X. Forbidden Transitions

A. Quantum Mechanics (Physics)

- Electric dipole selection rules
  - ◇ Matrix element

$$<\phi_f|\hat{\varepsilon}\cdot\vec{r}\,|\phi_i>$$

  - ◇ $\vec{r}$ is a rank 1 spherical vector
    - ▲ $\Delta\ell = 0, \pm 1$
    - ▲ $\ell : 0 \to 0$ is forbidden
    - ▲ $\Delta m = 0, \pm 1$
  - ◇ Spin: $\Delta S = 0$
  - ◇ Parity: $\Delta\ell = 0$ is forbidden
- Electric Quadrapole
  - ◇ Expand $e^{i\vec{k}\cdot\vec{r}}$ beyond the dipole approximation

$$e^{i\vec{k}\cdot\vec{r}} = 1 + i\vec{k}\cdot\vec{r} + \ldots \tag{1}$$

  - ◇ Forbidden transition → The '1' term vanishes in the matrix element
  - ◇ Quadrapole matrix element

$$<\phi_f|i\vec{k}\cdot\vec{r}\,\hat{\varepsilon}\cdot\vec{p}\,|\phi_i> = i\vec{k}\cdot<\phi_f|\vec{r}\vec{p}\,|\phi_i>\cdot\hat{\varepsilon} \tag{2}$$

  - ◇ Following E+M treatment of higher order moments, express as the sum of a symmetric and antisymmetric operator

$$\vec{r}\vec{p} = \frac{1}{2}\left(\vec{r}\vec{p}+\vec{p}\vec{r}\right) + \frac{1}{2}\left(\vec{r}\vec{p}-\vec{p}\vec{r}\right) \tag{3}$$

  - ◇ Examine the symmetric operator

$$\vec{r}\vec{p}+\vec{p}\vec{r} = \vec{r}\frac{im}{\hbar}[H_0,\vec{r}\,] + \frac{im}{\hbar}[H_0,\vec{r}\,]\vec{r} \tag{4}$$

$$= \frac{im}{\hbar}[H_0,\vec{r}\vec{r}\,] \tag{5}$$

  - ◇ For correspondence with classical E+M, consider

$$\vec{Q} \equiv -\left(3\vec{r}\vec{r} - |r|^2\hat{\varepsilon}\right) \tag{6}$$

    - ▲ Clearly, $\vec{k}\cdot<\phi_f|r^2\hat{\varepsilon}|\phi_i>\cdot\hat{\varepsilon} = 0$
    - ▲ Replace our symmetric piece with $\vec{Q}$

◇ Altogether now, for the electric quadrapole

$$<\phi_f|\vec{r}\vec{p}|\phi_i> = \frac{m}{6\hbar}<\phi_f|[H_0,\vec{Q}]|\phi_i> \tag{7}$$
$$= \frac{m}{6\hbar}\left(E_f - E_i \right)\vec{Q}_{fi} \tag{8}$$
$$= \frac{m\omega_{fi}}{6}\vec{Q}_{fi} \tag{9}$$

◇ $\vec{Q}$ is a rank two spherical tensor: $T_q^{(2)}$

▲ Recall Wigner-Eckert

▲ Selection rules

$$<\alpha, j'm'|T_q^{(2)}|\alpha, jm> \tag{10}$$

- $\Delta j = 0, \pm 1, \pm 2$
- $0 \to 0$ is forbidden
- $\Delta m = q = 0, \pm 1, \pm 2$

▲ Parity: $\vec{Q}$ is symmetric under the exchange $\vec{r} \to -\vec{r}$

- Initial and final states must have the same parity
- $\Delta\ell \neq \pm 1$ for Hydrogenic ions

- Magnetic Dipole Transitions

◇ Consider the antisymmetric part of $\vec{r}\vec{p}$

$$\vec{k}\cdot\left(\vec{r}\vec{p} - \vec{p}\vec{r}\right)\cdot\hat{\varepsilon} = \left(\vec{k}\times\hat{\varepsilon}\right)\cdot\left(\vec{r}\times\vec{p}\right) \tag{11}$$

◇ Identifying $\vec{r}\times\vec{p} = \vec{L}$, we define

$$\vec{M} = -\frac{e}{2m_e c}\vec{L} \tag{12}$$

◇ Selection rules

▲ Express

$$\vec{L} = \frac{1}{2}L_+\left(\hat{x} + i\hat{y}\right) + \frac{1}{2}L_-\left(\hat{x} - i\hat{y}\right) + L_z\hat{z} \tag{13}$$

- L_+, L_-, L_z all leave ℓ unchanged
- L_+, L_- change m by ± 1

▲ Rules

$$\Delta\ell = 0$$
$$\Delta m = 0, \pm 1$$

- Because the matrix element has no $\vec{r}$ dependence,

$$\Delta n = 0 \tag{14}$$

- Complementary of the multipole transitions
  - ◇ Selection rules of one multipole generally preclude the others
  - ◇ Therefore, mixing of the terms is rare
  - ◇ One exception (to be discussed shortly) are the forbidden [OIII] lines where the states are linear combinations of the 'pure' multipole states
- Strictly forbidden transitions
  - ◇ Definition: Transitions for which the matrix element vanishes to all perturbational order
  - ◇ e.g. $2s \to 1s$ in Hydrogen
  - ◇ Requires two photon process
- Astrophysics
  - ◇ Violation of $\Delta S = 0 \Rightarrow$ semi-forbidden transition: CIII]
  - ◇ Violation of other rules (e.g. parity) $\Rightarrow$ forbidden: [OIII]

B. Astrophysical Forbidden Lines

- These states are generally excited by collisions
  - ◇ Important diagnostics of density and temperature
  - ◇ e.g. [OIII], [OII]
- [OIII]
  - ◇ Configuration: $1s^2 2s^2 2p^2$
  - ◇ Two equivalent p electrons (sound familiar?)
    - ▲ Allowed states: ${}^1S_0; {}^3P_{0,1,2}; {}^1D_2$
    - ▲ Other states are excluded by Pauli
  - ◇ Relative energies: Hund's Rules
    - (a) Higher $S \Rightarrow$ Lower energy
      ${}^3P_J$ has lowest energy
    - (b) Higher $L \Rightarrow$ Lower energy
      ${}^1D_2$ has lower energy than ${}^1S_0$
    - (c) Higher $J \Rightarrow$ Higher energy for less than half filled
      ${}^3P_0$ has lower energy than ${}^3P_1$, etc.
  - ◇ Wavelengths
    ${}^1S_0 \to {}^1D_2 \quad \lambda = 4363$Å
    ${}^1D_2 \to {}^3P_2 \quad \lambda = 5007$Å
    ${}^1D_2 \to {}^3P_1 \quad \lambda = 4959$Å
    ${}^1D_2 \to {}^3P_0 \quad \lambda = 4931$Å
  - ◇ Fig
  - ◇ Transitions between any two of these states is forbidden

- ▲ No change in parity
- ▲ Parity of two p electrons is always even

- [OII]
  - ◇ Configuration: $1s^2 2s^2 2p^3$
  - ◇ Three equivalent p electrons
    - ▲ Add 1 equivalent p electron to the $2p^2$ states
    - ▲ Allowed states: ${}^4S_{\frac{3}{2}}$; ${}^2P_{\frac{1}{2},\frac{3}{2}}$; ${}^2D_{\frac{3}{2},\frac{5}{2}}$
  - ◇ Relative energies: Hund's Rules
    (a) Higher $S \Rightarrow$ Lower energy
        ${}^4S_{\frac{3}{2}}$ has lowest energy
    (b) Higher $L \Rightarrow$ Lower energy
        ${}^2D_{\frac{3}{2},\frac{5}{2}}$ are second
    (c) Half full $\Rightarrow$ All bets are off ${}^2P_{\frac{1}{2}}$ is higher than ${}^3P_{\frac{3}{2}}$
        ${}^2D_{\frac{3}{2}}$ is higher than ${}^2D_{\frac{5}{2}}$
  - ◇ Wavelengths
    ${}^2D_{\frac{3}{2}} \rightarrow {}^4S_{\frac{3}{2}} \quad \lambda = 3726\text{Å}$
    ${}^2D_{\frac{5}{2}} \rightarrow {}^4S_{\frac{3}{2}} \quad \lambda = 3729\text{Å}$
  - ◇ Fig
  - ◇ Transitions between any two of these states is forbidden
    - ▲ No change in parity
    - ▲ Parity of three p electrons is always odd

C. Astrophysical Implications of Forbidden Lines

- Key concepts
  (a) Gas is optically thin to forbidden lines (no radiative transfer)
  (b) Excited levels of forbidden lines are populated by collisions $\Rightarrow$ sensitive to n_e or T

- Collisional excitation
  - ◇ Cross-section (velocity)
    - ▲ Excitation

$$\sigma_{12}(v) = \frac{\pi\hbar^2}{m^2v^2}\frac{\Omega(1,2)}{g_1} \qquad \left(\frac{1}{2}mv^2 > \chi\right) \tag{15}$$

      - ○ $\Omega(1,2)$ is the 'collision strength' (Quantum)
      - ○ $\chi = h\nu_{12}$
    - ▲ De-excitation
      - ○ Detailed balance (Milne's relation)

$$g_1 v_1^2 \sigma_{12}(v_1) = g_2 v_2^2 \sigma_{21}(v_2) \tag{16}$$

- where

$$\frac{1}{2}mv_1^2 = \frac{1}{2}mv_2^2 + \chi \tag{17}$$

- Cross-section (thermal equilibrium)
  - De-excitation rate per unit time per unit volume

$$n_e n_2 q_{21} = n_e n_2 \int_0^\infty v\sigma_{21}(v) f(v) dv \tag{18}$$

$$= n_e n_2 \frac{8.629 \times 10^{-6}}{T^{\frac{1}{2}}} \frac{\Omega(1,2)}{g_2} \tag{19}$$

  - Excitation rate: Boltzmann population

$$q_{12} = \frac{g_2}{g_1} q_{21} \mathrm{e}^{-\chi/kT} \tag{20}$$

- Collision strengths: $\Omega(1,2)$
  - Computed via quantum mechanics (order unity)
  - Complicated by resonances, but generally have slow T dependence
  - Tabulated in Osterbrock
  - Useful relation

$$\Omega(S'L'J', SLJ) = \frac{(2J+1)}{(2S+1)(2L+1)}\, \Omega(S'L', SL) \tag{21}$$

    - Primes refer to excited state
    - Holds only if $S = 0$ or $L = 0$
    - Factors $(2J+1)$, etc. are simply the degeneracy
- Equilibrium equation
  - De-excitations balance excitations
  - Two level system

$$n_e n_1 q_{12} = n_e n_2 q_{21} + n_2 A_{21} \tag{22}$$

    - First term is collisional de-excitation
    - A_{21} is spontaneous emission (dominant for low n_e)
  - Rearranging

$$\frac{n_2}{n_1} = \frac{n_e q_{12}}{A_{21}} \left[\frac{1}{1 + \frac{n_e q_{21}}{A_{21}}} \right] \tag{23}$$

    - $n_e q_{21}/A_{21}$ is referred to as the critical density
    - Marks transition from spontaneous $\rightarrow$ collisional de-excitation

▲ Multi-level system

$$\sum_{j\neq i} n_j n_e q_{ji} + \sum_{j>i} n_j A_{ji} = \sum_{j\neq i} n_i n_e q_{ij} + \sum_{j<i} n_i A_{ij} \tag{24}$$

∘ Constraint: $\sum n_j = n$

∘ Messy algebra but otherwise straightforward

• [OIII]: Temperature diagnostic

⋄ Low density limit ($n_e < 10^5\,\mathrm{cm}^{-3}$)

⋄ Key: Every excitation is followed by spontaneous emission of a photon

⋄ Excitation of ^1D level

▲ Followed by emission of λ_{5007} or λ_{4959} photon

▲ Relative probabilities $\to A_{^1D,^3P_2} : A_{^1D,^3P_1} \approx 3$

⋄ Excitation of ^1S level

▲ Emission of $\lambda_{4363}(^1D_2)$ or $\lambda_{2321}(^3P_1)$ photon

▲ Relative probabilities $\to A_{^1S,^1D} : A_{^1S,^3P_1} \approx 10$

▲ Emission of λ_{4363} is followed by λ_{5007} or λ_{4959} photon (small contribution)

⋄ Emission line strength (energy/s/volume)

▲ Consider $^1S \to {}^1D$

$$j_{4363} = \left[\text{rate}^1S \text{ is populated}\right] \times \left[\,h\nu(4363)\,\right] \times \left[\text{rate}\,^1S \to\ ^1D\right] \tag{25}$$

∘ Collisional excitation rate

$$n_{^3P}\ q_{^3P,^1S} = \frac{n_{^3P}\ 8.629 \times 10^{-6}\ \Omega(^3P,^1S)\ \mathrm{e}^{-h\nu(^1S,^1D)/kT}}{T^{\frac{1}{2}} g_{^3P}} \tag{26}$$

∘ Rate $^1S \to\ ^1D_2$: Ratio of spontaneous emission coefficient

$$\frac{A_{^1S,^1D}}{A_{^1S,^1D} + A_{^1S,^3P_1}} \tag{27}$$

∘ Altogether

$$j_{4363} \propto \frac{n_{^3P}\Omega(^3P,^1S)\ \mathrm{e}^{h\nu(^1S,^1D)/kT}}{T^{\frac{1}{2}} g_{^3P}}\ \frac{\nu(^1S,^1D) A_{^1S,^1D}}{A_{^1S,^1D} + A_{^1S,^3P_1}} \tag{28}$$

▲ Consider $^1D \to {}^3P$

∘ Convenient to consider the two channels together

$$j_{4959} + j_{5007} \propto \frac{n_{^3P}\Omega(^3P,^1D)\ \mathrm{e}^{-h\nu(^1D,^3P)/kT}}{T^{\frac{1}{2}} g_{^3P}}\ \bar{\nu}(^1D,^3P) \tag{29}$$

- where

$$\bar{\nu}(^1D,^3P) = \frac{\nu(^1D,^3P_2)A_{^1D,^3P_2} + \nu(^1D,^3P_1)A_{^1D,^3P_1}}{A_{^1D,^3P_2} + A_{^1D,^3P_1}} \tag{30}$$

- For higher accuracy, we should include the contribution of de-excitations from the $^1S \rightarrow {}^1D$ transition
- But, these are small for $T < 30000$K

◇ Emission-line ratio

$$\frac{j_{4959} + j_{5007}}{j_{4363}} = \frac{\Omega(^3P,^1D)}{\Omega(^3P,^1S)} \frac{A_{^1S,^1D} + A_{^1S,^3P}}{A_{^1S,^1D}} \frac{\bar{\nu}(^3P,^1D)}{\nu(^1S,^1D)} e^{\Delta E/kT} \tag{31}$$

▲ $\Delta E = h\nu(^1S,^1D)$

▲ The only physical dependence of the line ratio is temperature

▲ Excellent T diagnostic for low density regimes

▲ At higher n_e, collisional de-excitation is important and ^1D is preferentially weakened.

▲ Can correct equation (31) by a factor

$$f = [\text{See Osterbrock p. 121}] \tag{32}$$

◇ Useful expression (not quite exact)

$$\frac{j_{4959} + j_{5007}}{j_{4363}} = \frac{6.91 \exp\left[\,(2.5 \times 10^4)/T\,\right]}{1 + 2.5 \times 10^{-3}(n_e/T^{\frac{1}{2}})} \tag{33}$$

- [OII]: Density diagnostic

◇ Pair of emission lines with very nearly the same energy $\Rightarrow$ $e^{\Delta E/kT} \approx 1$

◇ Low density limit: Every collisional excitation is followed by a spontaneous emission

$$\frac{j_{3729}}{j_{3726}} \propto \frac{\Omega(^4S,^2D_{\frac{5}{2}})\ \nu(^4S,^2D_{\frac{5}{2}})}{\Omega(^4S,^2D_{\frac{3}{2}})\ \nu(^4S,^2D_{\frac{3}{2}})} e^{-\Delta E/kT} \tag{34}$$

▲ $\Delta E \ll kT$ for reasonable T $\Rightarrow$ $e^{-\Delta E/kT} \approx 1$

▲ $\nu(^4S,^2D_{\frac{5}{2}})/\nu(^4S,^2D_{\frac{3}{2}}) \approx 1$

▲ Equation (21) $\Rightarrow$ $\Omega(^4S,^2D_{\frac{5}{2}}) = \frac{3}{2}\Omega(^4S,^2D_{\frac{3}{2}})$

▲ Therefore

$$\frac{j_{3729}}{j_{3726}} \propto 1.5 \qquad (n_e \ll 10^3\,\text{cm}^{-3}) \tag{35}$$

◇ High density limit: Levels are Boltzmann populated

$$\frac{j_{3729}}{j_{3726}} = \frac{g_{3729}}{g_{3726}} \frac{A_{3729}}{A_{3726}} = 0.3 \tag{36}$$

◇ Transition between these two regimes occurs at the critical density

$$n_e = \frac{A}{q} \approx \begin{cases} 3 \times 10^3\,\mathrm{cm}^{-3} & {}^2D_{\frac{5}{2}} \\ 1.6 \times 10^4\,\mathrm{cm}^{-3} & {}^2D_{\frac{3}{2}} \end{cases} \tag{37}$$

◇ Fig