Fine structure in one-electron atoms.

Magnetic moments, Stern-Gerlach experiment: SP 2.1.4, McM 8.1-8.3

$$\hat{\mu}_L = -\frac{e}{2m}\hat{L}$$

$$\hat{\mu}_S = -g_s \cdot \frac{e}{2m} \cdot \hat{S}, \quad g_s = 2$$

$$\hat{\mu}_{\text{tot}} = -\frac{e}{2m} \cdot (\hat{L} + 2\hat{S})$$

Spin-orbit interaction and other fine structure effects: McM 8.4, SP 2.1.4, Foot 2.3.2 - 2.3.5 (Fig 2.6) Exercises: 16 and 18

$$E_{SO} = \langle \hat{H}_{so} \rangle = \beta_{n,\ell} \cdot \frac{1}{2}[j(j+1) - \ell(\ell+1) - s(s+1)], \; j = \ell \pm \frac{1}{2}$$

$$\beta_{n,\ell} = R \cdot \frac{\alpha^2 Z^4}{n^3 \ell(\ell+1/2)(\ell+1)}. \text{ NOTE } \beta \sim Z^4, n^{-3} \text{ and } \ell^{-3}$$

Lande' interval rule: $\Delta E_{SO} = \beta_{n,\ell} \cdot j_{\max}$

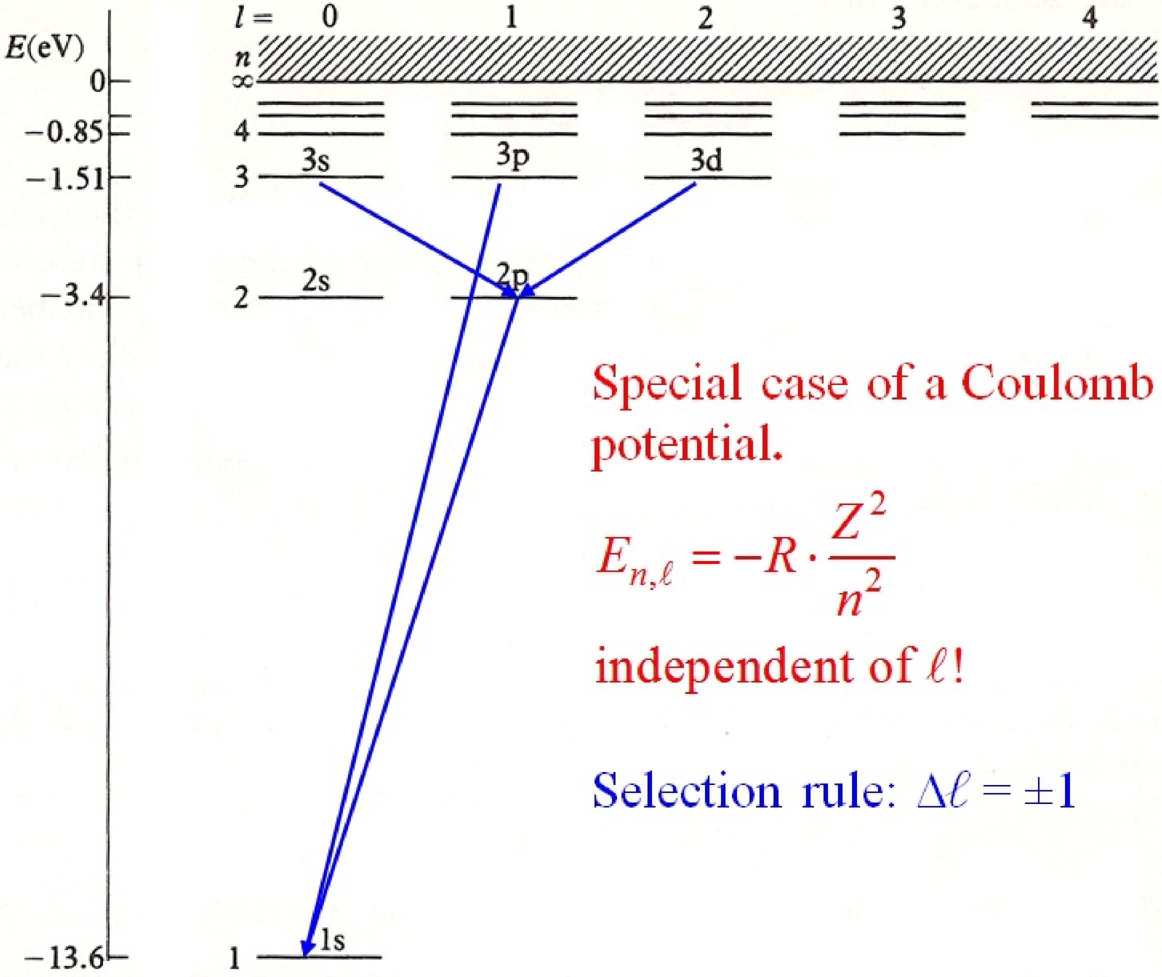
Total fine structure including all relativistic effects of order $\alpha^2 Z^4$.

$$E_{n,j} = -R \cdot [\frac{Z^2}{n^2} + \frac{\alpha^2 Z^4}{4n^4}(\frac{4n}{j+1/2} - 3)]$$

And then QED to reach perfect agreement with experiments within the estimated uncertainties.

Energy structure one-electron systems.

Numerical values for H



Special case of a Coulomb potential.

$$E_{n,\ell} = -R \cdot \frac{Z^2}{n^2}$$

independent of ℓ!

Selection rule: $\Delta\ell = \pm 1$

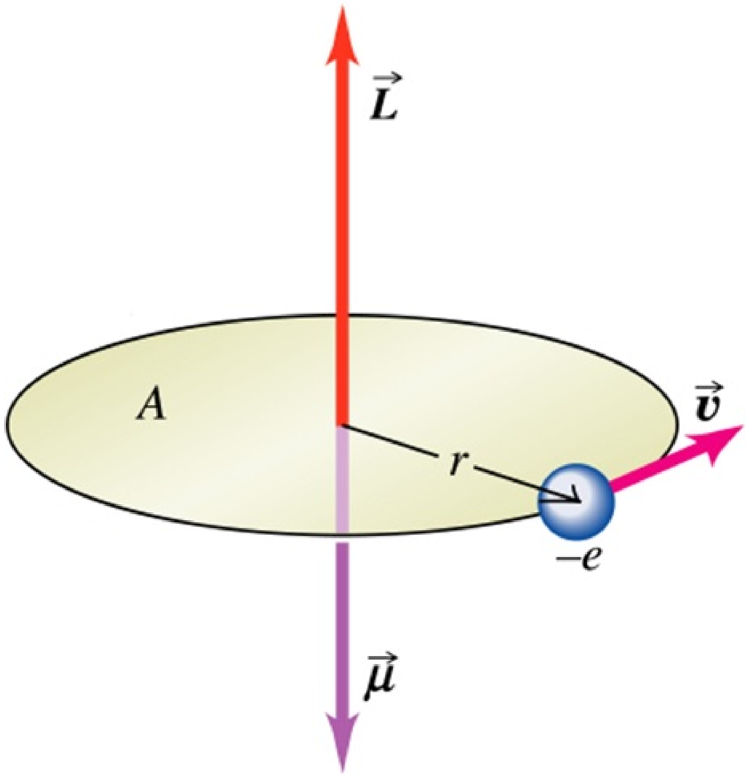
Comparison theory – experiments for the 1s – 2p transition in H.

All wavelengths in nm

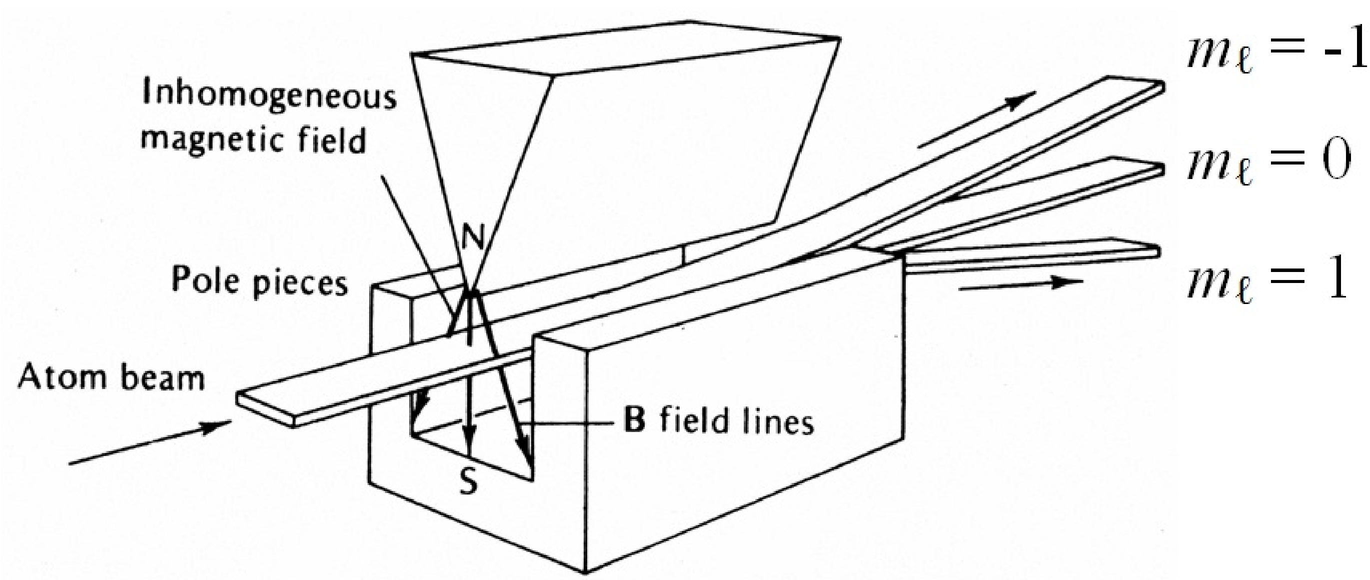
λ_{exp}	$\Delta\lambda_{exp}$	Model	λ_{th}	λ_{th} - λ_{exp}	$\Delta\lambda_{th}$
121.56682	0.00054	el-stat [a]	121.56845	0.00163	0
121.56736				0.00109	

a) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}}$

Magnetic moment of the electron due to its orbital motion



Stern-Gerlach experiment with an orbital angular momentum $\ell = 1$

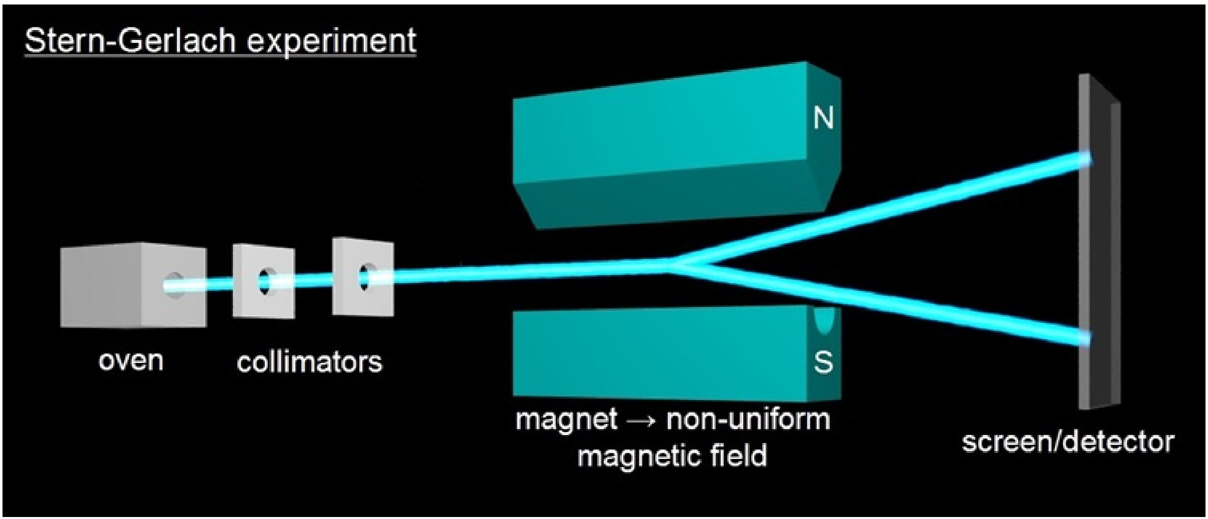


$$F_z = -\frac{e\hbar}{2m} \cdot m_\ell \cdot \frac{dB}{dz}$$

Stern-Gerlach experiment. Electron spin.

A beam of neutral silver atoms pass through an inhomogeneous magnetic field directed in the z-direction.

Silver has a ground configuration with filled orbitals (spherically symmetric) and an unpaired 5s outer electron, hence $L = 0$ and $\mu_L = 0$



Spin angular momentum, S

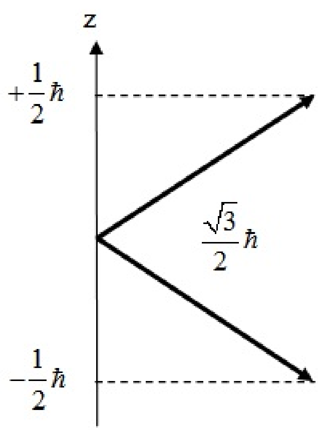
McMurry Ch 6.2

Magnitude quantum number $s = ½$

$$\mathbf{S} = \hbar\sqrt{s(s+1)} \Rightarrow S = |\mathbf{S}| = \frac{\sqrt{3}}{2}\hbar$$

Projection quantum number $m_s = \pm ½$

$$S_z = m_s\hbar = \pm\frac{1}{2}\hbar$$



$$\chi_{1/2,m_s}(sz) = \delta_{m_s,sz} \Leftrightarrow \begin{cases} \chi_{1/2,\pm1/2}(\pm1/2) = 1 \\ \chi_{1/2,\pm1/2}(\mp1/2) = 0 \end{cases}$$

Mean values of powers of the radius for hydrogenic electron orbits

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Department of Physics, Lund Institute of Technology, Lund, Sweden
(Received 24 September 1973)

$$\langle r^3\rangle = \left(\frac{a_0}{Z}\right)^3 \frac{n^2}{8}\{35n^4 - n^2[30l(l+1) - 25] + 3(l-1)l(l+1)(l+2)\} ,$$

$$\langle r^4\rangle = \left(\frac{a_0}{Z}\right)^4 \frac{n^4}{8}\{63n^4 - n^2[70l(l+1) - 105] + 15(l-1)l(l+1)(l+2) - 20l(l+1) + 12\} ,$$

$$\langle r^5\rangle = \left(\frac{a_0}{Z}\right)^5 \frac{n^4}{16}\{231n^6 - n^4[315l(l+1) - 735] + n^2[105(l-1)l(l+1) \times(l+2) - 315l(l+1) + 294] - 5(l-2)(l-1)l(l+1)(l+2)(l+3)\} ,$$

$$\left\langle\frac{1}{r}\right\rangle = \frac{Z}{a_0}\frac{1}{n^2},$$

$$\left\langle\frac{1}{r^2}\right\rangle = \left(\frac{Z}{a_0}\right)^2 \frac{1}{n^3(l+\frac{1}{2})} ,$$

$$\left\langle\frac{1}{r^3}\right\rangle = \left(\frac{Z}{a_0}\right)^3 \frac{1}{n^3 l(l+\frac{1}{2})(l+1)} \quad (l>0) ,$$

$$\left\langle\frac{1}{r^4}\right\rangle = \left(\frac{Z}{a_0}\right)^4 \frac{3n^2 - l(l+1)}{2n^5(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})} \quad (l>0) ,$$

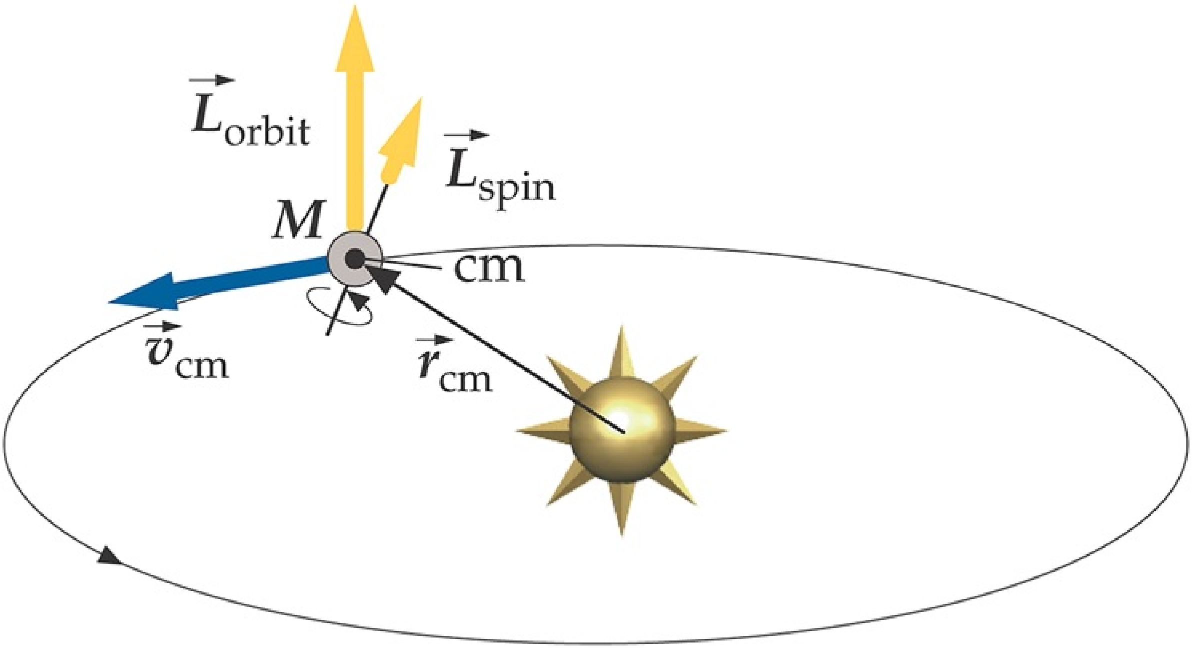
$$\left\langle\frac{1}{r^5}\right\rangle = \left(\frac{Z}{a_0}\right)^5 \frac{5n^2 - 3l(l+1) + 1}{2n^5(l-1)(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})(l+2)} \quad (l>1) ,$$

$$\left\langle\frac{1}{r^6}\right\rangle = \left(\frac{Z}{a_0}\right)^6 \frac{35n^4 - n^2[30l(l+1) - 25] + 3(l-1)l(l+1)(l+2)}{8n^7(l-\frac{3}{2})(l-1)(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})(l+2)(l+\frac{5}{2})} \quad (l>1) ,$$

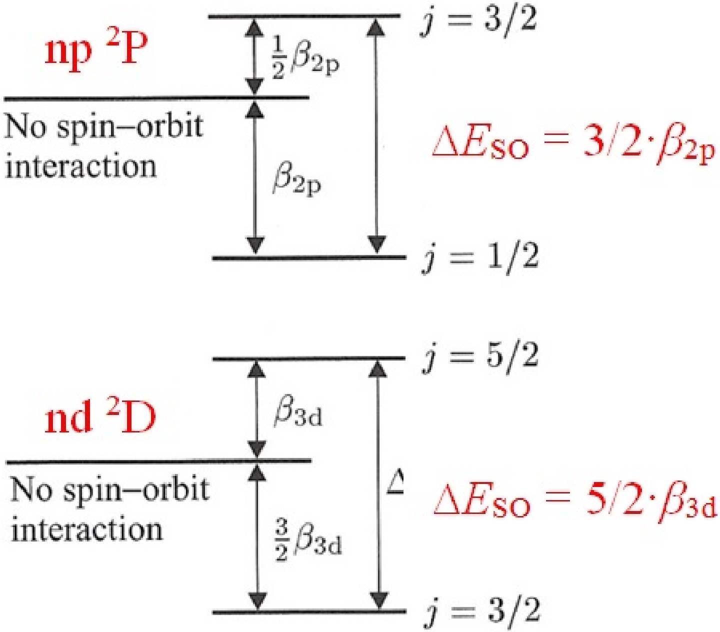
$$\left\langle\frac{1}{r^7}\right\rangle = \left(\frac{Z}{a_0}\right)^7 \frac{63n^4 - n^2[70l(l+1) - 105] + 15(l-1)l(l+1)(l+2) - 20l(l+1) + 12}{8n^7(l-2)(l-\frac{3}{2})(l-1)(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})(l+2)(l+\frac{5}{2})(l+3)} \quad (l>2) ,$$

Classical example of the addition of angular momenta.

$$\mathbf{L}_{\text{system}} = \mathbf{L}_{\text{orbit}} + \mathbf{L}_{\text{spin}} = \mathbf{r}_{\text{cm}} \times M \cdot \mathbf{v}_{\text{cm}} + \mathbf{L}_{\text{spin}} =$$
$$\mathbf{r}_{\text{cm}} \times M \cdot \mathbf{v}_{\text{cm}} + I \cdot \boldsymbol{\omega}$$



Examples of Lande' interval rule - from Foot fig 2.5.



Comparison theory – experiments for the 1s – 2p transition in H.

All wavelengths in nm

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121.56682	0.00054	el-stat [a]	121.56845	0.00163	0
121.56736				0.00109	
		SO [b]	121.56827	0.00145	0.00054
			121.56881	0.00145	

a) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}}$

b) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}}$

Fine structure energies one-electron atoms.

Spin-orbit interaction:

$$E_{SO} = R\cdot\frac{\alpha^2 Z^4}{n^3\ell(\ell+1/2)(\ell+1)}\cdot\frac{1}{2}[j(j+1)-\ell(\ell+1)-s(s+1)]$$

Relativistic mass:

$$E_{mass} = R\cdot\frac{\alpha^2 Z^4}{n^4}(\frac{3}{4}-\frac{n}{\ell+1/2})$$

Darwin:

$$E_D = R\cdot\frac{\alpha^2 Z^4}{n^3}\cdot\delta_{\ell,0}$$

Total fine structure including all relativistic effects of order $\alpha^2 Z^4$.

$$E_{n,j} = -R\cdot[\frac{Z^2}{n^2}+\frac{\alpha^2 Z^4}{4n^4}(\frac{4n}{j+1/2}-3)],\quad j=\ell\pm\frac{1}{2},\ell>0$$

Fine structure for $n = 3$ as a sum of Darwin, relativistic mass and spin-orbit effects. Note the coincidence that although all 3 effects depends on ℓ, the sum happens to be independen of ℓ and depends only on n and j.

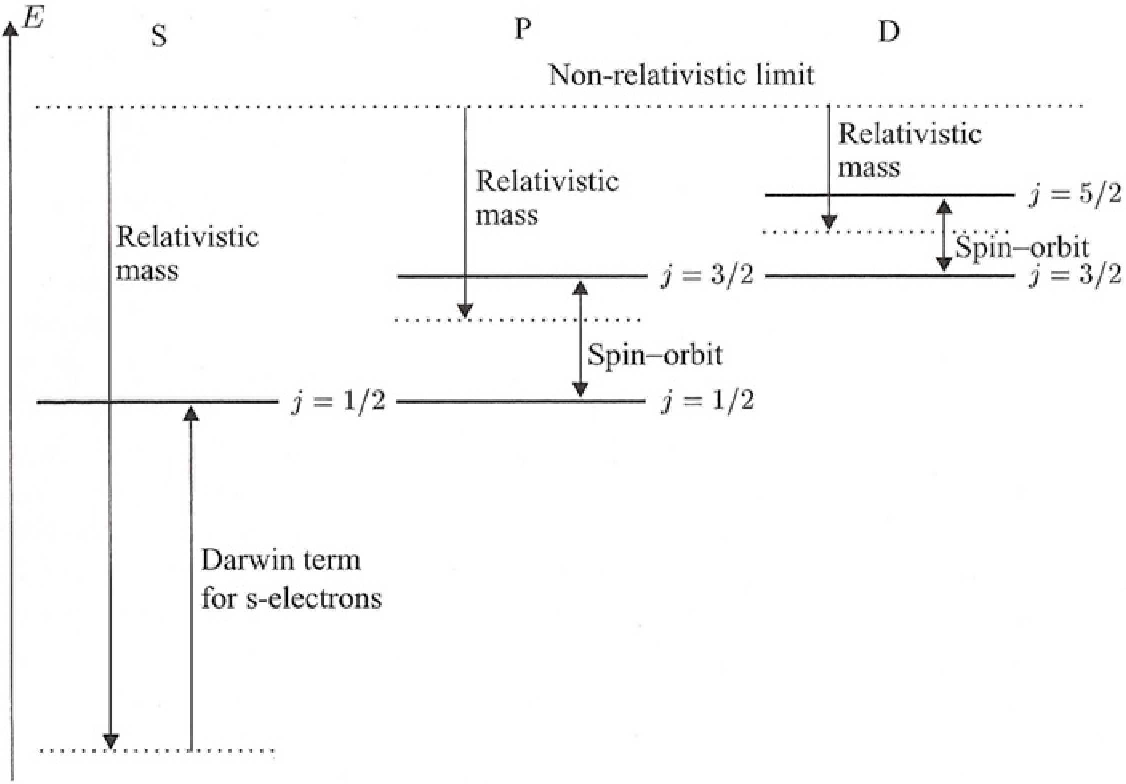


Fig 2.6 in Foot

Comparison theory – experiments for the 1s – 2p transition in H.

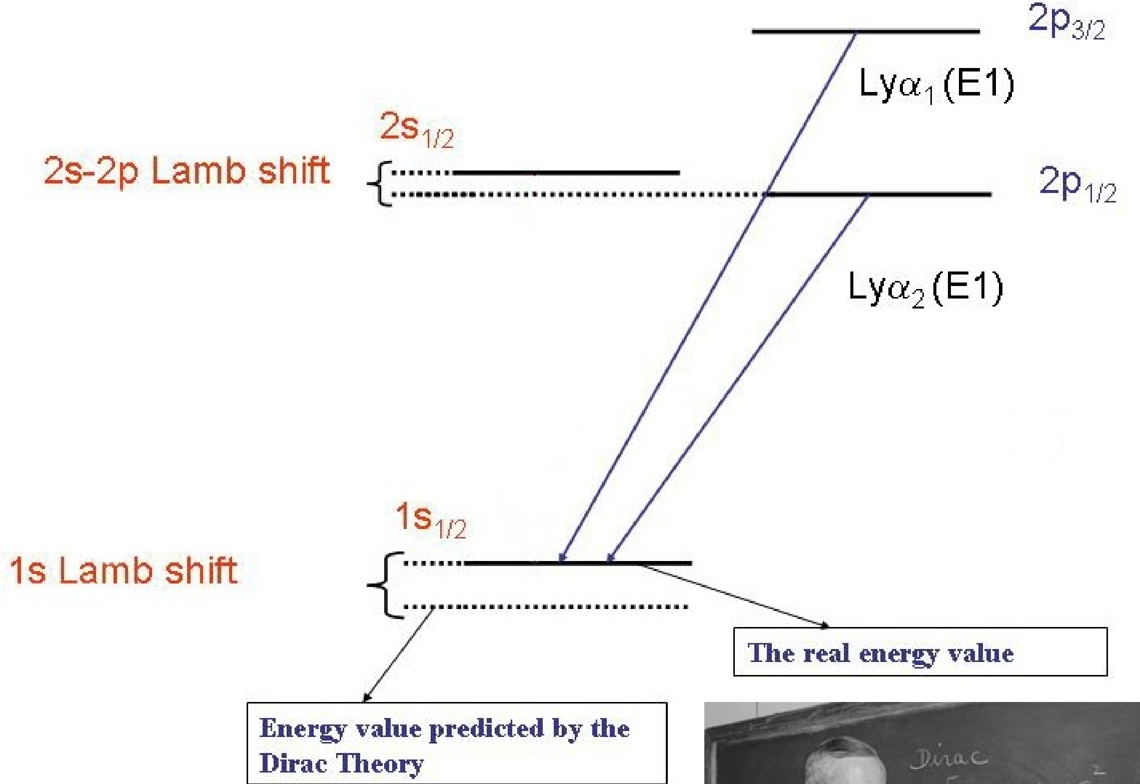
All wavelengths in nm

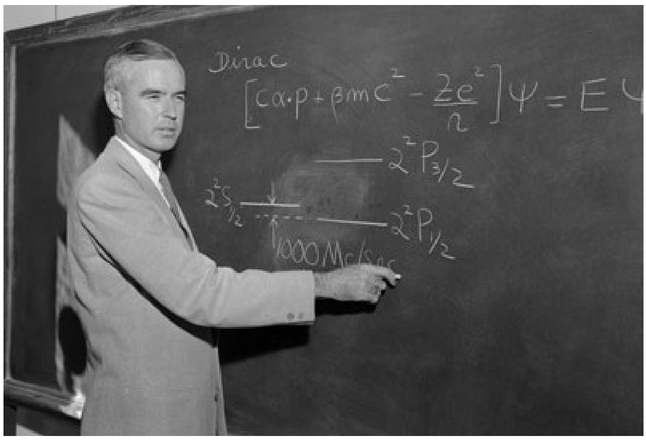
λ_{exp}	$\Delta\lambda_{exp}$	Model	λ_{th}	$\lambda_{th} - \lambda_{exp}$	$\Delta\lambda_{th}$
121.56682	0.00054	el-stat [a]	121.56845	0.00163	0
121.56736				0.00109	
		SO [b]	121.56827	0.00145	0.00054
			121.56881	0.00145	
		all $\alpha^2 Z^4$ [c]	121.56643	-0.00039	0.00054
			121.56697	-0.00039	

a) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}}$

b) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}}$

c) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}} + \hat{H}_{\text{mass}} + \hat{H}_{\text{Darwin}}$


2p3/2
Lyα1 (E1)
2s1/2
2s-2p Lamb shift
2p1/2
Lyα2 (E1)
1s1/2
1s Lamb shift
The real energy value
Energy value predicted by the Dirac Theory


Dirac
2²P3/2
2²S1/2
2²P1/2
1000 Mc/sec

Comparison theory – experiments for the 1s – 2p transition in H.

All wavelengths in nm

λ_{exp}	$\Delta\lambda_{exp}$	Model	λ_{th}	λ_{th} - λ_{exp}	$\Delta\lambda_{th}$
121.56682	0.00054	el-stat [a]	121.56845	0.00163	0
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			121.56881	0.00145	
		all $\alpha^2 Z^4$ [c]	121.56643	-0.00039	0.00054
			121.56697	-0.00039	
		QED[d]	121.56682	0	0.00054
			121.56736	0	

a) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}}$

b) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}}$

c) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}} + \hat{H}_{\text{mass}} + \hat{H}_{\text{Darwin}}$

d) $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{Coulomb}} + \hat{H}_{\text{SO}} + \hat{H}_{\text{mass}} + \hat{H}_{\text{Darwin}} + \text{QED}$

QED corrections. Vacuum polarization

$$\Delta E \cdot \Delta t = \frac{1}{2}\hbar$$

According to quantum field theory, the vacuum between interacting particles is not simply empty space. Rather, it contains short-lived virtual particle-antiparticle pairs (leptons or quarks and gluons) which are created out of the vacuum in amounts of energy constrained in time by the energy-time version of the Heisenberg uncertainty principle. After the constrained time, having duration inversely correlated with the amount of energy of the fluctuation, the virtual particles annihilate each other.

These particle–antiparticle pairs carry various kinds of charges, such as color charge if they are subject to QCD such as quarks or gluons, or the more familiar electromagnetic charge if they are electrically charged leptons or quarks, the most familiar charged lepton being the electron and since it is the lightest in mass, the most numerous due to the energy-time uncertainty principle as mentioned above; e.g., virtual electron–positron pairs. Such charged pairs act as an electric dipole. In the presence of an electric field, e.g., the electromagnetic field around an electron, these particle–antiparticle pairs reposition themselves, thus partially counteracting the field (a partial screening effect, a dielectric effect). The field therefore will be weaker than would be expected if the vacuum were completely empty. This reorientation of the short-lived particle-antiparticle pairs is referred to as *vacuum polarization*.

From Wikipedia