Perturbation methods

2018/6/7

Outline

- Basic principle
- Degenerate case
- Stark Effect
- Fine structure
- Hyperfine structure

Time independent

- Assume that the Hamiltonian is a sum of two terms,

$$H = H_0 + \lambda H_1$$

- Let {IΦ_n>} be a complete set of eigenstates of the unperturbed Hamiltonian H_0 with energy eigenvalues $E^{(0)}{}_n$

$$H_0 \left| \phi_n \right\rangle = E_n^{(0)} \left| \phi_n \right\rangle$$

- The eigenstates {Iψ>} and eigenvalues {E_n} of the complete Hamiltonian H

$$H \left| \psi_n \right\rangle = E_n \left| \psi_n \right\rangle$$

To express H with a matrix

- choose basis of $|\Phi_n>$
- The diagonal elements are original eigenvalues

$$H_{mn} = \langle \phi_m | H | \phi_n \rangle = E_m^{(0)} \delta_{mn} + \langle \phi_m | \lambda H_1 | \phi_n \rangle$$

Non-degenerate case

- unperturbed results

$$\lambda << 1 \qquad |\psi_n\rangle \simeq |\phi_n\rangle \qquad E_n \simeq E_n^{(0)}$$

- To express Iψ> using complete set IΦ_n>

$$|\psi_n\rangle = N(\lambda)\left(|\phi_n\rangle + \sum_{k\neq n} C_{nk}(\lambda)|\phi_k\rangle\right)$$

$$\langle\psi_n|\psi_n\rangle = 1$$

power series expansion

- Perturbation theory evaluates the eigenvalues E_n, and the coefficients C_{nk}, as power series in λ

- coefficients

$$C_{nk}(\lambda) = \lambda C_{nk}^{(1)} + \lambda^2 C_{nk}^{(2)} + \cdots$$

- eigenenergy

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

Expansion

- The Schrodinger equation

$$\left(H_0+\lambda H_1\right)\left\{\left|\phi_n\right\rangle+\sum_{k\neq n}\lambda C_{nk}^{(1)}\left|\phi_k\right\rangle+\sum_{k\neq n}\lambda^2 C_{nk}^{(2)}\left|\phi_k\right\rangle+\cdots\right\}$$

$$=\left(E_n^{(0)}+\lambda E_n^{(1)}+\lambda^2 E_n^{(2)}+\cdots\right)\left\{\left|\phi_n\right\rangle+\sum_{k\neq n}\lambda C_{nk}^{(1)}\left|\phi_k\right\rangle+\sum_{k\neq n}\lambda^2 C_{nk}^{(2)}\left|\phi_k\right\rangle+\cdots\right\}$$

- the 1st order

$$H_0\sum_{k\neq n}\lambda C_{nk}^{(1)}\left|\phi_k\right\rangle+\lambda H_1\left|\phi_n\right\rangle=E_n^{(0)}\sum_{k\neq n}\lambda C_{nk}^{(1)}\left|\phi_k\right\rangle+\lambda E_n^{(1)}\left|\phi_n\right\rangle$$

energy shift

$$H_0 \sum_{k \neq n} \lambda C_{nk}^{(1)} \left| \phi_k \right\rangle + \lambda H_1 \left| \phi_n \right\rangle = E_n^{(0)} \sum_{k \neq n} \lambda C_{nk}^{(1)} \left| \phi_k \right\rangle + \lambda E_n^{(1)} \left| \phi_n \right\rangle$$

$$E_k \sum_{k \neq n} C_{nk}^{(1)} \left| \phi_k \right\rangle + H_1 \left| \phi_n \right\rangle - E_n^{(0)} \sum_{k \neq n} C_{nk}^{(1)} \left| \phi_k \right\rangle = E_n^{(1)} \left| \phi_n \right\rangle$$

$$H_1 \left| \phi_n \right\rangle + \sum_{k \neq n} \left(E_k^{(0)} - E_n^{(0)} \right) C_{nk}^{(1)} \left| \phi_k \right\rangle = E_n^{(1)} \left| \phi_n \right\rangle$$

$$E_n^{(1)} \simeq \left\langle \phi_n \right| H_1 \left| \phi_n \right\rangle$$

- energy shift

$$\lambda E_n^{(1)} \simeq \left\langle \phi_n \right| \lambda H_1 \left| \phi_n \right\rangle$$

wavefunction change

- choose m<>n

$$\langle \phi_m | H_1 | \phi_n \rangle + \left(E_m^{(0)} - E_n^{(0)} \right) C_{nm}^{(1)} = 0$$

$$C_{nm}^{(1)} = \frac{\langle \phi_m | H_1 | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}}$$

- wavefunction change

$$\lambda C_{nm}^{(1)} = \frac{\langle \phi_m | \lambda H_1 | \phi_n \rangle}{E_n^{(0)} - E_m^{(0)}}$$

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{k \neq n} \frac{\langle \phi_k | \lambda H_1 | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} |\phi_k\rangle$$

2nd order

- 2nd order

$$H_0 \sum_{k\neq n} C_{nk}^{(2)} \left|\phi_k\right\rangle + H_1 \sum_{k\neq n} C_{nk}^{(1)} \left|\phi_k\right\rangle$$

$$= E_n^{(2)} \left|\phi_n\right\rangle + E_n^{(1)} \sum_{k\neq n} C_{nk}^{(1)} \left|\phi_k\right\rangle + E_n^{(0)} \sum_{k\neq n} C_{nk}^{(2)} \left|\phi_k\right\rangle$$

- energy change

$$H_0 \sum_{k\neq n} C_{nk}^{(2)} \left|\phi_k\right\rangle = \sum_{k\neq n} E_k^{(0)} C_{nk}^{(2)} \left|\phi_k\right\rangle$$

$$E_n^{(2)} = \left\langle\phi_n\right| H_1 \sum_{k\neq n} C_{nk}^{(1)} \left|\phi_k\right\rangle = \sum_{k\neq n} C_{nk}^{(1)} \left\langle\phi_n\right| H_1 \left|\phi_k\right\rangle$$

$$= \sum_{k\neq n} \frac{\left\langle\phi_n\right| H_1 \left|\phi_k\right\rangle \left\langle\phi_k\right| H_1 \left|\phi_n\right\rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$= \sum_{k\neq n} \frac{\left|\left\langle\phi_n\right| H_1 \left|\phi_k\right\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$$

Degenerate case

- When there are degenerate states, the perturbation breaks down $E_n = E_k$
- To solve this problem, we may diagonize the perturbation in the degeneracy subspace

Example: 3-level system

- consider a model Hamiltonian

degeneracy subspace

$$H_0 = \begin{pmatrix} E^{(0)} & 0 & 0 \\ 0 & E^{(0)} & 0 \\ 0 & 0 & E_3^{(0)} \end{pmatrix} \qquad H_1 = \begin{pmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{pmatrix}$$

- Diagonize H using a unitary transformation

$$UHU^{\dagger} = H_D$$

$$H_D = \begin{pmatrix} E^{(0)} + \lambda w_1 & 0 & \lambda h_{13} \\ 0 & E^{(0)} + \lambda w_2 & \lambda h_{23} \\ \lambda h_{31} & \lambda h_{32} & E_3^{(0)} + \lambda h_{33} \end{pmatrix}$$

$$w_1, w_2 = \frac{h_{11} + h_{22}}{2} \pm \sqrt{\left(\frac{h_{11} - h_{22}}{2}\right)^2 + h_{12}h_{21}}$$

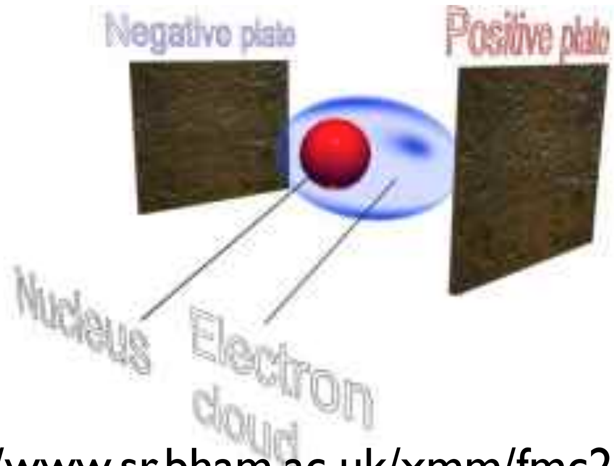
- then the degeneracy is lifted

The Stark effect

- Atom in the E-field

$$H_0 = \frac{p^2}{2\mu} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\lambda H_1 = e\mathcal{E} z$$



http://www.sr.bham.ac.uk/xmm/fmc2.html

- 1st order energy shift for ground state

$$E_{100}^{(1)} = e\mathcal{E} \langle \phi_{100} | z | \phi_{100} \rangle = e\mathcal{E} \int d^3 r \left| \phi_{100}(r) \right|^2 z = 0$$

because of parity symmetry

2nd order shift

- 2nd order shift

$$E_{100}^{(2)} = e^2 \mathcal{E}^2 \left\{ \sum_{nlm} \frac{\left| \langle \phi_{nlm} | z | \phi_{100} \rangle \right|^2}{E_1^{(0)} - E_n^{(0)}} + \sum_k \frac{\left| \langle \phi_k | z | \phi_{100} \rangle \right|^2}{E_1^{(0)} - \dfrac{\hbar^2 k^2}{2m}} \right\}$$

$E > 0$ $\quad |\phi_k\rangle$ unbound state

$E < 0$ $\quad |\phi_{nlm}\rangle$ bound state

$$E_{100}^{(2)} = e^2 \mathcal{E}^2 \sum_{E \neq E_1} \frac{\left| \langle \phi_E | z | \phi_{100} \rangle \right|^2}{E_1^{(0)} - E}$$

2nd order shift

- The upper-bound of energy shift

$$-E_{100}^{(2)} \le e^2\mathcal{E}^2 \frac{1}{E_2^{(0)} - E_1^{(0)}} \sum_{E \neq E_1} \left|\langle \phi_{100} | z | \phi_E \rangle\right|^2 = e^2\mathcal{E}^2 \frac{1}{E_2^{(0)} - E_1^{(0)}} \sum_{E} \left|\langle \phi_{100} | z | \phi_E \rangle\right|^2$$

$$-E_{100}^{(2)} \le e^2\mathcal{E}^2 \frac{1}{E_2^{(0)} - E_1^{(0)}} \langle \phi_{100} | z^2 | \phi_{100} \rangle$$

$$\langle \phi_{100} | z^2 | \phi_{100} \rangle = \langle \phi_{100} | x^2 | \phi_{100} \rangle = \langle \phi_{100} | y^2 | \phi_{100} \rangle$$
$$= \frac{1}{3} \langle \phi_{100} | r^2 | \phi_{100} \rangle = a_0^2$$

$$E_2^{(0)} - E_1^{(0)} = -\frac{1}{2} m_e c^2 \alpha^2 \left(\frac{1}{4} - 1 \right) = \frac{3}{8} m_e c^2 \alpha^2$$

2nd order shift

- energy shift

$$-E_{100}^{(2)} \le e^2 \mathcal{E}^2 \frac{8}{3} \frac{a_0^2}{m_e c^2 \alpha^2} = \frac{8}{3}\left(4\pi\varepsilon_0 \mathcal{E}^2\right) a_0^3$$

$$-E_{100}^{(2)} = (\mathrm{cosnt})\left(4\pi\varepsilon_0 \mathcal{E}^2\right) a_0^3 = \frac{9}{4}\left(4\pi\varepsilon_0 \mathcal{E}^2\right) a_0^3$$

n=2 state

- 4-level degeneracy

$$|\phi_{200}\rangle$$
$$|\phi_{211}\rangle$$
$$|\phi_{210}\rangle$$
$$|\phi_{2,1,-1}\rangle$$

- parity: *l*=0 even, *l*=1 odd

symmetry of H_1

- the perturbation commute with L_z

$$[z, L_z] = 0$$

- matrix elements of H_1 involving states with different m are zero

$$\langle l,m | L_z H_1 - H_1 L_z | l',m' \rangle = 0 \qquad (m - m') \langle l,m | H_1 | l',m' \rangle = 0$$

- Only the matrix elements need to be considered

$$\langle \phi_{200} | H_1 | \phi_{210} \rangle \qquad \langle \phi_{200} | H_1 | \phi_{200} \rangle \qquad \langle \phi_{210} | H_1 | \phi_{210} \rangle$$

degenerate case

- With the technique of degenerate perturbation

$$e\mathcal{E}\begin{pmatrix} \langle\phi_{200}|z|\phi_{200}\rangle & \langle\phi_{200}|z|\phi_{210}\rangle \\ \langle\phi_{210}|z|\phi_{200}\rangle & \langle\phi_{210}|z|\phi_{210}\rangle \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = E^{(1)}\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

$$e\langle\phi_{200}|z|\phi_{210}\rangle = \left[\int \frac{e^{-r/a_0}}{(2a_0)^3}\frac{2r}{\sqrt{3}a_0}\left(1-\frac{r}{2a_0}\right)rr^2dr\right]\left[\int d\Omega Y_{00}^{*}\sqrt{\frac{4\pi}{3}}Y_{10}Y_{10}\right] = -3a_0$$

$$\langle\phi_{200}|H_1|\phi_{200}\rangle = \langle\phi_{210}|H_1|\phi_{210}\rangle = 0$$

energy shift for m=0 states

- The eigenvalues

$$-3e\mathcal{E}a_0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = E^{(1)}\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

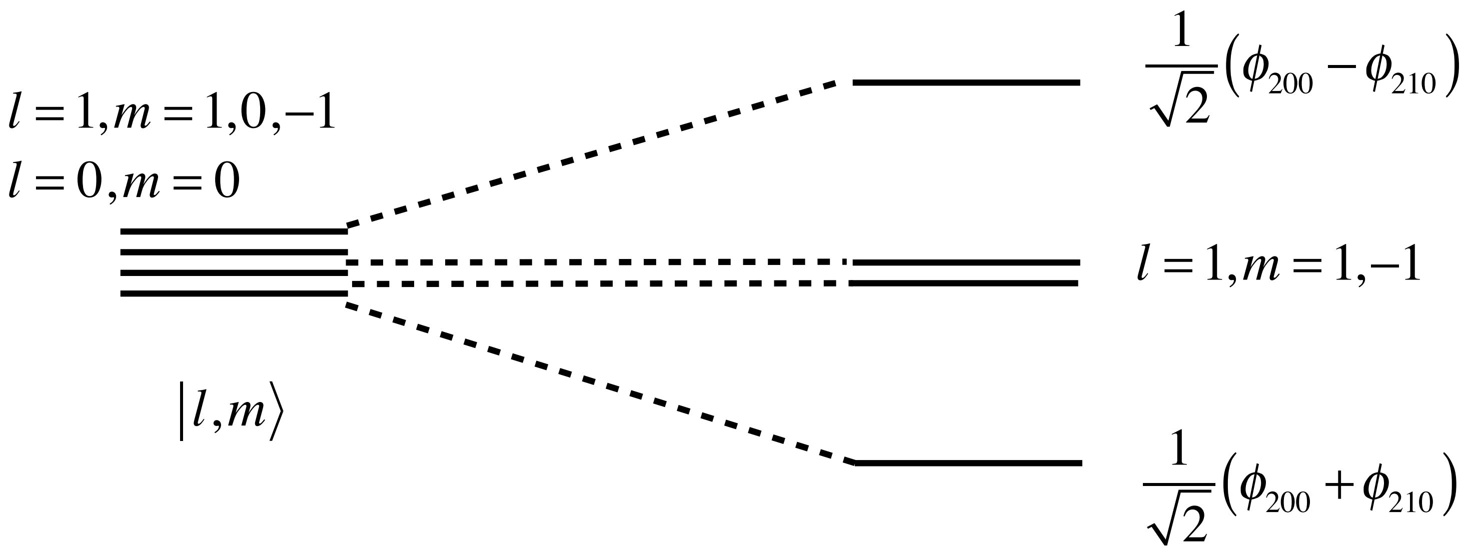
$$E^{(1)} = \pm 3e\mathcal{E}a_0$$

- The eigenstates

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

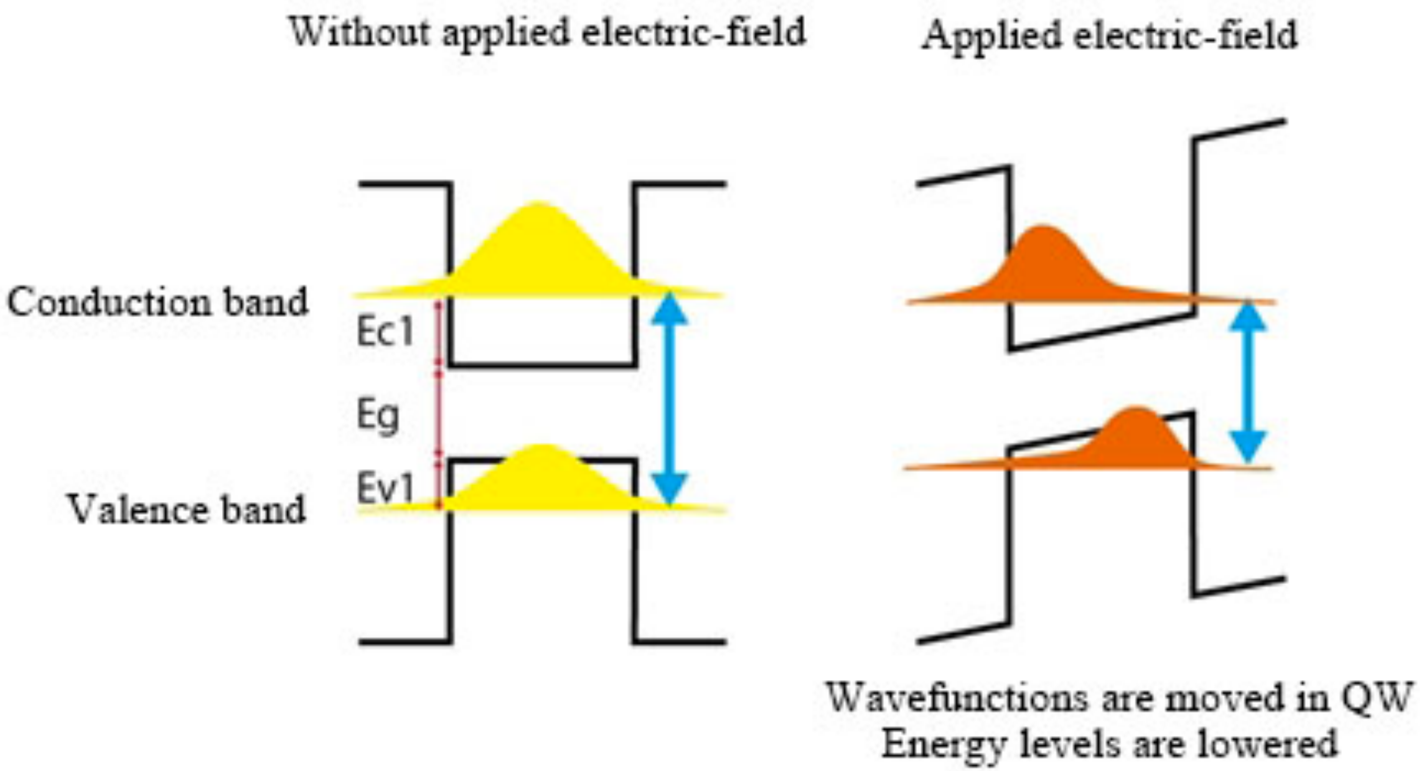
$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Stark shift for n=2 states



- The electron may tunnel out if E is strong

Stark effect in Q well



http://pweb.cc.sophia.ac.jp/shimolab/html-e/qcse-e.html

Fine structure

- The fine structure of hydrogen atom contains the relativistic correction and SOI
- The relativistic correction for the kinetic energy is

$$K = \sqrt{p^2c^2 + m_e^2c^4} - m_ec^2 = \frac{p^2}{2m_e} - \frac{1}{8}\frac{p^4}{m_e^3c^2} + \cdots$$

$$H_1 = -\frac{1}{8}\frac{p^4}{m_e^3c^2}$$

- spin orbital interaction(SOI)

$$H_2 = \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2m_e^2c^2r^3}\mathbf{S}\cdot\mathbf{L}$$

Relativistic correction

- 1st order energy correction

$$H_0 = \frac{p^2}{2m_e} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\begin{aligned}
\langle \phi_{nlm} | H_1 | \phi_{nlm} \rangle &= -\frac{1}{2m_e c^2} \langle \phi_{nlm} | \left(\frac{p^2}{2m_e} \right)^2 | \phi_{nlm} \rangle \\
&= -\frac{1}{2m_e c^2} \langle \phi_{nlm} | \left(H_0 + \frac{Ze^2}{4\pi\varepsilon_0 r} \right)^2 | \phi_{nlm} \rangle \\
&= -\frac{1}{2m_e c^2} \langle \phi_{nlm} | \left(E_n + \frac{Ze^2}{4\pi\varepsilon_0 r} \right)^2 | \phi_{nlm} \rangle \\
&= -\frac{1}{2m_e c^2} \left[E_n^2 + 2E_n \frac{Ze^2}{4\pi\varepsilon_0} \langle \phi_{nlm} | \frac{1}{r} | \phi_{nlm} \rangle + \left(\frac{Ze^2}{4\pi\varepsilon_0} \right)^2 \langle \phi_{nlm} | \frac{1}{r^2} | \phi_{nlm} \rangle \right]
\end{aligned}$$

1st-order energy shift

$$\langle\phi_{nlm}|H_1|\phi_{nlm}\rangle = -\frac{1}{2m_ec^2}\left[E_n^2 + 2E_n\frac{Ze^2}{4\pi\varepsilon_0}\langle\phi_{nlm}|\frac{1}{r}|\phi_{nlm}\rangle + \left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2\langle\phi_{nlm}|\frac{1}{r^2}|\phi_{nlm}\rangle\right]$$

$$= -\frac{1}{2m_ec^2}\left[\left(\frac{m_ec^2\alpha^2}{2}\frac{Z^2}{n^2}\right)^2 + 2\frac{m_ec^2\alpha^2}{2}\frac{Z^2}{n^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\frac{Z}{a_0n^2} + \left(\frac{Ze^2}{4\pi\varepsilon_0}\right)^2\frac{2Z^2}{a_0^2n^3(2l+1)}\right]$$

$$= -\frac{1}{2m_ec^2}\left[\left(\frac{m_ec^2\alpha^2}{2}\frac{Z^2}{n^2}\right)^2 - 2\frac{m_ec^2\alpha^2}{2}\frac{Z^4}{n^4}(\alpha\hbar c)\left(\frac{\alpha m_ec}{\hbar}\right) + (\alpha\hbar c)^2\left(\frac{\alpha m_ec}{\hbar}\right)^2\frac{2Z^4}{n^3(2l+1)}\right]$$

$$= -\frac{m_ec^2\alpha^4}{2}\frac{Z^4}{n^4}\left[\frac{1}{4} - 1 + \frac{2n}{2l+1}\right] = -\frac{1}{2}m_ec^2\frac{\alpha^4Z^4}{n^4}\left[\frac{2n}{2l+1} - \frac{3}{4}\right]$$

$$\langle\phi_{nlm}|\frac{1}{r}|\phi_{nlm}\rangle = \frac{Z}{a_0n^2} \qquad \frac{e^2}{4\pi\varepsilon_0} = \alpha\hbar c$$

$$\langle\phi_{nlm}|\frac{1}{r^2}|\phi_{nlm}\rangle =^2 \frac{2Z^2}{a_0^2n^3(2l+1)} \qquad a_0 = \frac{\alpha m_ec}{\hbar}$$

$$m_ec^2 \sim 0.5\ \text{MeV} \qquad \alpha^4 \sim \left(\frac{1}{137}\right)^4 \sim 3\times10^{-9} \qquad \Delta E_1 \sim 10^{-4}\ \text{eV}$$

Spin-orbital coupling

- To calculate the SOI, we can use the result for addition of angular momenta

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$J_z = L_z + S_z$$

$$\mathbf{S}\cdot\mathbf{L} = \frac{1}{2}\left(J^2 - L^2 - S^2\right)$$

- The possible eigenstates

$$|l,m\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle \longrightarrow$$

$j = l + \frac{1}{2}$

$\left|l+\frac{1}{2}, m+\frac{1}{2}\right\rangle$ parallel

$\left|l-\frac{1}{2}, m+\frac{1}{2}\right\rangle$ anti-parallel

$j = l - \frac{1}{2}$

Eigenvalues

- The eigenstates gives different SOI
- Parallel $\left|l+\frac{1}{2},m+\frac{1}{2}\right\rangle$

$$\mathbf{S}\cdot\mathbf{L}\left|l+\frac{1}{2},m+\frac{1}{2}\right\rangle=\frac{1}{2}\left(J^2-L^2-S^2\right)\left|l+\frac{1}{2},m+\frac{1}{2}\right\rangle$$

$$=\frac{1}{2}\hbar^2\left[\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)-l(l+1)-\frac{1}{2}\frac{3}{2}\right]\left|l+\frac{1}{2},m+\frac{1}{2}\right\rangle$$

$$=\frac{1}{2}\hbar^2 l\left|l+\frac{1}{2},m+\frac{1}{2}\right\rangle$$

- Anti-parallel $\left|l-\frac{1}{2},m+\frac{1}{2}\right\rangle$

$$\mathbf{S}\cdot\mathbf{L}\left|l-\frac{1}{2},m+\frac{1}{2}\right\rangle=\frac{1}{2}\left(J^2-L^2-S^2\right)\left|l-\frac{1}{2},m+\frac{1}{2}\right\rangle$$

$$=\frac{1}{2}\hbar^2\left[\left(l-\frac{1}{2}\right)\left(l+\frac{1}{2}\right)-l(l+1)-\frac{1}{2}\frac{3}{2}\right]\left|l-\frac{1}{2},m+\frac{1}{2}\right\rangle$$

$$=-\frac{1}{2}\hbar^2(l+1)\left|l-\frac{1}{2},m+\frac{1}{2}\right\rangle$$

SOI energy shift

- The energy shift for the 1st order

$$\left\langle \phi_{jm_jl} \middle| H_2 \middle| \phi_{jm_jl} \right\rangle = \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2m_e^2c^2}\left\langle \phi_{jm_jl} \middle| (\mathbf{S}\cdot\mathbf{L})\frac{1}{r^3} \middle| \phi_{jm_jl} \right\rangle$$

$$= \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2m_e^2c^2}\frac{\hbar^2}{2}\left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}\left\langle \phi_{jm_jl} \middle| \frac{1}{r^3} \middle| \phi_{jm_jl} \right\rangle$$

$$= \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{2m_e^2c^2}\frac{\hbar^2}{2}\left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}\frac{Z^3}{a_0^3}\frac{2}{n^3 l(l+1)(2l+1)}$$

$$= (\alpha\hbar c)\left(\frac{m_e c\alpha}{\hbar}\right)^3 \frac{\hbar^2 Z^4}{2m_e^2c^2}\frac{\left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}}{n^3 l(l+1)(2l+1)}$$

$$= \frac{1}{2}m_e c^2 Z^4 \alpha^4 \frac{\left\{ \begin{matrix} l \\ -l-1 \end{matrix} \right\}}{n^3 l(l+1)(2l+1)} = \frac{1}{2}m_e c^2 Z^4\alpha^4 \frac{1}{n^3(2l+1)}\left\{ \begin{matrix} 1/(l+1) \\ -1/l \end{matrix} \right\} \quad \begin{matrix} \nearrow j = l + \frac{1}{2} \\ \searrow j = l - \frac{1}{2} \end{matrix}$$

$$= \pm\frac{1}{2}m_e c^2 Z^4 \alpha^4 \frac{1}{n^3(2l+1)\left(j+\frac{1}{2}\right)}$$

$$\Delta E_2 \sim 10^{-4}\ \text{eV}$$

Fine structure

- Total energy shift combining relativistic correction and SOI

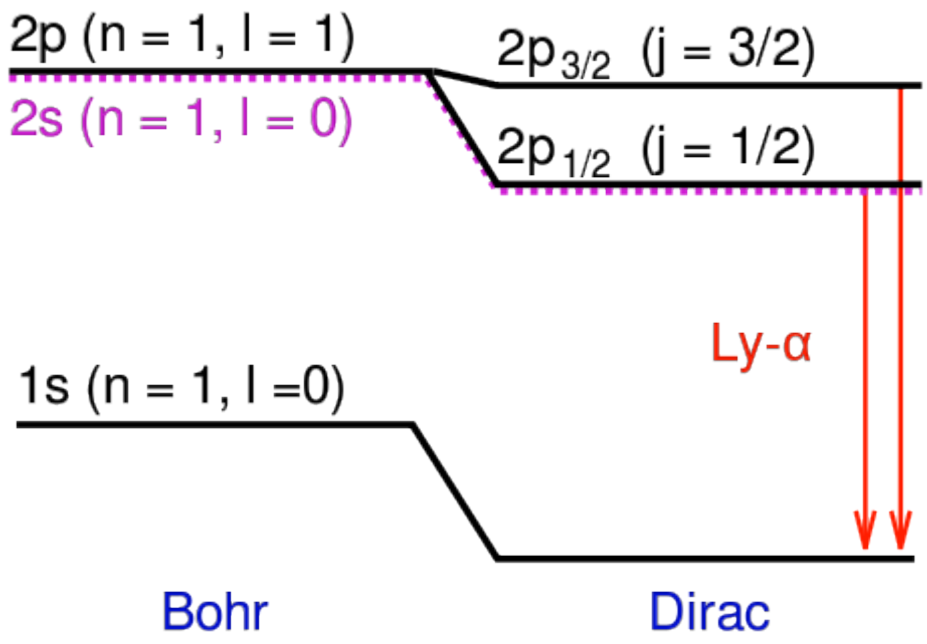
$$\left\langle \phi_{jm_jl} \middle| H_1 + H_2 \middle| \phi_{jm_jl} \right\rangle = -\frac{m_e c^2}{2}\frac{\alpha^4 Z^4}{n^4}\left[\frac{2n}{2l+1} - \frac{3}{4}\right] \pm \frac{1}{2} m_e c^2 Z^4 \alpha^4 \frac{1}{n^3(2l+1)(j+1/2)}$$

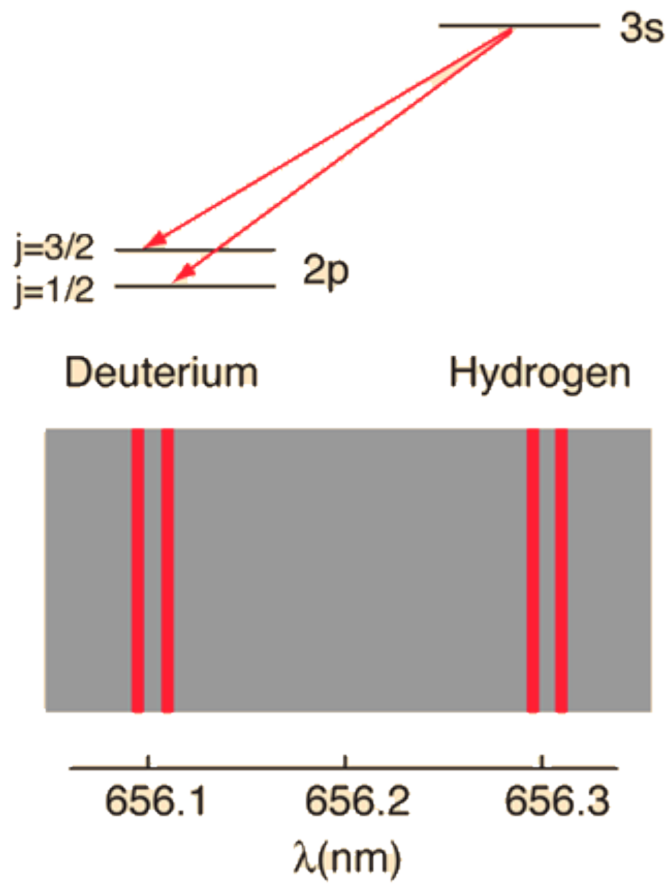
$$= -\frac{1}{2} m_e c^2 Z^4 \alpha^4 \frac{1}{n^3}\left[\frac{1}{(2l+1)}\left(\mp\frac{1}{j+1/2} + 2\right) - \frac{3}{4n}\right]$$

$$= -\frac{1}{2} m_e c^2 Z^4 \alpha^4 \frac{1}{n^3}\left[\frac{1}{(2l+1)(j+1/2)}\begin{pmatrix} 2j \\ 2j+2 \end{pmatrix} - \frac{3}{4n}\right]$$

$$= -\frac{1}{2} m_e c^2 Z^4 \alpha^4 \frac{1}{n^3}\left[\frac{1}{j+1/2} - \frac{3}{4n}\right]$$

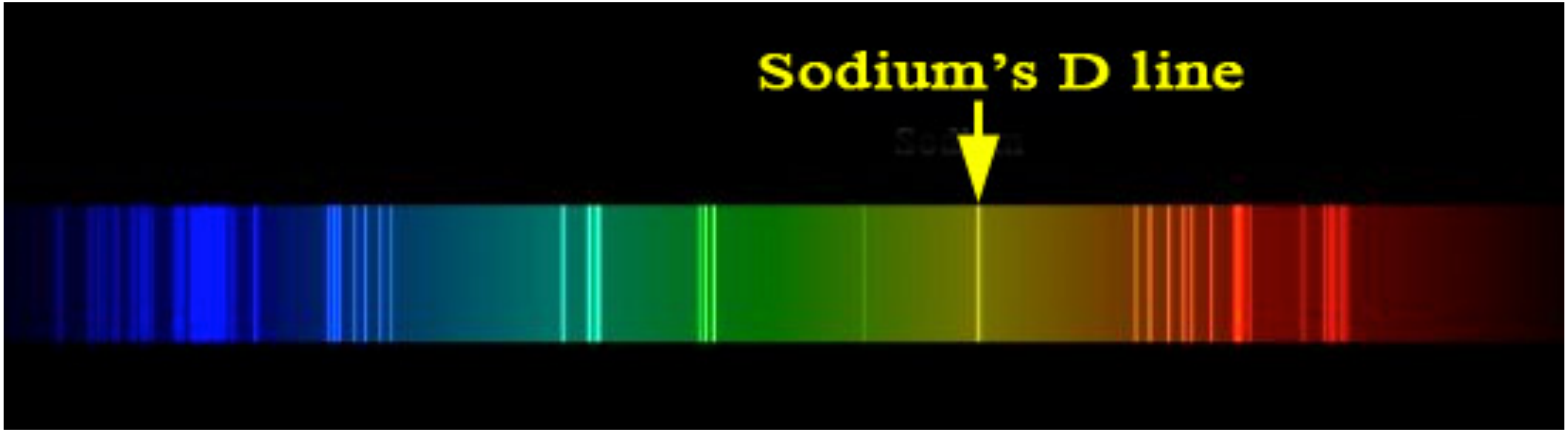
Fine structure

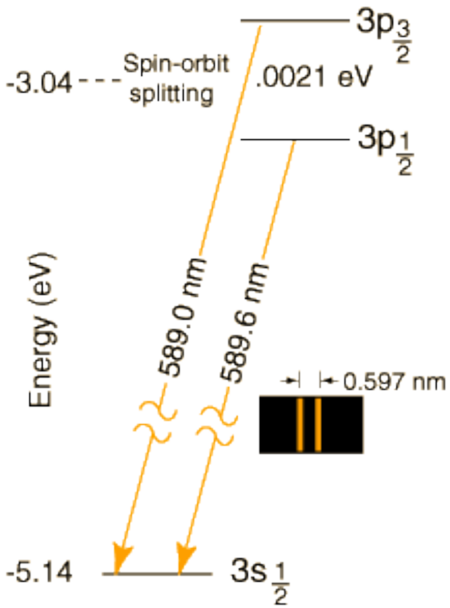




http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydfin.html

Sodium doublet





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Hyperfine structure

- The magnetic moment of nucleus produces a very tiny magnetic field to the electron
- The nuclear magnetic moment is related to its spin

$$\mathbf{M} = \frac{Zeg_N}{2M_N}\mathbf{I}$$

- the dipole field is $$\mathbf{B} = \frac{\mu_0}{4\pi}\left(\frac{3\mathbf{r}(\mathbf{r}\cdot\mathbf{M}) - r^2\mathbf{M}}{r^5} + \frac{8\pi}{3}\mathbf{M}\delta(\mathbf{r})\right)$$
- The energy is

$$H_{hf} = -\mathbf{m}\cdot\mathbf{B} = \frac{e}{2m_e}(\mathbf{L} + 2\mathbf{S})\cdot\mathbf{B}$$

$$\mathbf{m} = \frac{e}{2m_e}\mathbf{L} + \frac{eg}{2m_e}\mathbf{S}$$

perturbation

- The hyperfine perturbation

$$H_{hf} = \frac{e}{2m_e}\frac{Zeg_N}{2M_N}\frac{\mu_0}{4\pi}\left(\frac{3\mathbf{r}(\mathbf{r}\cdot\mathbf{I}) - r^2\mathbf{I}}{r^5} + \frac{8\pi}{3}\mathbf{I}\delta(\mathbf{r})\right)\cdot(\mathbf{L}+2\mathbf{S})$$

$$= \frac{Ze^2}{4\pi\varepsilon_0}\frac{g_N}{4M_N m_e c^2}\left(\frac{3\mathbf{r}(\mathbf{r}\cdot\mathbf{I}) - r^2\mathbf{I}}{r^5} + \frac{8\pi}{3}\mathbf{I}\delta(\mathbf{r})\right)\cdot(\mathbf{L}+2\mathbf{S})$$

- If L=0

$$H_{hf} = \frac{Ze^2}{4\pi\varepsilon_0}\frac{g_N}{2M_N m_e c^2}\left(\frac{3(\mathbf{r}\cdot\mathbf{I})(\mathbf{r}\cdot\mathbf{S}) - r^2\mathbf{I}}{r^5} + \frac{8\pi}{3}(\mathbf{I}\cdot\mathbf{S})\delta(\mathbf{r})\right)\cdot$$

- The energy shift

$$\langle\phi_{n00}|H_{hf}|\phi_{n00}\rangle = \frac{Ze^2}{4\pi\varepsilon_0}\frac{g_N}{2M_N m_e c^2}\frac{8\pi}{3}\langle\phi_{n00}|(\mathbf{I}\cdot\mathbf{S})\delta(\mathbf{r})|\phi_{n00}\rangle$$

energy shift

- For H-atom, n=1

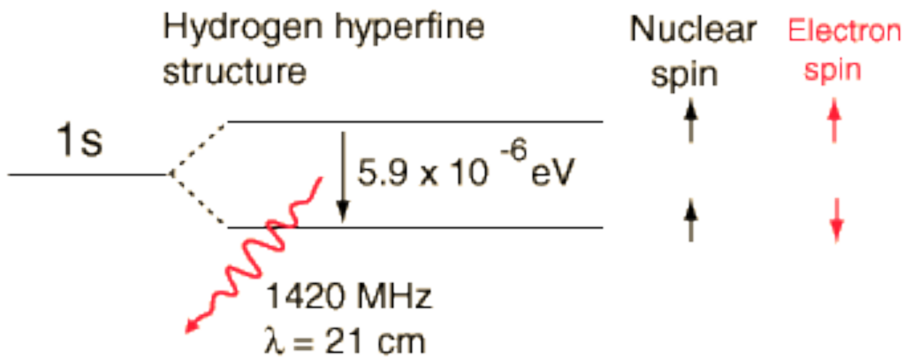
$$\langle \phi_{n00} | H_{hf} | \phi_{n00} \rangle = \frac{8\pi}{3} \frac{g_N}{2M_N m_e c^2} (\alpha \hbar c) \left(\frac{m_e \alpha c}{\hbar} \right)^3 \frac{1}{\pi} (\mathbf{I} \cdot \mathbf{S})$$

$$= \frac{4}{3} m_e c^2 \alpha^4 g_N \frac{m_e}{M_N} \frac{\langle \mathbf{I} \cdot \mathbf{S} \rangle}{\hbar^2}$$

- hyperfine splitting $\langle \mathbf{I} \cdot \mathbf{S} \rangle = \frac{1}{2} \langle F^2 - I^2 - S^2 \rangle = \begin{Bmatrix} 1/4 \\ -3/4 \end{Bmatrix}$ $\quad \mathbf{F} = \mathbf{I} + \mathbf{S}$

$$\Delta E_{hf} = \frac{4}{3} m_e c^2 \alpha^4 g_N \frac{m_e}{M_N} \left(\frac{1}{4} - \left(\frac{3}{4} \right) \right)$$

$$= \frac{4}{3} m_e c^2 \alpha^4 g_N \frac{m_e}{M_N}$$



energy splitting

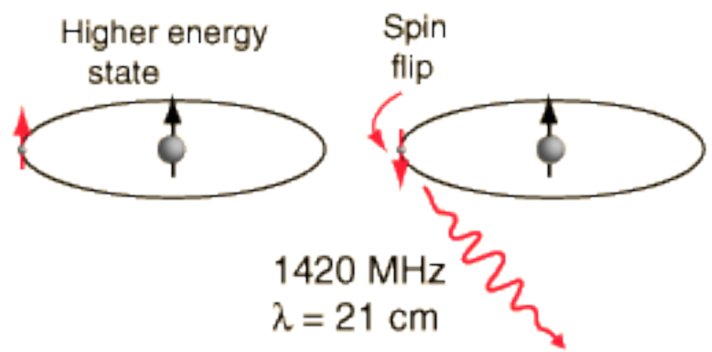
- Put in values $g_N = g_p = 5.56$ $\qquad \frac{m_e}{M_p} = \frac{1}{1830}$
- energy splitting

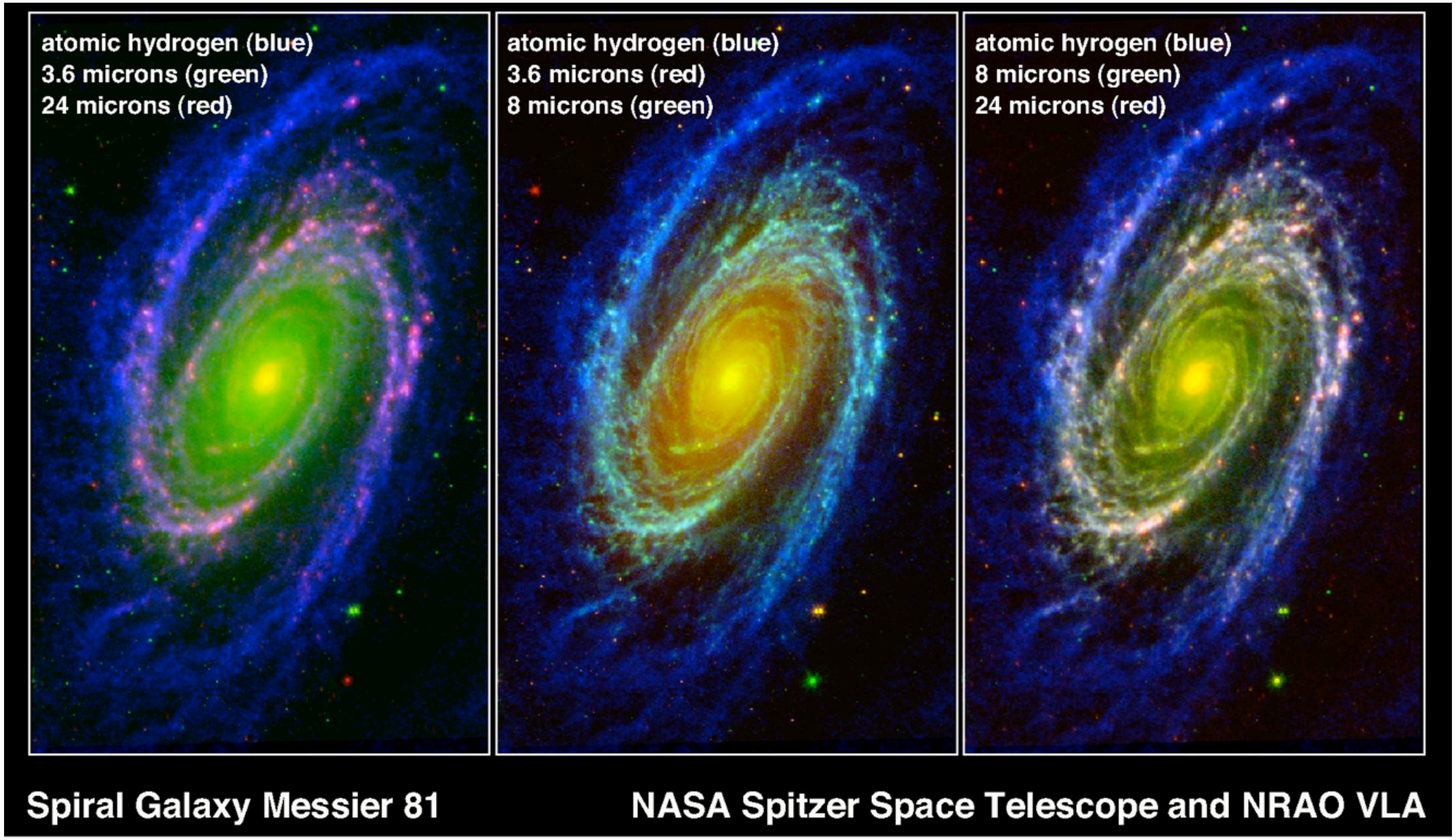
$$\Delta E_{hf} = \frac{4}{3}(0.5\text{M eV})\left(\frac{1}{137}\right)^4 (5.56)\left(\frac{1}{1830}\right)$$
$$= 5.7 \times 10^{-6}\ \text{eV}$$
$$\sim (1420\ \text{MHz})h$$

- transition between the splitting

$$\lambda = \sim 21\ \text{cm}$$

used in radio astronomy





Gallery

image of M81 made with the VLA for the THINGS

Very Large Array(VLA) National Radio Astronomy Observatory (NRAO)