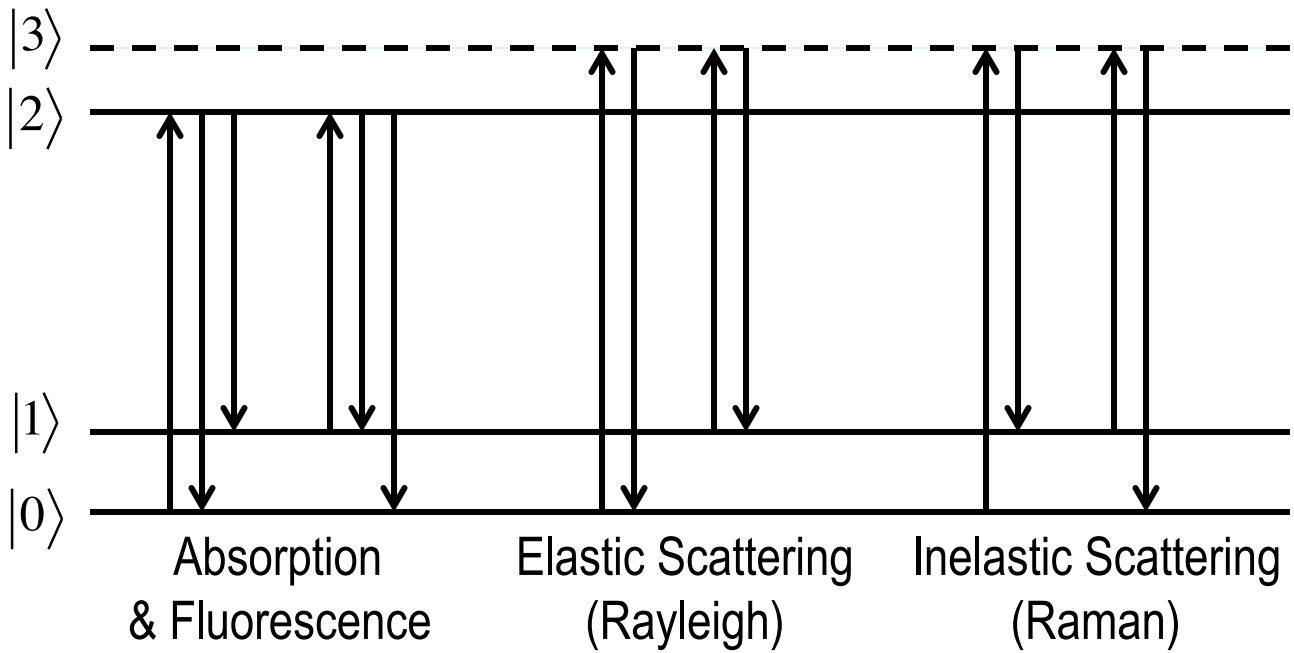
Lecture 10. Lidar Effective Cross-Section vs. Convolution

- Introduction
- Convolution in Lineshape Determination
  -- Voigt Lineshape (Lorentzian $\otimes$ Gaussian)
- Effective Cross Section for Single Isotope
  -- Na Resonance Fluorescence Lidar
- Effective Cross Section for multiple Isotopes
  -- K Resonance Fluorescence Lidar
- Convoluted Rayleigh Doppler Lineshape
  -- Influence of Laser Lineshape

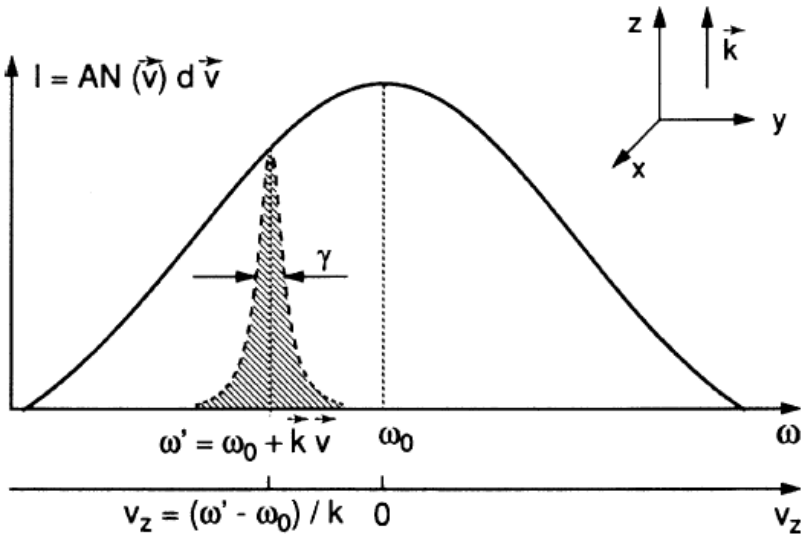
Introduction

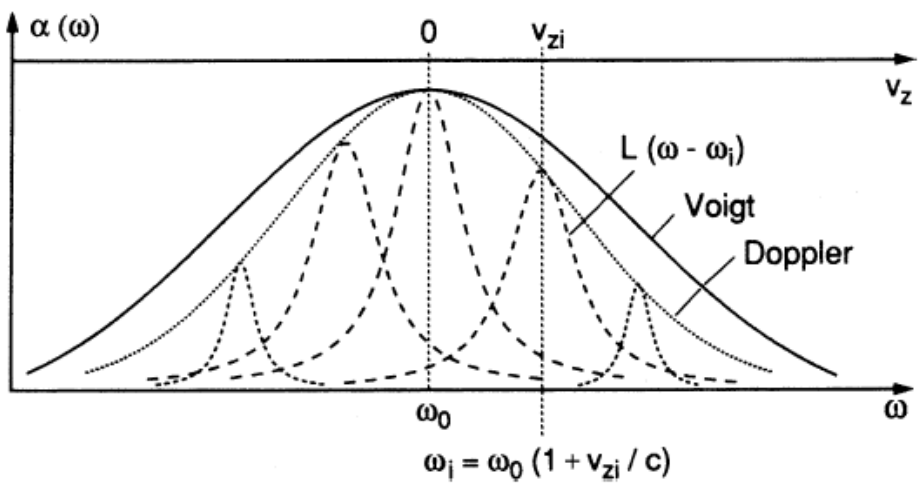


Here, 0, 1, and 2 are real energy states, while 3 is a virtual state.

- Resonance fluorescence contains two single-photon processes: Absorption of a photon by an atom, and spontaneous emission of another photon by the atom. Fluorescence can be quenched by collisions.
- Rayleigh scattering or Raman scattering is a two-photon process, in which two photons are involved simultaneously. Therefore, Rayleigh/Raman scattering has much smaller scattering cross-section than absorption, about 10^{14} & 10^{17} orders of magnitude smaller, respectively.

Atomic Absorption Lineshape Determined by Convolution

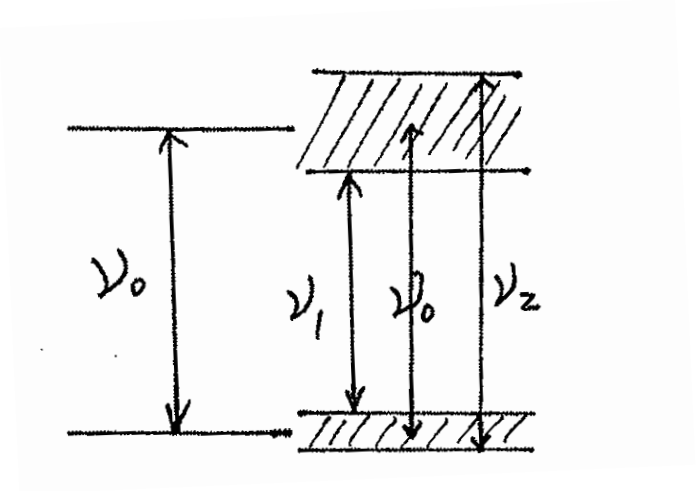


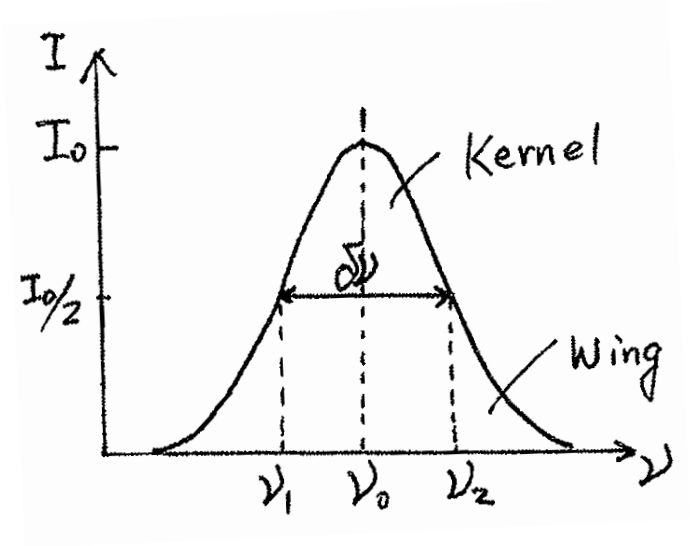


$$I(\omega) = I_0 \int_{-\infty}^{+\infty} n(\omega', \omega_0) g_{Lorentzian}(\omega', \omega) d\omega'$$

$$= \frac{I_0 (\gamma/2\pi) N_i}{\sqrt{2\pi}\,(2\pi\sigma_D)} \int_0^{\infty} \frac{\exp\left[-\frac{(\omega'-\omega_0)^2}{2(2\pi\sigma_D)^2}\right]}{(\omega-\omega')^2 + (\gamma/2)^2} d\omega'$$

Natural Linewidth Determined by Finite Radiative Lifetime

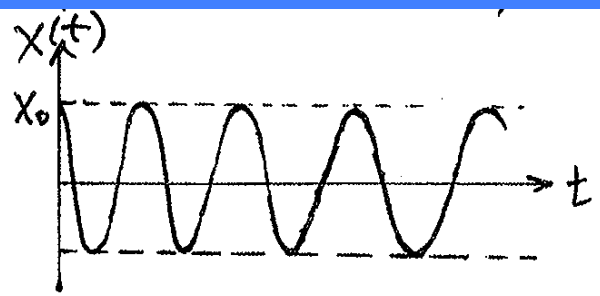


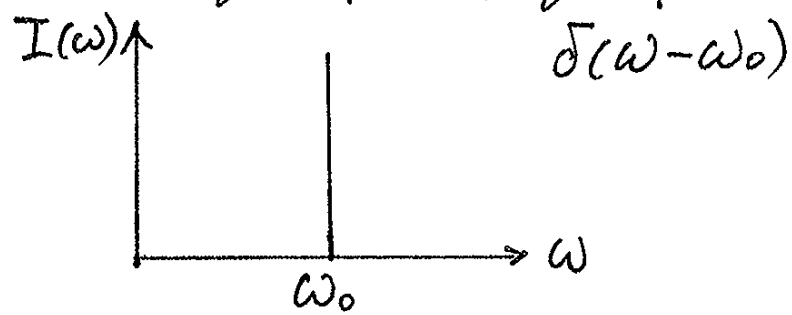


Usually only the ground state can have infinite radiative lifetime, therefore infinite thin energy level. Excited states all have finite radiative lifetime, therefore finite energy level widths.

Natural Linewidth Determined by Finite Radiative Lifetime

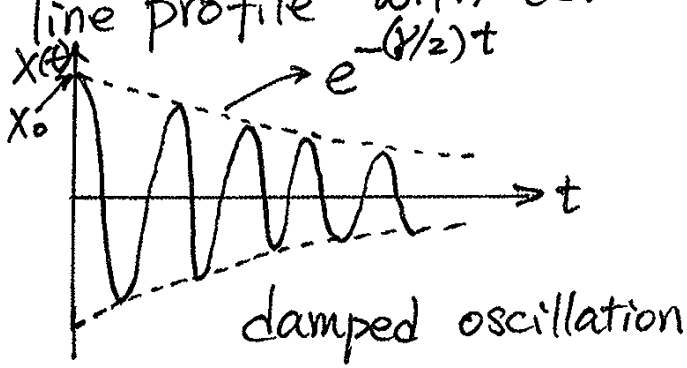
Infinite lifetime → harmonic oscillator → narrow linewidth

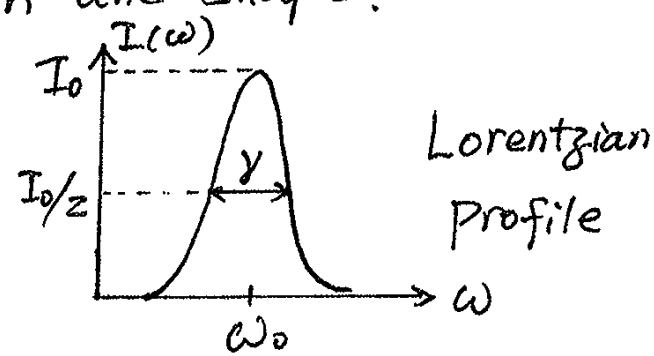




Finite radiative lifetime → damped oscillator → natural linewidth

In frequency domain, the $\delta(\omega-\omega_0)$ function is replaced by a line profile with certain width and shape.





Atomic Absorption Cross-Section

- σ_{abs} is proportional to the probability of a single-frequency photon being absorbed by an atom:

$$\sigma_{abs}(\nu,\nu_0) = A_{ki}\frac{\lambda^2}{8\pi n^2}\frac{g_k}{g_i}g_A(\nu,\nu_0) \qquad (10.1)$$

where A_{ki} is the spontaneous transition probability per unit time, i.e., the Einstein A coefficient; g_k and g_i are the degeneracy factors for the upper and lower energy levels k and i, respectively; λ is the wavelength; n is the refraction index, and g_A is the absorption lineshape. ν and ν_o are the laser frequency and the central frequency of the atomic absorption line, respectively.

- For single atom, the absorption lineshape g_A is determined by natural linewidth and collisional broadening, which has Lorentzian shape

$$g_A(\nu,\nu_0) = g_H(\nu,\nu_0) = \frac{\Delta\nu_H}{2\pi\left[(\nu-\nu_0)^2 + (\Delta\nu_H/2)^2\right]} \qquad (10.2)$$

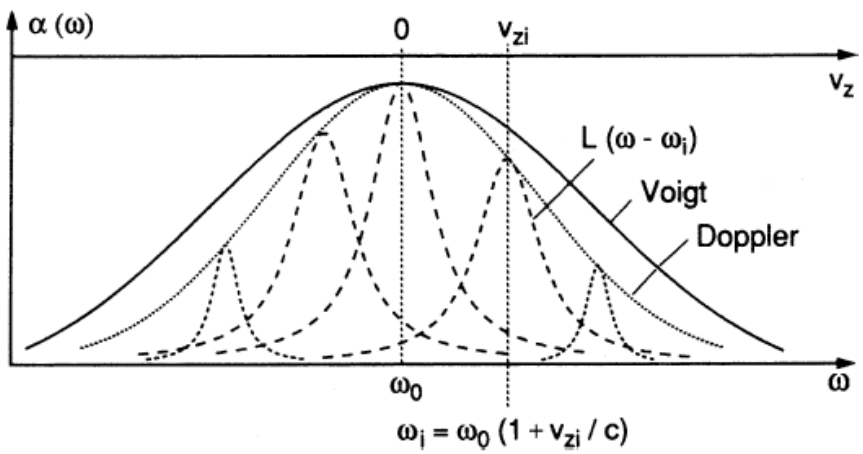
where $\Delta\nu_H$ is the homogeneous broadened linewidth.

Refer to our textbook Chapter 5 and references therein

Absorption Cross Section Under Doppler Effects

- For many atoms in thermal equilibrium, the lineshape is the integration of the Doppler broadening (Gaussian shape) with the Lorentzian natural lineshape. The absorption lineshape g_A is given by Voigt integration

$$g_A(\omega) = \int_{-\infty}^{+\infty} g_{Gaussian}(\omega_0, \omega') g_{Lorentzian}(\omega, \omega') d\omega'$$



Absorption Cross Section Under Doppler Effects

- When ignoring the Lorentzian natural linewidth (~10 MHz), the Doppler broadening (~1 GHz) dominates the lineshape. The statically averaged absorption cross section for each atomic transition line is then given by a Gaussian

$$\sigma_{abs}(\nu,\nu_o) = \sigma_o \exp\left(-\frac{\left[\nu(1-V_R/c)-\nu_o\right]^2}{2\sigma_D^2}\right) \quad (10.3)$$

where $\sigma_o = \frac{1}{\sqrt{2\pi}\sigma_D}\frac{e^2}{4\varepsilon_o m_e c} f_{ik}$ (10.4) and $\sigma_D = \sqrt{\frac{k_B T}{M\lambda_0^2}}$ (10.5)

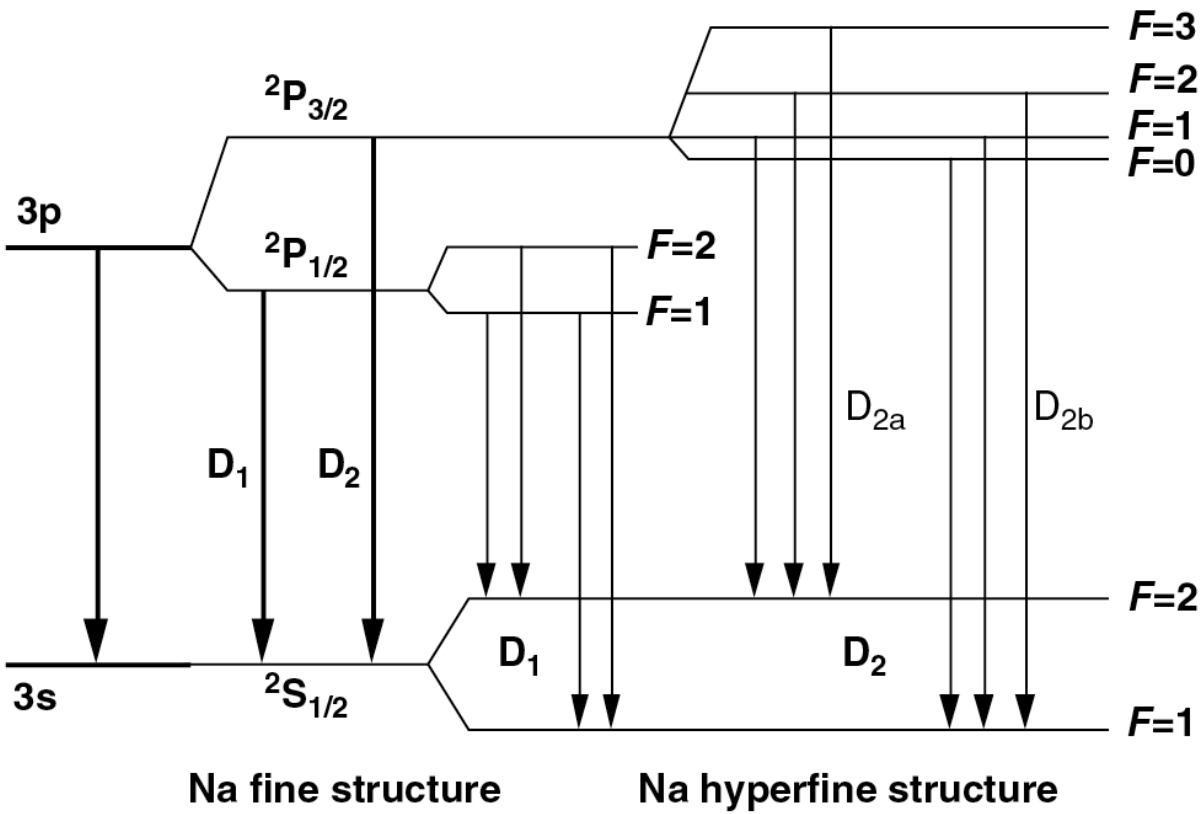
σ_o – peak absorption cross section (m^2 or cm^2)
e – charge of electron; m_e – mass of electron
ε_o – electric constant; c – speed of light
f_{ik} – absorption oscillator strength; V_R – radial velocity

σ_D – Doppler broadened line width
k_B – Boltzmann constant; T – temperature
M – mass of atom; λ_o – wavelength

Resonance Fluorescence Lidar: Effective Cross Section

- Refer to the textbook Section 5.2.1.3.1 for effective cross section σ_{eff}
- Resonance fluorescence contains two single-photon processes: Absorption of a photon by an atom, and spontaneous emission of another photon by the atom.
- Because resonance fluorescence is isotropic, the differential backscatter cross-section $d\sigma/d\Omega$ can be replaced by the total effective scattering cross-section σ_{eff} divided by 4π.
- The total effective scattering cross-section σ_{eff} is defined as the ratio of the average photon number scattered by an individual atoms (in all directions) to the total incident photon number per unit area.
- The σ_{eff} is determined by the convolution of the atomic absorption cross-section σ_{abs} and the laser spectral lineshape $g_L(\nu)$.
- The absorption cross-section σ_{abs} is defined as the ratio of the average absorbed single-frequency photons per atom to the total incident photons per unit area.

Na Atomic Energy Levels



- Na (sodium) is probably one of the most well studied alkali species. ^{23}Na is the only stable isotope for Na, and it has hyperfine structures.

Refer to our textbook Chapter 5 and references therein

Na Atomic Parameters

Table 5.1 Parameters of the Na D_1 and D_2 Transition Lines

Transition Line	Central Wavelength (nm)	Transition Probability ($10^8\ s^{-1}$)	Radiative Lifetime (nsec)	Oscillator Strength f_{ik}
D_1 ($^2P_{1/2} \rightarrow {}^2S_{1/2}$)	589.7558	0.614	16.29	0.320
D_2 ($^2P_{3/2} \rightarrow {}^2S_{1/2}$)	589.1583	0.616	16.23	0.641

Group	$^2S_{1/2}$	$^2P_{3/2}$	Offset (GHz)	Relative Line Strength[a]
D_{2b}	$F=1$	$F=2$	1.0911	5/32
		$F=1$	1.0566	5/32
		$F=0$	1.0408	2/32
D_{2a}	$F=2$	$F=3$	−0.6216	14/32
		$F=2$	−0.6806	5/32
		$F=1$	−0.7150	1/32

Doppler-Free Saturation–Absorption Features of the Na D_2 Line

f_a (MHz)	f_c (MHz)	f_b (MHz)	f_+ (MHz)	f_- (MHz)
−651.4	187.8	1067.8	−21.4	−1281.4

[a]Relative line strengths are in the absence of a magnetic field or the spatial average. When Hanle effect is considered in the atmosphere, the relative line strengths will be modified depending on the geomagnetic field and the laser polarization.

Doppler-Limited Na Spectroscopy

- Doppler-broadened Na absorption cross-section is approximated as a Gaussian with rms width σ_D

$$\sigma_{abs}(\nu) = \frac{1}{\sqrt{2\pi}\sigma_D}\frac{e^2 f}{4\varepsilon_0 m_e c}\sum_{n=1}^{6} A_n \exp\left(-\frac{[\nu_n - \nu(1 - V_R/c)]^2}{2\sigma_D^2}\right) \quad (10.6)$$

- Assume the laser lineshape is a Gaussian with rms width σ_L
- The effective cross-section is the convolution of the atomic absorption cross-section and the laser lineshape

$$\sigma_{eff}(\nu) = \frac{1}{\sqrt{2\pi}\sigma_e}\frac{e^2 f}{4\varepsilon_0 m_e c}\sum_{n=1}^{6} A_n \exp\left(-\frac{[\nu_n - \nu(1 - V_R/c)]^2}{2\sigma_e^2}\right) \quad (10.7)$$

where $\sigma_e = \sqrt{\sigma_D^2 + \sigma_L^2}$ (10.8) and $\sigma_D = \sqrt{\frac{k_B T}{M\lambda_0^2}}$ (10.5)

Effective Cross-Section

- The effective cross section is a convolution of the atomic absorption cross section and the laser line shape. When the laser has finite spectral linewidth with lineshape (its intensity distribution along frequency) of

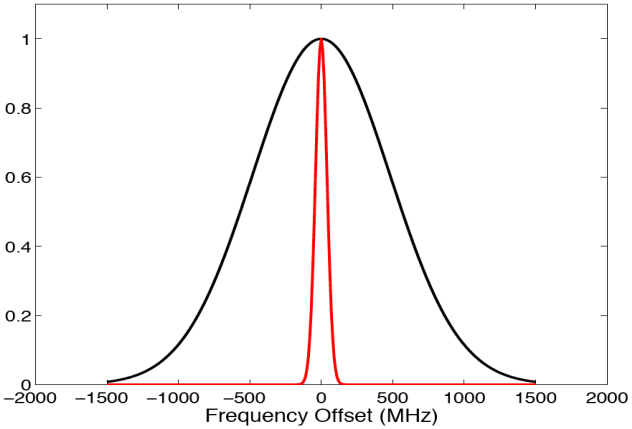
$$\int_0^{\infty} g_L(\nu,\nu_L)d\nu = 1 \qquad (10.9)$$

- The effective cross-section σ_{eff} is given by the convolution of σ_{abs} with the laser lineshape g_L:

$$\sigma_{eff}(\nu_L,\nu_o) = \int_{-\infty}^{+\infty} \sigma_{abs}(\nu,\nu_o) g_L(\nu,\nu_L)d\nu \qquad (10.10)$$

- If the laser spectral lineshape is a Gaussian shape:

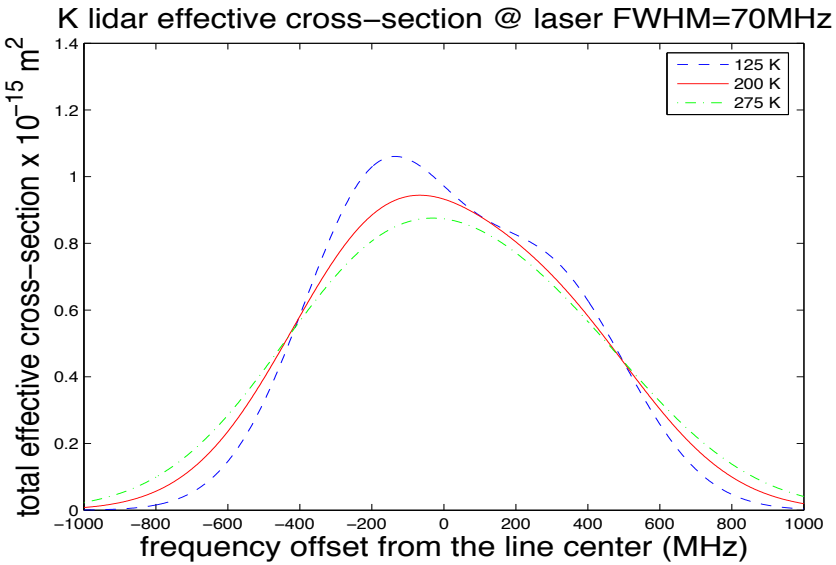
$$g_L(\nu,\nu_L) = \frac{1}{\sqrt{2\pi}\sigma_L}\exp\left(-\frac{(\nu-\nu_L)^2}{2\sigma_L^2}\right) \qquad (10.11)$$

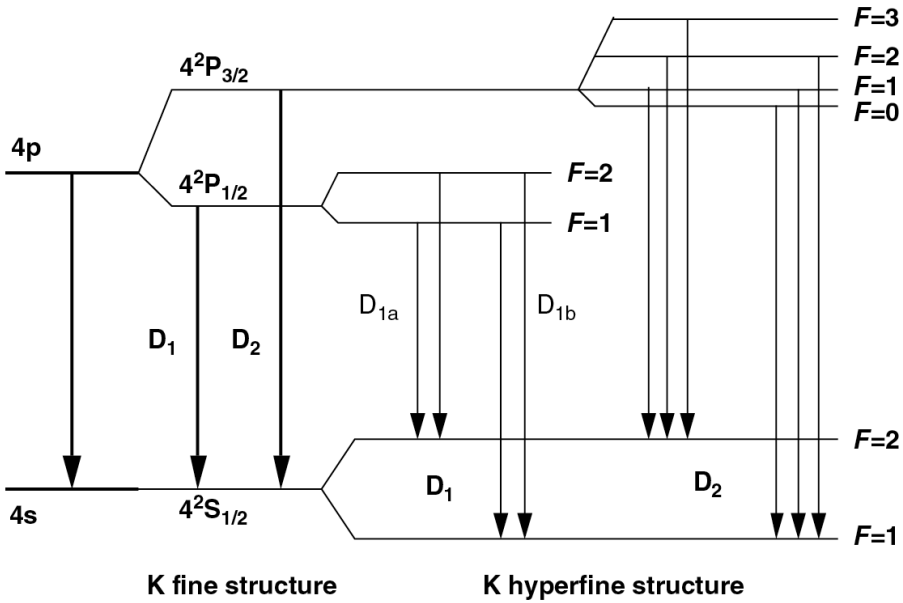


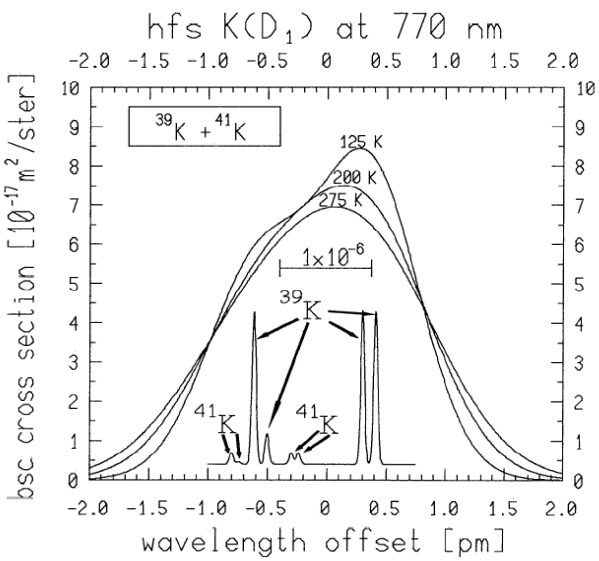
- then σ_{eff} can be written as

$$\sigma_{eff}(\nu_L,\nu_0) = \frac{\sigma_D\sigma_0}{\sqrt{\sigma_D^2+\sigma_L^2}}\exp\left(-\frac{\left[\nu_L(1-V_R/c)-\nu_0\right]^2}{2(\sigma_D^2+\sigma_L^2)}\right) \qquad (10.12)$$

Effective Cross-Section for K Atoms







Atomic K energy levels
Reference our textbook Chapter 5

- K (potassium) is another alkali species, and it has several stable isotopes (^{39}K, ^{40}K, and ^{41}K) with hyperfine structures.

Effective Cross-Section for K Atoms

- Absorption cross section of K atom's D1 line is given by

$$\sigma_{abs}(\nu) = \sum_{A=39}^{41}\left\{IsotopeAbdn(A)\frac{1}{\sqrt{2\pi}\sigma_D}\frac{e^2 f}{4\varepsilon_0 m_e c}\sum_{n=1}^{4}A_n \exp\left(-\frac{[\nu_n - \nu(1-V_R/c)]^2}{2\sigma_D^2}\right)\right\} \quad (11.9)$$

Isotope abundance: 93.2581% (^{39}K), 0.0117% (^{40}K), 6.7302% (^{41}K)
Line strength: An = 5/16, 1/16, 5/16, 5/16
Oscillator strength: f, Doppler broadening: σ_D

- The effective total scattering cross section of K atom's D1 line is the convolution of the absorption cross section and the laser lineshape. Under the assumption of Gaussian lineshape of the laser, it is given by

$$\sigma_{eff}(\nu) = \sum_{A=39}^{41}\left\{IsotopeAbdn(A)\frac{1}{\sqrt{2\pi}\sigma_e}\frac{e^2 f}{4\varepsilon_0 m_e c}\sum_{n=1}^{4}A_n \exp\left(-\frac{[\nu_n - \nu(1-V_R/c)]^2}{2\sigma_e^2}\right)\right\} \quad (11.10)$$

where $\sigma_e = \sqrt{\sigma_D^2 + \sigma_L^2}$ (11.11) and $\sigma_D = \sqrt{\frac{k_B T}{M\lambda_0^2}}$ (11.12)

Refer to our textbook Chapter 5 and references therein

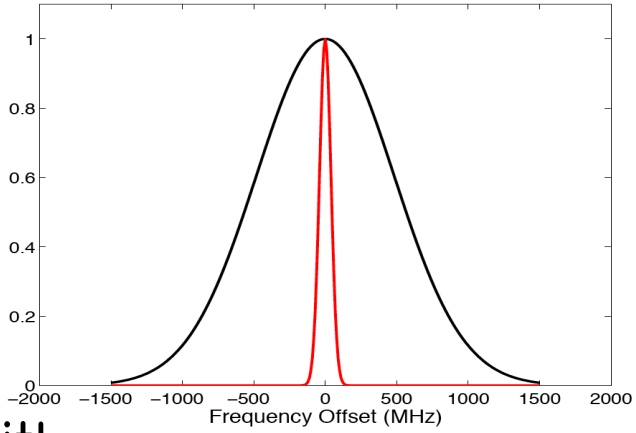
Convoluted Rayleigh Doppler Lineshape

- If scattering is produced with a single-frequency laser beam and without pressure broadening, Rayleigh scattering from atmosphere molecules experiences pure Doppler effects (Doppler shift and Doppler broadening) and exhibits a Gaussian shape.
- When the laser has finite spectral linewidth with lineshape, the return Rayleigh Doppler lineshape is a convolution of the pure Doppler Gaussian with the laser line shape.

$$\sigma_{eff}(\nu_L,\nu_o) = \int_{-\infty}^{+\infty} \sigma_{abs}(\nu,\nu_o) g_L(\nu,\nu_L) d\nu$$

where the laser spectral lineshape is normalized:

$$\int_0^{\infty} g_L(\nu,\nu_L) d\nu = 1$$



- If the laser spectral lineshape is a Gaussian,

$$g_L(\nu,\nu_L) = \frac{1}{\sqrt{2\pi}\sigma_L} \exp\left(-\frac{(\nu-\nu_L)^2}{2\sigma_L^2}\right)$$

then the convolution leads to another Gaussian with RMS linewidth

$$\sigma_{convoluted} = \sqrt{\sigma_D^2 + \sigma_L^2}$$