Line Shapes and Broadening

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Books and reviews

- S. Alexiou, HEDP 5, 225 (2009)
- E. Stambulchik and Y. Maron, HEDP 6, 9 (2010)

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Line broadening

- Instrumental
- Collisonal (broadening) – Stark – Van der Waals – Resonance
- Doppler
- Natural

Many-body problem:
QM picture of line broadening is described in terms of a complete QM system of radiator + all perturbers

Doppler broadening

Doppler shift: $\frac{\nu}{\nu_0} = 1 - \frac{v}{c}$

Fraction of atoms with $v_N \leq v \leq v_N + dv_N$:

$N = \int f_N \exp \left( \frac{\nu - \nu_0}{\Delta \nu} \right) dv_N$

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$\delta \nu_{1/2} = \frac{\Delta \nu}{2} = \frac{c}{2v_N}$

FWHM = $2\sqrt{2} \delta \nu_{1/2} = a_0 = 7.715 \times 10^{-5} \text{ m}$

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Energy spectrum:

Radiator loses energy:

Lorentz profile:

Classical atomic oscillator

$f(t) = f_0 \exp(i \omega t)$

Energy spectrum:

$L(\omega) = \int_0^\infty f(t) e^{-i \omega t} dt$

Radiator losas energy:

$f(\omega) = f_0 \exp(i \omega t)$

$L(\omega) = \int_0^\infty f(t) e^{-i \omega t} dt$
Interaction between atom and perturber is a classical particle. No transitions are produced by the perturber.

Atom is embedded in plasma. Atom is unperturbed between collisions.

Perturber moves with a constant velocity,\( \text{moving} \) charged perturbers of motionless (slowly moving) charged perturbers. Of motionless (slowly moving) charged perturbers.

Convolution of G and L: Voigt profile

\[ \varphi_v(\omega) = \int_{-\infty}^{\infty} \varphi_G(\omega - x) \varphi_L(x) dx \]

\[ = \frac{\gamma}{2\pi} \int_{0}^{\infty} \frac{\exp(-x^2)}{\sqrt{x^2} + \alpha^2} dx \]

\[ H(\alpha, v) = \frac{\gamma}{\pi} \int_{0}^{\infty} \frac{\exp(-x^2)}{\sqrt{x^2} + \alpha^2} dx \]

\[ H(\alpha, v) \approx e^{-\alpha^2} + \alpha^2/(\pi^{1/2} v^2) \]

At 1%: \( \delta_{\text{FWHM}} = \left[ \frac{\delta_{\text{FWHM}}}{2} \right]^2 + \delta_{\text{FWHM}}^2 \]

Gauss+Lorentz? Voigt!

Lorentz profile

\[ \varphi_L(\omega) = \frac{1}{\pi} \frac{\gamma/2}{(\omega - \omega_0)^2 + (\gamma/2)^2} \]

FWHM = \( \gamma \)

peak x FWHM = 0.64

Pressure broadening: classical approach

Impact theory

- Oscillator
- Emitted wavetrain is interrupted
- Instantaneous phase shift
- Transition to another level
- Oscillator "starts" and "stops"
- Duration of collision is small compared to the mean time between collisions

Quasi-static theory

- Atom is embedded in plasma of motionless (slowly moving) charged perturbers.
- The field fluctuates
  - Spectral line position shifts
  - Final shape is obtained from the distribution of microfields

Impact (cont'd)

Lindholm-Foley approximation:

\[ f(t) = \exp \left[ i \omega_0 t + \frac{1}{2} \int_{t_{-\infty}}^{t} \Delta \omega(t') dt' \right] = \exp \left[ i \omega_0 t + \frac{1}{2} \int_{t_{-\infty}}^{t} \Delta \omega(t') dt' \right] \]

\[ I(\omega) = \frac{N \sigma_0}{(\omega - \omega_0)^2 + (N \sigma_0)^2} \]

\[ \sigma_0 = 2 \pi \int_{0}^{\infty} \left[ 1 - \cos \theta(\alpha) \right] d\alpha; \quad \sigma_1 = 2 \pi \int_{0}^{\infty} \sin \theta(\alpha) \alpha d\alpha; \]

\[ \text{Width: } \Gamma = 2N \sigma_0; \quad \text{Shift: } \Delta \omega_0 = N \sigma_0 \]

Natural Broadening: QM

Quantum mechanics gives the same result as classical theory although it is the finite width of the discrete energy levels rather than decay of the wave train.

\[ \Delta E \geq \hbar/2 \]

\[ \gamma = \hbar (\gamma = 2 \Delta E, \tau = 1/\Sigma A) \]

\[ \delta \omega = \gamma; \quad \frac{\delta A}{A} = \frac{\lambda}{2 \pi c} \gamma; \quad \frac{\lambda}{2 \pi c} \Delta A \]

Weisskopf & Wigner

Generally, natural broadening is negligible compared to Doppler but: sum over \( A \)'s includes autoionization (if present)

Collisional (pressure) broadening

Interaction of the atom(-ic oscillator) with other plasma particles:

- Electric fields are most important and therefore "Stark broadening"
- Van der Waals: two dipole moments (neutrals); short-range interaction

Weisskopf theory:

- Atom is unperturbed between collisions (\( \tau_c \))
- Perturber is a classical particle
- Perturber moves with a constant velocity, straight line, velocity \( v \), impact parameter \( \rho \)
- No transitions are produced by the perturber (phase shifts only)
- Interaction between atom and perturber is described by: \( \Delta \omega(t) = \Delta \omega_0 \gamma, \gamma = v \rho/2 \gamma \)

Lorentz:

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

\[ \Gamma = 2 \pi \hbar \left[ \frac{N \sigma_0}{\rho} \right]^{3/2} \]

Impact Approximation

Problems with the classical impact approximation

- Time of interest \( \tau = 1/\Delta \omega \) becomes smaller than the collision time \( \tau_c = \rho/v \) for large \( \Delta \omega \): problem at large displacements!
- Low densities preferred
- Collisions overlap at \( \rho \rightarrow \infty \) (\( \tau_c \) exceeds the mean time between collisions)
- Classical impact theory is adiabatic
Impact Approximation: quantum

M. Baranger, 1958:

\[ \Delta \omega = n_x \int_0^\infty v f_x(v) \left( \sum_{i,j} \sigma_{i,j}(v) + \sum_j \sigma_{j,j}(v) \right) dv + \]

\[ n_x \int_0^\infty v f_x(v) \left( \int f_i(\theta, v) - f_i(\theta, v)^2 \right) dv \]

Impact Approximation: FWHM

M. Baranger, 1958:

\[ \Delta \omega \approx n_x \int_0^\infty v f_x(v) \left( \sum_{i,j} \sigma_{i,j}(v) + \sum_j \sigma_{j,j}(v) \right) dv + \]

\[ n_x \int_0^\infty v f_x(v) \left( \int f_i(\theta, v) - f_i(\theta, v)^2 \right) dv \]

Example: problems in isolated lines

- **Isolated** ion lines, which are purely \( e^+ \) impact broadened, show factor of \( \sim 2 \) discrepancies between theory and experiment.
  - Techniques used to resolve this issue are:
    - sophisticated semiclassical calculations
    - fully quantum mechanical (close coupling) calculations, different formulations
    - population effects
  - However, there has been no resolution yet

\[ \text{via a collision} \quad \text{2p} \quad \text{via a collision} \quad \text{2s} \]

Stark effect

From: MA Gigosos (2014)

Linear for H, quadratic for others (weak field)

Nearest Neighbor Approximation

- Only nearest neighbor is important
- No interaction between the perturbers
- Not really a “statistical” model

\[ W(r) dr = \left( 1 - \int_0^r W(x) dx \right) 4\pi r^2 N dr \]

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

Simple...and wrong!

Quasi-static approximation

- Electric field (by the ions) is considered (almost) constant at the radiator during emission
- Plasma microfield splits and shifts level via Stark effect
- \( E \) is not constant but has some distribution \( \Rightarrow \) components smeared \( \Rightarrow \) line profile

\[ \text{From: MA Gigosos (2014)} \]

Holtsmark model (1919)

- Ensemble of perturbers; statistically independent; interaction isotropic
- No interaction between perturbers
- Calculation steps
  - Probability of finding the nearest ion at distance \( r \): \( P(r) \)
  - Probability of the emitter being subjected to field \( F(\theta) \)
  - Shift of levels calculated for each field, result convolved

\[ F_0 = 2.603 \alpha N^{2/3} \]

\[ \beta = \frac{P}{F_0}, \quad \int_0^\infty H(\beta) d\beta = 1 \]

\[ H(\beta) = \frac{2}{\beta} \int_0^\infty x \cdot \sin(\beta x) \cdot e^{-x^2} dx \]

\[ \text{Wings: } \sim (\Delta \omega)^{-5/2} \]
How good is Holtsmark?..  

Holtsmark vs Hooper  
(ion-ion correlations, Debye shielding)  
\[ a = \frac{R_0}{\rho} \]  
\[ R_0 = \frac{3}{\gamma E_{\text{CEF}}} \]

Wkh (1975)  

\[ N_e = 8 \times 10^{16} \text{ cm}^{-3} \]  
Quasi-static theory works quite well for hydrogen but ion dynamics is important (sometimes electrons are important too)

Modern computer simulations  

\[ i\hbar \frac{d}{dt} U(t) = H(t) U(t) = (\hat{H}_0 + qE \cdot \hat{R}) U(t) \]  
\[ D(t) = U^\dagger(t) D(0) U(t) \]  
\[ \Phi(t) = Tr[D(0) \cdot D(t) \beta] \]  
\[ I(\Delta \omega) = \frac{1}{\pi} R \int_0^{\infty} e^{i \Delta \omega t} \Phi(t) dt \]

Exp vs theory (CSM)  

\[ H_3 \]  
\[ n_e = 1.2 \times 10^{13} \text{ cm}^{-3} \]  
\[ T_e = 0.16 \text{ eV} \]

Inglis-Teller effect  

Weise et al (1972)  

\[ \lg n_2 [\text{cm}^{-3}] = 23.12 + 4.5 \lg Z - 1.5 \lg z - 7.5 \lg n_{\text{max}} \]

Modern CS  

- Trivial MD  
  - Electrons and protons move along straight lines  
- Full MD  
  - All perturbers interact  
- 200 e and 200 p; a cube with mirror walls

Where's good data?  

- Hydrogen atoms  
  - Griem (1974)  
- Non-hydrogenic ions  
  - Griem (1974)  
  - Modified semiclassical approach, Dimitrijevic and Konjevic (1980)

- NIST Atomic Spectral Line Broadening Bibliographic Database  
  - http://physics.nist.gov/cgi-bin/ASHBib1/LineBroadBib.cgi  
- Stark-B Database  
  - http://stark-b.obspm.fr/