Classical Oscillator, I

Transition between energy levels $\Longrightarrow$ Line emission!

Emission of radiation will occur at frequency

$$h\nu = E_2 - E_1 \tag{9.34}$$

where $E_{1,2}$ energy of two levels. During transition, electron behaves as oscillator with that frequency

$\Longrightarrow$ Do semi-classical calculations, and later apply "fudge factors" (aka oscillator strength) to obtain correct quantum-mechanical result.

Line emission for transition $m \longrightarrow n$ described with Einstein A coefficient:

Power emitted per unit volume is

$$\frac{\mathrm{d}P}{\mathrm{d}V} = N_m h\nu_{mn} A_{mn} \tag{9.35}$$

where

N_m: number density of atoms in level m,

$h\nu_{mn}$: energy of transition.

Classical Oscillator, II

For harmonic oscillator, dipole moment of electron is

$$d(t) = ex(t) = ex_0 \cos(2\pi\nu_{mn}t) \tag{9.36}$$

where charge e (=electron) moves in x-direction.

Differentiation of $d(t)$ twice gives

$$\ddot{d}(t) = -4\pi^2\nu_{mn}^2 ex_0 \cos(2\pi\nu_{mn}t) \stackrel{\langle\cos^2\omega t\rangle=2}{\Longrightarrow} \langle\ddot{d}\rangle = 32\pi^4 e^2 x_0^2 \tag{9.37}$$

Compute emitted power using Larmor formula (Eq. 4.6):

$$P_{\text{oscill}} = \frac{2}{3}\frac{\langle|\ddot{d}(t)|^2\rangle}{c^3} = \frac{64\pi^4\nu_{mn}^4}{3c^3}(ex_0)^2 \tag{9.38}$$

(time averaged!).

Note that $\mathrm{d}P/\,\mathrm{d}V = P_{\text{oscill}}/N_m$, and thus

$$A_{mn} = \frac{P_{\text{oscill}}}{h\nu_{mn}} = \frac{64\pi^4\nu_{mn}^3}{3hc^3}(ex_0)^2 \tag{9.39}$$

Classical Oscillator, III

Quantum-mechanically, a formula similar to Eq. (9.39) can be derived, often written in the form

$$A_{mn} = \frac{P_{\text{oscill}}}{h\nu_{mn}} = \frac{64\pi^4\nu_{mn}^3}{3hc^3}|\mu_{mn}|^2 \sim 1.2\times10^{-2}\nu_{mn}^3\,|\mu_{mn}|^2\ \mathrm{s}^{-1} \tag{9.40}$$

where μ_{mn} is called the electric dipole matrix element, defined via

$$\mu_{mn}^2 = e^2|\langle\psi_n|r|\psi_m\rangle|^2 \tag{9.41}$$

where the ψ are the wave functions of the initial and final state.

Derivation of this formula using (time dependent) quantum mechanical perturbation theory.

From previous slide,

$$\mu_{mn}^2 \sim e^2 x_0^2 \tag{9.42}$$

For the ground state of H, $\nu_{mn} \sim 3.3\times10^{15}$ Hz and $x_0 \sim r_0$, thus

$$|\mu_{mn}|^2 \sim e^2 r_0^2 \sim 6.46\times10^{-36}\,\mathrm{cm^2esu^2} \tag{9.43}$$

and therefore

$$A_{mn} \sim 10^9\,\mathrm{s}^{-1} \tag{9.44}$$

Classical Oscillator, IV

Emission changes kinetic energy of harmonic oscillator:

$$T(t) = m_{\mathrm{e}}\dot{x}^2/2 = 2\pi^2 m_{\mathrm{e}}\nu_{mn}^2 x_0^2\cos^2(2\pi\nu_{mn}t) \tag{9.45}$$

Squaring $\ddot{d}$ from Eq. (9.37),

$$\ddot{d}^2(t) = 16\pi^4\nu_{mn}^4 e^2 x_0^2\cos^2(2\pi\nu_{mn}t) = 8\pi^2\nu_{mn}^2 e^2 T(t)/me \tag{9.46}$$

but Larmor (Eq. 4.6):

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -P_{\text{oscill}} = -\frac{2q^2\langle|\ddot{d}(t)|\rangle^2}{3c^3} = -\frac{8\pi^2e^2\nu_{mn}^2}{3m_{\mathrm{e}}c^3}\cdot T(t) = -\gamma T(t) \tag{9.47}$$

(factor 2 from taking into account the $|\ldots|$; γ is called the classical damping constant).

Because of definition of Einstein coefficient:

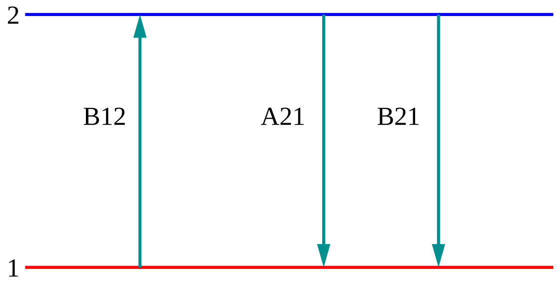
$$A_{mn,\text{classical}} = \frac{P_{\text{oscill}}}{h\nu_{mn}} = \frac{P_{\text{oscill}}}{T} = -\gamma \tag{9.48}$$

Quantum mechanics gives same result for A_{mn}, write (using exact theory):

$$A_{mn} = -3\gamma f_{mn} = \left(\frac{8\pi^2e^2}{m_{\mathrm{e}}c^3}\right)\nu_{mn}^2 f_{mn} \tag{9.49}$$

where f_{mn} is called the oscillator strength (=effective number of electrons per atom)

Einstein coefficients



Knowing the coefficient for spontaneous emission, A_{12}, calculate other Einstein coefficients with the Einstein relations

$$g_1 B_{12} = g_2 B_{21} \quad \text{and} \quad A_{21} = \frac{2h\nu_{21}^3}{c^2} B_{21} \qquad (5.27b, 5.27a)$$

such that

$$A_{mn} = \left(\frac{8\pi^2 e^2}{m_e c^3}\right) \nu_{mn}^2 f_{mn} \quad \text{and} \quad B_{mn} = \frac{4\pi^2 e^2}{h\nu_{mn} m_e c} f_{mn} = B_{nm} \qquad (9.50)$$

Reiche-Thomas-Kuhn Sum Rule

Due to the interpretation of f_{mn}, for a system with Z active electrons,

$$\sum_{n<m} f_{mn} + \sum_{n>m} f_{mn} = Z \qquad (9.51)$$

(Reiche-Thomas-Kuhn sum rule)

(total number of equivalent electrons cannot exceed total number of electrons...)

For two levels m, n the oscillator strength has the property

$$g_m f_{mn} = -g_n f_{nm} \qquad (9.52)$$

where g_m is called the statistical weight.

For a level ℓ, $g = 2\ell + 1$, for the nth shell of a H-atom, $g_n = 2n^2$.

For the H-atom, f_{mn} given to good precision by Kramers' formula (Kramers, 1923; Menzel & Pekeris, 1935):

$$f_{nm} = -\frac{g_m}{g_n} f_{mn} = \frac{2^5}{3\sqrt{3}\pi} \frac{1}{m^2} \left(\frac{1}{m^2} - \frac{1}{n^2}\right)^{-3} \left| \frac{1}{n^3} \frac{1}{m^3} \right| g_{bb} \qquad (9.53)$$

where $g_{bb} \sim 1$ is Gaunt factor for a bound-bound transition.

f-values are available on the WWW, especially at the collections of the NIST atomic data centers, `http://physics.nist.gov/PhysRefData/datarefs/introdatacen.html`.

Line Width, I

To obtain spectrum emitted by oscillator, need to take into account radiation reaction of radiating oscillator.

In dipole approximation, emission was

$$\frac{dP}{d\Omega} = \frac{2e^2 \ddot{r}^2}{3c^3} \qquad (4.92)$$

But: Emission of radiation corresponds to force

$$\boldsymbol{F} = \frac{2}{3}\frac{e^2}{c^3}\frac{d^3\boldsymbol{r}}{dt^3} \qquad (9.54)$$

on oscillator $\Longrightarrow$ damping!

Proof for this conjecture: look at work done by $\boldsymbol{F}$:

$$\langle \boldsymbol{F} \cdot \dot{\boldsymbol{r}} \rangle = \left\langle \frac{2e^2}{3c^3}\frac{d^3\boldsymbol{r}}{dt^3} \cdot \frac{d\boldsymbol{r}}{dt} \right\rangle = \left\langle \frac{2e^2}{3c^3}\frac{d}{dt}(\dot{\boldsymbol{r}} \cdot \ddot{\boldsymbol{r}}) - \frac{2e^2}{3c^3}\ddot{r}^2 \right\rangle = \frac{dP}{d\Omega} \qquad (9.55)$$

since $\langle \dot{r} \cdot \ddot{r} \rangle = 0$ because $\dot{r}$ and $\ddot{r}$ are out of phase for harmonic motion.

Line Width, II

Thus, equation of motion of oscillator:

$$m_e \ddot{r} = -m_e \omega_{mn}^2 r + \frac{2e^2}{3c^3}\frac{d^3 r}{dt^3} \qquad (9.56)$$

For weak damping, the motion is approximately harmonic $\Longrightarrow$

$$\frac{d^3 r}{dt^3} = -\omega_{mn}^2 \dot{r} \qquad (9.57)$$

such that

$$\ddot{r} = -\omega_{mn}^2 r - \gamma \dot{r} \quad \text{where} \gamma = \frac{2}{3}\frac{e^2 \omega_{mn}^2}{m_e c^3} = \frac{8\pi^2 e^2 \nu_{mn}^2}{3 m_e c^3} \ll \omega_{mn} \qquad (9.58)$$

where γ is again the classical damping constant (Eq. (9.47))

The approximate solution to Eq. (9.58) is

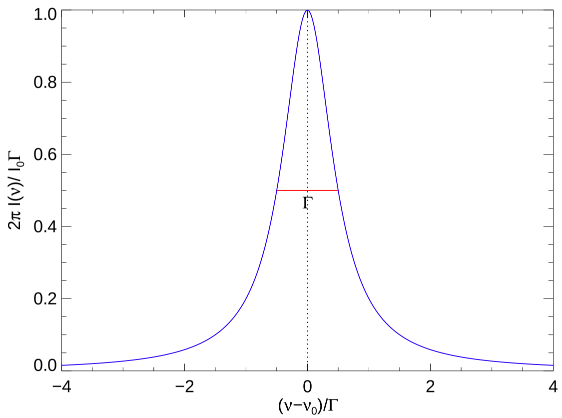
$$r(t) = r_0 \, e^{-\gamma t/2} \, e^{-i\omega_0 t} \qquad (9.59)$$

such that the electric field of the oscillator is

$$E(t) = \begin{cases} E_0 \, e^{-\gamma t/2} \, e^{-i\omega_0 t} & \text{for } t \geq 0 \\ 0 & \text{for } t < 0 \end{cases} \qquad (9.60)$$

(use real part only).

Line Width, III



The spectrum is obtained by Fourier transforming $E(t)$, to yield

$$E(\omega) = \frac{1}{2\pi}\frac{E_0}{i(\omega-\omega_0)-\gamma/2} \tag{9.61}$$

Since $I(\omega) = |E(\omega)|^2$ and inserting $\omega = 2\pi\nu$,

$$I(\nu) = I_0\left(\frac{\Gamma}{2\pi}\right)\frac{1}{(\nu-\nu_0)^2+\Gamma^2/4} \tag{9.62}$$

where

$$\Gamma = \frac{\gamma}{2\pi} = \frac{4\pi}{3}\frac{e^2\nu_0^2}{m_e c^3} \tag{9.63}$$

The profile $I(\nu)$ is called a Lorentz profile, Γ is its full width at half maximum (FWHM) and is called the natural line width.

Doppler Broadening

Many astrophysical systems are hot $\Longrightarrow$ Doppler broadening caused by the thermal motion of ions.

Number of ions at radial velocity v_r is given by Maxwell-Boltzmann distribution,

$$n(v_r)\,\mathrm{d}v_r = N\sqrt{\frac{m}{2\pi kT}}\exp\left(-\frac{mv_r^2}{2kT}\right)\,\mathrm{d}v_r \tag{9.64}$$

Doppler effect (ν_0: rest frame frequency):

$$\nu-\nu_0 = \nu_0\frac{v_r}{c} \quad\Longrightarrow\quad v_r = \frac{c(\nu-\nu_0)}{\nu_0} \tag{9.65}$$

If the natural line width is negligible $\Longrightarrow$ line profile with Doppler width, $\Delta\nu_\mathrm{D}$:

$$\phi(\nu) = \frac{1}{\Delta\nu_\mathrm{D}\sqrt{\pi}}\exp\left(-\frac{(\nu-\nu_0)^2}{\Delta\nu_\mathrm{D}^2}\right) \quad \text{where} \quad \Delta\nu_\mathrm{D} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}} \tag{9.66}$$

Often, also turbulent velocity field from macroscopic velocity fields. "microturbulence": characteristic size of turbulence $<$ mean free path $\Longrightarrow$ if stochastic (Gaussian) motions, effective Doppler width

$$\Delta\nu_\mathrm{D} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}+\xi} \tag{9.67}$$

where ξ rms measure of turbulent velocities.

Allowed Lines

Allowed lines are lines that are allowed in the dipole approximation:

- $\Delta S = 0$ (no spin flip)
- $\Delta L = 0, \pm 1$ (ang. momentum)
- $\Delta l = \pm 1$ for jumping electron
- $\Delta J = 0, \pm 1$ (but $0 \not\to 0$)
- $\Delta M_J = 0, \pm 1$ (but $0 \not\to 0$ if $\Delta J = 0$).

If from ground state, allowed lines are also called resonance lines, typically $A \sim 10^8$–$10^{13}\,\mathrm{s}^{-1}$. Mainly lie in the ultraviolet.

Example: Lyman-Series of Hydrogen (e.g., H Lα 1216Å)

Kramers' formula (Eq. 9.53) gives $f_{1n} \propto 1/n^3$, i.e., lines from higher levels to the ground state get rapidly weaker.

Lines where the dipole selection rules are not obeyed are called forbidden lines

Generally, forbidden lines observed in emission (after collisional excitation).

Forbidden Lines: M1

M1: magnetic dipole transitions: spin flip possible: $\Delta S = 1$.

For a magnetic dipole, assume a dipole moment of

$$m(t) = m_0\cos(2\pi\nu_{mn}t) \tag{9.68}$$

A similar reasoning as for electric dipoles then shows that the spontaneous emission coefficient for magnetic dipole radiation is

$$A_{mn} = \frac{64\pi^4\nu_{mn}^3}{3hc^3}|\mu_{mn}|^2 \tag{9.69}$$

where μ_{mn} is the magnetic dipole matrix element, which is generally on the order of the Bohr magneton.

For an order of magnitude estimate, take again $\nu_{mn} \sim 3.3\times10^{15}$ Hz, and

$$|\mu_{mn}|^2 = \mu_\mathrm{B}^2 = \left(\frac{eh}{4\pi m_e c}\right) = 8.6\times10^{-41}\,\mathrm{erg}^2\,\mathrm{G}^{-2} \tag{9.70}$$

such that for magnetic dipole radiation

$$A_{mn} \sim 10^4\,\mathrm{s}^{-1} \tag{9.71}$$

If A for a magnetic dipole line is much larger than $10^4\,\mathrm{s}^{-1}$: lines is called a "semi-forbidden line" (e.g., C III] 1909)

Forbidden Lines: E2

Finally, there are also electric quadrupole transitions:
$\Delta L = 0, \pm 1, \pm 2$, $\Delta J = 0, \pm 1, \pm 2$ (but still $0 \not\to 0$!).

The radiated power of a quadrupole is given by

$$P = \frac{32\pi^6 \nu_{mn}^6}{5c^5} \left(\frac{ex_0^2}{2}\right)^2 \quad (9.72)$$

where $ex_0^2/2$ is the average quadrupole moment. Thus

$$A_{mn} = \frac{32\pi^6 \nu_{mn}^5}{5hc^5} \cdot \mu \quad (9.73)$$

where μ is the quadrupole matrix element.

For the H-atom, take again $\nu_{mn} \sim 10^{15}$ Hz and note

$$\mu \sim a_0^4 e^2 \sim 1.6 \times 10^{-52}\,\mathrm{cm}^4\,\mathrm{esu}^2 \quad (9.74)$$

where a_0 is the radius of the first Bohr orbit. Thus

$$A_{mn} \sim 10\,\mathrm{s}^{-1} \quad (9.75)$$

(e.g., [O III] 5007Å)

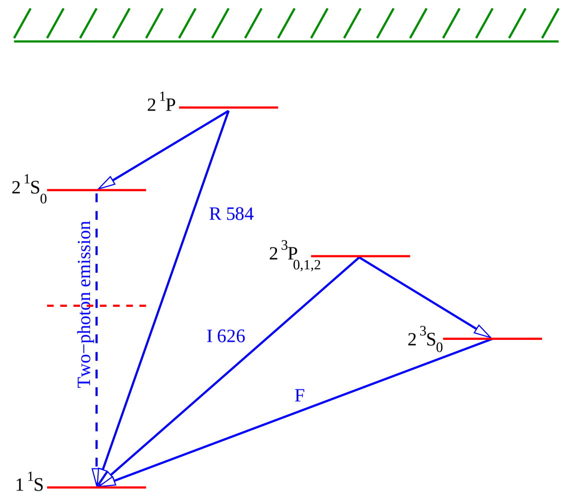
Some further lingo

Fine-structure lines are forbidden lines within ground state multiplet, usually seen in IR (e.g., C II 158μm, ${}^2P_{3/2} \to {}^2P_{1/2}$), seen from cool gas.

Hyperfine-structure lines: nucleus also has influence, e.g., electron spin-flip to produce 21 cm line.

Satellite lines: lines produced from excited ions (e.g., atoms where inner-shell electrons are missing)
$\Longrightarrow$ perturbed energy levels
$\Longrightarrow$ slightly different line energies
$\Longrightarrow$ Lines are "satellites" to the lines from ions in the ground state.

Summary



He term scheme, I: "intercombination line"