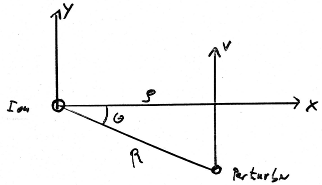
calculation of γ_n

- with $\rho = R\cos\Theta \rightarrow$

$$\Phi = 2\pi \int C_n \cos^2\Theta \frac{dt}{\rho^n}$$

- with

$$v = \frac{dy}{dt} = (\rho/\cos^2\Theta)\frac{d\Theta}{dt}$$



- $\rightarrow$

$$dy = (\rho/v)\frac{d\Theta}{\cos^2\Theta}$$

calculation of γ_n

- this gives

$$\Phi = \frac{2\pi C_n}{v\rho^{n-1}} \int_{-\pi/2}^{\pi/2} \cos^{n-2}(\Theta)\, d\Theta$$

- integral for different n:

$$\begin{aligned} n = 2 &\rightarrow \pi \\ n = 3 &\rightarrow 2 \\ n = 4 &\rightarrow \pi/2 \\ n = 6 &\rightarrow 3\pi/8 \end{aligned}$$

calculation of γ_n

- consider only phase shifts $> 1\,\text{rad} \rightarrow$
- limiting impact parameter

$$\rho_0 = \left(\frac{2\pi C_n}{v} \int_{-\pi/2}^{\pi/2} \cos^{n-2}\Theta \, d\Theta \right)^{\frac{1}{n-1}}$$

- consider only collisions with $\rho \leq \rho_0$
- $\rightarrow$ number of collisions

$$(\pi \rho_0^2 v) N T$$

- N: number density of perturbers
- T: time interval over which collisions are counted

calculation of γ_n

- set $T = W_0 \rightarrow$ number of collisions is ≈ 1
- thus
$$(\pi\rho_0^2 v)NW_0 = 1$$
- $\rightarrow$
$$\gamma_n = \frac{2}{W_{0,n}} = 2\pi\rho_0^2 vN$$
with
$$v = \sqrt{\frac{8kT}{\pi}\left(\frac{1}{m_A} + \frac{1}{m_B}\right)}$$

Example 1: quadratic Stark

$$\rho_0 = (\pi C_4 / 2v)^{1/3}$$

and

$$\gamma_4 = 2\pi v N (\pi^2 C_4 / v)^{2/3} = 29 v^{1/3} C_4^{2/3} N$$

- better theory *Lindholm approximation* $\rightarrow$

$$\gamma_4 = 39 v^{1/3} C_4^{2/3} N$$

Example 1: quadratic Stark

- perturbers: electrons, ions

$$
\begin{aligned}
\gamma_4 &= 39 C_4^{2/3} \left[\frac{8kT}{\pi} \left(\frac{1}{m} + \frac{1}{m_e} \right) \right]^{1/6} N_e \\
&+ 39 C_4^{2/3} \sum_i \left[\frac{8kT}{\pi} \left(\frac{1}{m} + \frac{1}{m_i} \right) \right]^{1/6} N_i
\end{aligned}
$$

Example 2: van der Waals

$$\gamma_6 = 17 v^{3/5} C_6^{2/5} N$$

- typically induced by H, He (cool objects: also H_2)
- experimental result:

$$\left[\frac{C_6(\mathrm{He})}{C_6(\mathrm{H})}\right]^{2/5} = 0.619$$

- also $(v_{\mathrm{He}}/v_{\mathrm{H}})^{3/5} = 0.684$
- gives an expression of the form

$$\log \gamma_6 = 19.6 + \log C_6(\mathrm{H}) + \log P_{\mathrm{gas}} - 0.7 \log T$$

Example 2: van der Waals

- Unsöld C_6 approximation:

$$C_6(\mathrm{H}) = 0.3 \times 10^{-30} \left[\frac{1}{(I - \chi - \chi_\lambda)^2} - \frac{1}{(I - \chi)^2} \right]$$

- I: ionization potential
- χ: excitation potential (lower level)
- χ_λ: energy of line photon

Example 2: van der Waals

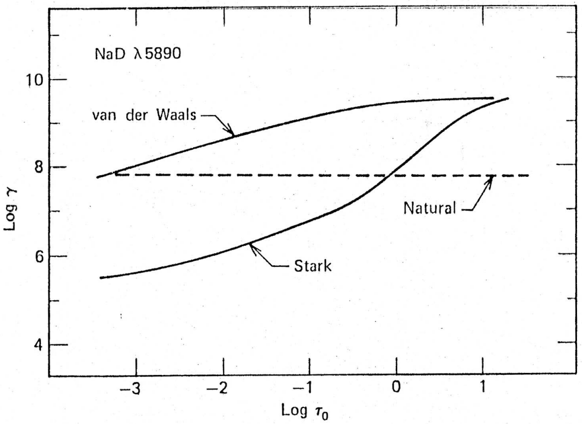


Fig. 11.6. Damping constants for the Na I D_1 line are shown as a function of depth in a solar model. The van der Waals constant is computed using eqs. (11.35) and (11.36). The Stark constant comes from eq. (11.33). For comparison, the natural radiation damping according to eq. (11.19) is shown.

statistical theory

- impact theory in stellar atmospheres valid for metal lines
- not for Balmer lines!
- reason: duration of collisions long compared to time between collisions!
- statistical theory:
  - radiating particle embedded in statistically fluctuating field of randomly distributed perturbers
- if motion of perturbers is ignored
- $\rightarrow$ 'quasi-static approximation'

statistical theory

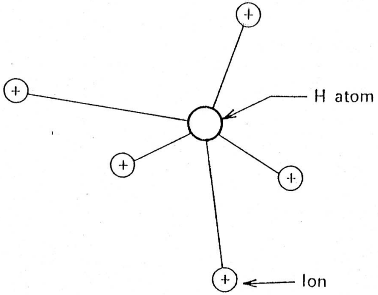


Fig. 11.7. The distribution of ions in space gives a nonzero electric field at the position of the atom. This field causes a perturbation in the energy levels of the atom.

nearest neighbor approximation

- main effect by perturbation of nearest neighbor
- neglect everything else
- $W(r)$: probability that nearest neighbor is at $(r, r + dr)$
- $\rightarrow$ frequency spectrum

$$I(\Delta\omega)d(\Delta\omega) \propto W(r)[dr/d(\Delta\omega)]d(\Delta\omega)$$

with $\Delta\omega = C_n/r^n$

nearest neighbor approximation

- uniform density $\rightarrow$

$$W(r) = 4\pi r^2 N \exp\left(-\frac{4}{3}\pi r^3 N\right)$$

- write interparticle distance $r_0 = (4/3\pi N)^{1/3}$,
- define $\Delta\omega_0 = C_n/r_0^n$
- $\rightarrow (\Delta\omega/\Delta\omega_0) = (r_0/r)^n$
- so that

$$W(r)dr = \exp\left(-(\Delta\omega/\Delta\omega_0)^{3/n}\right) d(\Delta\omega/\Delta\omega_0)^{3/n}$$

nearest neighbor approximation

- for linear Stark effect ($n = 2$)
- 'normal field strength'

$$F_0 = \frac{e}{r_0^2} = e\left(\frac{4}{3}\pi N\right)^{2/3} = 2.59N^{2/3}$$

- define $\beta = F/F_0 \rightarrow$

$$W(\beta)dr = \frac{3}{2}\beta^{-5/2}\exp\left(\beta^{-3/2}\right)\, d\beta$$

nearest neighbor approximation

- $\beta \to \infty$ gives $W(\beta) \to (3/2)\beta^{-5/2}$
- $\to$ profile drops off like $\Delta\omega^{-5/2}$
- impact approximation: $\Delta\omega^{-2}$

Holtsmark theory

- consider effect of ensemble of perturbers $\rightarrow$

$$W(\beta) = \frac{2\beta}{\pi} \int_0^\infty \exp\left(-y^{3/n}\right) y \sin(\beta y)\, dy$$

- where $F_0 = \gamma C_n N^{n/3}$ and

$$\gamma = \left[\frac{2\pi^2 n}{3(n+3)\Gamma(3/n)\sin(3\pi/2n)} \right]^{n/3}$$

- $\int$ can be computed analytically only for $n = 3/2$ and $n = 3$
- for $n = 2$ use expansions etc.

Holtsmark theory

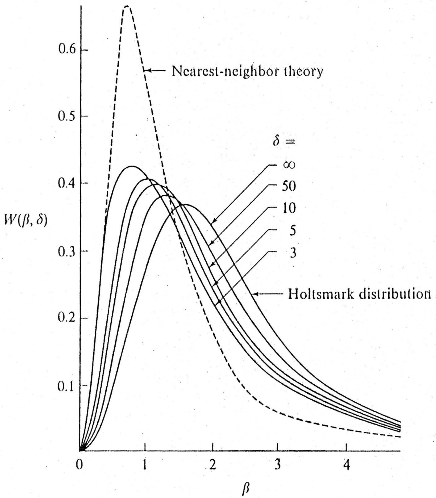


FIGURE 9-1
Probability distribution of field strength at a test point, including shielding effects; δ is the number of charged particles within the Debye sphere. From **(205)**, by permission.

quasi-static broadening

- consider H I lines
- $\rightarrow$ permanent dipole moment
- $\rightarrow$ linear Stark effect
- $\rightarrow$ energy shifts of levels $\propto$ field strength F
- Stark components overlap
- each has characteristic shift

$$\Delta\lambda_k = \frac{2h\lambda^2 n_k}{8\pi^2 c m_e Z} F = C_k F$$

- and relative strength I_k

quasi-static broadening

- total line profile

$$
\begin{aligned}
I(\Delta\lambda)d(\Delta\lambda) &= \sum_k I_k W(F/F_0)dF/F_0 \\
&= \sum_k I_k W(\Delta\lambda/C_k F_0)d(\Delta\lambda)/C_k F_0
\end{aligned}
$$

quasi-static broadening

- set $\alpha = \Delta\lambda / F_0$
- profile function

$$S(\alpha) d(\alpha) = \sum_k I_k W(\alpha / C_k F_0) d(\alpha) / C_k F_0$$

- absorption cross section

$$\sigma(\Delta\lambda) = \frac{\pi e^2}{mc} f_{ij} S(\Delta\lambda / F_0) \frac{\lambda^2}{c F_0}$$

- $S(\alpha)$ must be tabulated

Stark profiles

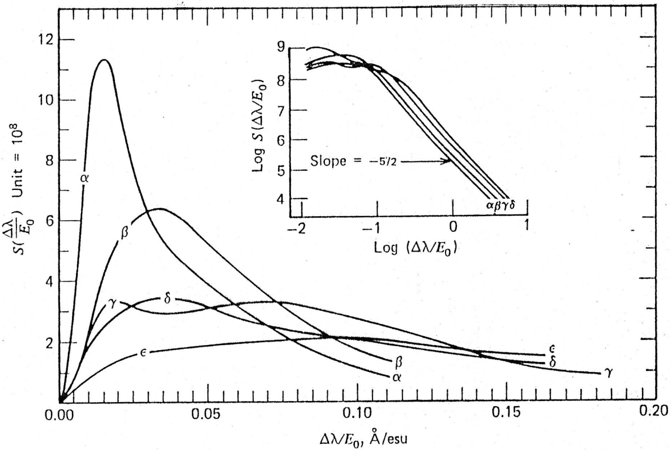
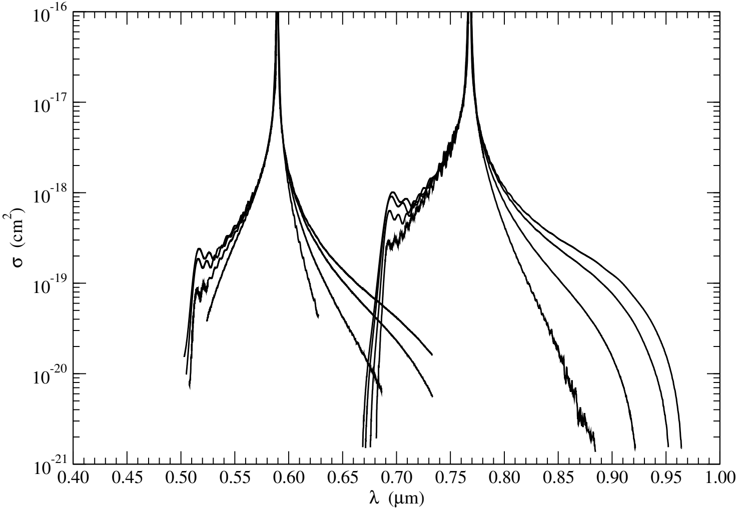


Fig. 11.10. Stark profiles $S(\Delta\lambda/E_0)$ are shown for the first few Balmer lines. Only half the profiles are shown since they are symmetric. The inset shows the same functions on logarithmic coordinates where the $\Delta\lambda^{-\frac{5}{2}}$ behavior in the wing is apparent. Data from Underhill and Waddell (1959).

detailed line profiles



Importance of line profiles