Quantum Mechanics II

H-Atom Details (2)

Hyperfine Structure; Quantum Field Corrections

Tristan Hübsch

Department of Physics and Astronomy, Howard University, Washington DC

http://physics1.howard.edu/~thubsch/

H-Atom Details (2)

Hyperfine Structure

Extra!

- To first order in perturbation theory,

$$E_{n,\ell} = -\frac{1}{2}\alpha_e^2 m_e c^2 \frac{1}{n^2}\left\{1 + \frac{\alpha_e^2}{4n^2}\left[\frac{4n}{(j+\frac{1}{2})} - 3\right] + \ldots\right\} \quad j = \ell \pm \tfrac{1}{2}$$

"fine structure" "hyperfine structure"

1st order

1st order

- Corrections stem from:

$$\hat{H}'_{\rm rel} = -\frac{\hbar^4}{8m_e^3c^2}(\vec{\nabla}^2)^2 \qquad \hat{H}''_{\rm rel} = +\frac{\hbar^6}{16m_e^5c^4}(\vec{\nabla}^2)^3 \qquad \ldots\ldots\ldots$$

$$\hat{H}_{S_eO} = \tfrac{1}{4}g_e\alpha_e{}^4 m_e c^2 \frac{1}{(r/a_0)^3}\,\vec{L}\cdot\vec{S}_e \qquad \hat{H}_{S_pO} = g_p\alpha_e{}^4 m_e c^2 \frac{m_e}{m_p}\frac{1}{(r/a_0)^3}\,\vec{L}\cdot\vec{S}_p$$

$$\hat{H}_{S_eS_p} = \tfrac{1}{2}g_e g_p\,\alpha_e{}^4 m_e c^2 \frac{m_e}{m_p}\left[\Big(3(\vec{S}_e\cdot\hat{r})(\vec{S}_p\cdot\hat{r}) - \vec{S}_e\cdot\vec{S}_p\Big)\frac{1}{(r/a_0)^3} + \frac{8\pi}{3}\vec{S}_e\cdot\vec{S}_p\,\delta^3(\vec{r}/a_0)\right]$$

- 1st order: $\hat{H}''_{\rm rel}$, $\hat{H}_{SpO}$, $\hat{H}_{SeSp}$; 2nd order: $\hat{H}'_{\rm rel}$, $\hat{H}_{SeO}$ … etc.
- <u>*Estimate*</u> and order these contributions by magnitude

H-Atom Details (2)

Hyperfine Structure

Extra!

- Corrections:

$$E_n^{(1,r_2)} = \langle H''_{\mathrm{rel}} \rangle \sim \frac{1}{m_e^2 c^4} \left\langle \left(\frac{e^2}{4\pi\epsilon_0 \, r} \right)^3 \right\rangle \sim \frac{1}{m_e^2 c^4} \frac{(\alpha_e \hbar c)^3}{n^3 \, a_0^3} \sim \frac{1}{m_e^2 c^4} \frac{(\alpha_e \hbar c)^3}{(n\hbar / \alpha_e m_e c)^{\,3}}$$

H-Atom Details (2)

Hyperfine Structure

Extra!

- Corrections:

$$E_n^{(1,r_2)} = \langle H''_{\rm rel}\rangle \sim \frac{1}{m_e^2 c^4}\left\langle\left(\frac{e^2}{4\pi\epsilon_0\, r}\right)^3\right\rangle \sim \frac{\alpha_e^6\, m_e c^2}{n^3}$$

$$E_n^{(2,r_1)} = \sum_{n'\cdots\neq n\cdots}\frac{|\langle n',\cdots|H'_{\rm rel}|n,\cdots\rangle|^2}{E_n^{(0)}-E_m^{(0)}} \sim \frac{|E_n^{(1,r1)}|^2}{|E_n^{(0)}|} \sim \frac{\left(\alpha_e^4 m_e c^2/n^3\right)^2}{\alpha_e^2 m_e c^2/n^2}$$

H-Atom Details (2)

Hyperfine Structure

Extra!

- Corrections:

relativity

$$E_n^{(1,r_2)} = \langle H''_{\rm rel} \rangle \sim \frac{1}{m_e^2 c^4} \left\langle \left(\frac{e^2}{4\pi\epsilon_0\, r} \right)^3 \right\rangle \sim \frac{\alpha_e^6\, m_e c^2}{n^3}$$

$$E_n^{(2,r_1)} = \sum_{n'\cdots\neq n\cdots} \frac{|\langle n', \cdots | H'_{\rm rel} | n, \cdots \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \sim \frac{|E_n^{(1,r1)}|^2}{|E_n^{(0)}|} \sim \frac{\alpha_e^6 m_e c^2}{n^4}$$

$$E_n^{(1,S_pO)} = \langle H_{S_pO} \rangle = \frac{g_p\, e^2}{4\pi\epsilon_0} \frac{\hbar^2}{m_e m_p c^2} \left\langle \frac{1}{r^3}\, \vec{L} \cdot \vec{S}_p \right\rangle \sim \frac{g_p\, \alpha_e \hbar^3}{m_e m_p c} \cdot \frac{1}{n^3 a_0^3}$$

H-Atom Details (2)

Hyperfine Structure

Extra!

- Corrections:

relativity

$$E_n^{(1,r_2)} = \langle H''_{\rm rel} \rangle \sim \frac{1}{m_e^2 c^4} \left\langle \left(\frac{e^2}{4\pi\epsilon_0\, r} \right)^3 \right\rangle \sim \frac{\alpha_e^6\, m_e c^2}{n^3}$$

$$E_n^{(2,r_1)} = \sum_{n'\cdots \neq n\cdots} \frac{|\langle n', \cdots | H'_{\rm rel} | n, \cdots \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \sim \frac{|E_n^{(1,r1)}|^2}{|E_n^{(0)}|} \sim \frac{\alpha_e^6 m_e c^2}{n^4}$$

$$E_n^{(1,S_pO)} = \langle H_{S_pO} \rangle = \frac{g_p\, e^2}{4\pi\epsilon_0} \frac{\hbar^2}{m_e m_p c^2} \left\langle \frac{1}{r^3} \vec{L} \cdot \vec{S}_p \right\rangle \sim g_p \left(\frac{m_e}{m_p} \right) \frac{\alpha_e^4 m_e c^2}{n^3}$$

H-Atom Details (2)

Hyperfine Structure

Extra!

- Corrections:

relativity

$$E_n^{(1,r_2)} = \langle H''_{\text{rel}} \rangle \sim \frac{1}{m_e^2 c^4} \left\langle \left(\frac{e^2}{4\pi\epsilon_0\, r} \right)^3 \right\rangle \sim \frac{\alpha_e^6\, m_e c^2}{n^3}$$

$$E_n^{(2,r_1)} = \sum_{n'\cdots \neq n\cdots} \frac{|\langle n', \cdots | H'_{\text{rel}} | n, \cdots \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \sim \frac{|E_n^{(1,r1)}|^2}{|E_n^{(0)}|} \sim \frac{\alpha_e^6 m_e c^2}{n^4}$$

magnetic

$$E_n^{(1,S_pO)} = \langle H_{S_pO} \rangle = \frac{g_p\, e^2}{4\pi\epsilon_0} \frac{\hbar^2}{m_e m_p c^2} \left\langle \frac{1}{r^3} \vec{L} \cdot \vec{S}_p \right\rangle \sim g_p \left(\frac{m_e}{m_p} \right) \frac{\alpha_e^4 m_e c^2}{n^3}$$

$$E_n^{(1,S_eS_p)} = \langle H_{S_eS_p} \rangle \sim \frac{g_p\, e^2}{4\pi\epsilon_0} \frac{\hbar^2}{m_e m_p c^2} \left\langle \vec{S}_e \cdot \vec{S}_p \frac{1}{r^3} \right\rangle \sim g_p \left(\frac{m_e}{m_p} \right) \frac{\alpha_e^4 m_e c^2}{n^3}$$

- Expect:

$$E_n^{(1,r_2)} : E_n^{(2,r_1)} : E_n^{(1,S_pO)} : E_n^{(1,S_eS_p)} \approx n\alpha_e^2 : \alpha_e^2 : g_p \left(\frac{m_e}{m_p} \right) : g_p \left(\frac{m_e}{m_p} \right)$$

|——smaller——|———–bigger———–|

$\alpha_e^2 \approx 5.33 \times 10^{-5}$ $\quad g_p \left(\frac{m_e}{m_p} \right) \approx 1.52 \times 10^{-3}$

- The latter two dominate the "hyperfine structure"

QM II

H-Atom Details (2)

Hyperfine Structure

Extra!

- For magnetic corrections, $\vec{F} := \vec{J} + \vec{S}_p = \vec{L} + \vec{S}_e + \vec{S}_p.$

$$E_n^{\rm hfs} = E_n^{(1,S_eS_p)} + E_n^{(1,S_pO)}$$
$$= \Big(\frac{m_e}{m_p}\Big)\alpha_e^4\, m_e c^2\, \frac{g_p}{2n^3}\, \frac{\pm 1}{(f+\frac{1}{2})(\ell+\frac{1}{2})} \qquad \begin{cases} f = j + 1/2 \\ f = j - 1/2 \end{cases}$$

H-Atom Details (2)

Hyperfine Structure

Extra!

$\vec{Z} := \vec{S}_e + \vec{S}_p$

- For magnetic corrections, $\vec{F} := \vec{J} + \vec{S}_p = \vec{L} + \vec{S}_e + \vec{S}_p$

$$E_n^{\text{hfs}} = E_n^{(1,S_eS_p)} + E_n^{(1,S_pO)}$$

$$= \left(\frac{m_e}{m_p}\right)\alpha_e^4\, m_e c^2\, \frac{g_p}{2n^3}\, \frac{\pm 1}{(f+\frac{1}{2})(\ell+\frac{1}{2})} \overset{\ell\to 0}{=} \begin{cases} +\frac{4}{3} \\ -4 \end{cases} \qquad \begin{cases} z=1 \text{ (triplet)} \\ z=0 \text{ (singlet)} \end{cases}$$

- This contribution splits energy levels w/same n
  - allowing an $n=1 \to 1$ transition, w/21.0807 cm wavelength ("HI-line")
  - to within 1% of the measured value (microwave radio astronomy)
  - The deuteron (p^+ & n^0) has spin-1 and $g_D = 0.8574\ldots$
  - Thus, 21.807 cm → 91.7… cm (→ composition of distant stars)
- The relativistic 2nd order corrections
  - ~ 25–30 × smaller than (~ 3.6% of) the hyperfine structure
- "Exotic atoms": substitute e^- & p^+ and trace the changes.

H-Atom Details (2)

Quantum Field Corrections

Extra!

~ D. Park & F. Dyson

- $2^2s_{1/2}$ & $2^2p_{1/2}$ states are still degenerate
  - …but, in fact, *do* differ in energy & permit a transition
  - [W. Lamb & R.C. Retherford, 1947, exp.]: 1,057.8 MHz ($\approx 4 \times 10^{-6}$ eV)
  - owing to “vacuum fluctuations” in the EM field [T.A. Welton, 1948]
- Gauging the scalar potential to zero,

$$\vec{E}(\vec{r},t) = \vec{E}_0 \cos(\vec{k}\cdot\vec{r} - \omega t) \quad u(\vec{r},t) = \varepsilon_0 \vec{E}^2 = \tfrac{1}{2}\varepsilon_0 \vec{E}_0^2 \overset{!}{=} \tfrac{1}{2}\hbar\omega = \tfrac{1}{2}\hbar c|\vec{k}|$$

- Two polarizations, x- and y-component. $\quad E_0^2 = \frac{\hbar c k}{\varepsilon_0}$
- Jiggles an electron:

$$m_e\,\ddot{x} = e|\vec{E}_0|\cos(\omega t) \qquad x = -\frac{e|\vec{E}_0|}{m_e\omega^2}\cos(\omega t)$$

$$\overline{x^2} = \frac{1}{2}\left(\frac{eE_0}{m_e c^2 k^2}\right)^2 = 2\pi\alpha_e\left(\frac{\hbar}{m_e c}\right)^2\frac{1}{k^3} = \overline{y^2}$$

- # of photons:

$$\mathrm{d}N_{[k,\,k+\mathrm{d}k]} = \mathrm{Vol}\cdot\int_{\text{angles}}\frac{\mathrm{d}^3\vec{k}}{(2\pi)^3} = \mathrm{Vol}\cdot 4\pi\frac{k^2\mathrm{d}k}{(2\pi)^3} = \mathrm{Vol}\cdot\frac{k^2\mathrm{d}k}{2\pi^2}$$

H-Atom Details (2)

$a_0 = \frac{\hbar}{\alpha_e m_e c}$

Quantum Field Corrections

Extra!

- Adding the jiggling effect from both polarizations of ∞ modes

$$\overline{(\triangle\vec{r})^2} = \frac{2\alpha_e}{\pi}\left(\frac{\hbar}{m_e c}\right)^2 \int_a^b \frac{k^2 \mathrm{d}k}{k^3} = \frac{2\alpha_e}{\pi}\left(\frac{\hbar}{m_e c}\right)^2 \ln\left(\frac{b}{a}\right)$$

- Relativistic effects suggest the upper limit: $b \le m_e c/\hbar$
- Lower (wave-number) limit = long wavelength limit $a \ge k_0$
  - such that $\hbar c k_0$ is the mean excitation energy of the atom ~¼ Ry = ¼ $|E_2|$
- The hydrogen electron is then jiggled by the effective potential

$$\overline{V(\vec{r}+\triangle\vec{r})} - \overline{V(\vec{r})} = \overline{\triangle\vec{r}\cdot\vec{\nabla}V(\vec{r})} + \tfrac{1}{2}\overline{(\triangle\vec{r}\cdot\vec{\nabla})^2 V(\vec{r})} + \ldots$$

$$= \tfrac{1}{2}\tfrac{1}{3}\overline{(\triangle\vec{r})^2}\vec{\nabla}^2 V(\vec{r}) + \ldots \quad = \tfrac{1}{6}\overline{(\triangle\vec{r})^2}\Big(4\pi\alpha_e\hbar c\,\delta^3(\vec{r})\Big) + \ldots$$

- …which corrects the energy, to first order in perturbation theory,

$$\triangle E_{\text{FC}} = \left\langle \Psi \middle| \overline{\triangle V(\vec{r})} \middle| \Psi \right\rangle = \left[\frac{2\pi}{3}\alpha_e \hbar c\right]\left[\frac{2\alpha_e}{\pi}\left(\frac{\hbar}{m_e c}\right)^2 \ln\left(\frac{b}{a}\right)\right]|\Psi(0)|^2$$

$$= \frac{4\alpha_e^2\hbar^3}{3m_e^2 c}\ln\left(\frac{b}{a}\right)\frac{1}{8\pi a_0^3} = \frac{\alpha_e^2\hbar^3}{6\pi m_e^2 c}\ln\left(\frac{b}{a}\right)\frac{\alpha_e^3 m_e^3 c^3}{\hbar^3}$$

S-states only

Why?

H-Atom Details (2)

$$a_0 = \frac{\hbar}{\alpha_e m_e c}$$

Quantum Field Corrections

Extra!

- Adding the jiggling effect from both polarizations of ∞ modes

$$\overline{(\triangle\vec{r})^2} = \frac{2\alpha_e}{\pi}\Big(\frac{\hbar}{m_e c}\Big)^2 \int_a^b \frac{k^2 \mathrm{d}k}{k^3} = \frac{2\alpha_e}{\pi}\Big(\frac{\hbar}{m_e c}\Big)^2 \ln\Big(\frac{b}{a}\Big)$$

  - Relativistic effects suggest the upper limit: $b \le m_e c/\hbar$
  - Lower (wave-number) limit = long wavelength limit $a \ge k_0$
    - such that $\hbar c k_0$ is the mean excitation energy of the atom ~¼ Ry = ¼ $|E_2|$
  - The hydrogen electron is then jiggled by the effective potential

$$\overline{V(\vec{r}+\triangle\vec{r})} - \overline{V(\vec{r})} = \overline{\triangle\vec{r}\cdot\vec{\nabla}V(\vec{r})} + \tfrac{1}{2}\overline{(\triangle\vec{r}\cdot\vec{\nabla})^2 V(\vec{r})} + \ldots$$

$$= \tfrac{1}{2}\tfrac{1}{3}\overline{(\triangle\vec{r})^2}\vec{\nabla}^2 V(\vec{r}) + \ldots \quad = \tfrac{1}{6}\overline{(\triangle\vec{r})^2}\Big(4\pi\alpha_e\hbar c\,\delta^3(\vec{r})\Big) + \ldots$$

  - …which corrects the energy, to first order in perturbation theory,

$$\triangle E_{\mathrm{FC}} = \Big\langle \Psi \Big| \overline{\triangle V(\vec{r})} \Big| \Psi \Big\rangle = \Big[\frac{2\pi}{3}\alpha_e\hbar c\Big]\Big[\frac{2\alpha_e}{\pi}\Big(\frac{\hbar}{m_e c}\Big)^2 \ln\Big(\frac{b}{a}\Big)\Big]|\Psi(0)|^2$$

$$= \frac{\alpha_e^3}{3\pi}\ln\Big(\frac{b}{a}\Big)\Big[\frac{1}{2}\alpha_e^2 m_e c^2\Big]$$

S-states only

Why?

H-Atom Details (2)

Quantum Field Corrections

Extra!

- This semi-classical analysis produces

$$\triangle E_{\text{FC}} = \frac{\alpha_e^3}{3\pi} \ln\left(\frac{b}{a}\right) \left[\frac{1}{2}\alpha_e^2 m_e c^2\right]$$

odd power of α_e!! ~7–8 13.6 eV

$$E_n^{(1,r_2)} : E_n^{(2,r_1)} : E_n^{(1,S_p O)} : E_n^{(1,S_e S_p)} : E_n^{(QED)} \approx n\alpha_e^2 : \alpha_e^2 : g_p\left(\frac{m_e}{m_p}\right) : g_p\left(\frac{m_e}{m_p}\right) : \alpha_e$$

$$(5.33\times10^{-5}\cdot n) : (5.33\times10^{-5}) : (1.52\times10^{-3}) : (1.52\times10^{-3}) : (7.30\times10^{-3})$$

- The quantum field correction (Lamb shift) seems ~5 × ***larger*** than the hyperfine splitting; in fact, they are comparable.
- Dipole-dipole interaction: "21 cm line" at 1.42 GHz
- Lamb shift permits the $2^2p_{1/2} \to 2^2s_{1/2}$ transition at 1.06 GHz
- Odd power of α_e: beyond Sommerfeld's semi-classical result

Quantum Mechanics II

Now, go forth and calculate!!

Tristan Hübsch
Department of Physics and Astronomy, Howard University, Washington DC
http://physics1.howard.edu/~thubsch/