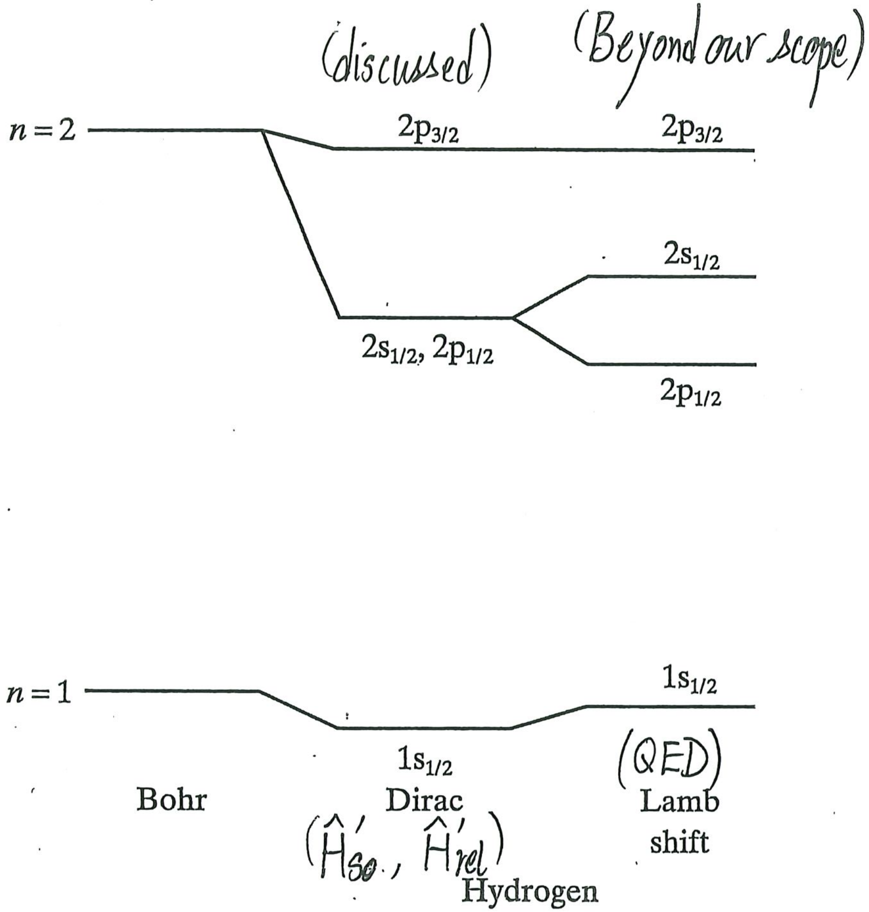
J. Hyperfine Structure

So far



(Not to scale)

[and the story continues] As spectroscopy becomes increasingly precise, even finer details are observed.

Q: The nucleus (proton for hydrogen) has Spin Angular momentum. How does nucleus spin affect the energy levels?

[Note: Study effects of nucleus]

Let's take stock ...

- Up to now, the nucleus provides

$$U(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$$

(in $\hat{H}_{atom}$)

$-e^2$ comes from $(+e)(-e)$

and $U(r)$ also enters into

$$\hat{H}_{so} \sim \vec{S}\cdot(\vec{\nabla}U \times \vec{p}) \sim \frac{1}{r}\frac{dU(r)}{dr}\,\vec{S}\cdot\vec{L}$$

in spin-orbit interaction

[both related to the charge +e of the proton (nucleus)] gives ($\vec{\nabla}U$)

- But proton is a spin-½ particle of +e charge
  $\Rightarrow \vec{\mu}_p$ (magnetic dipole moment)   What is its effect?

A Useful/Correct Viewpoint

See an atom as a whole [(nucleus + electron) is the whole atom system]

Allowed energies: Allowed energies that the atom can take on

not focusing on what an electron is doing

This is useful when things are interacting

e.g. electrons in atoms (other than hydrogen) are interacting

Hyperfine splitting (Hydrogen 1s states) $(1s\ ^2S_{1/2})$ [this is the electron]

- **Proton**: $+e$, spin-half $s=\frac{1}{2}$. $\vec{S}_p$ = spin AM of proton

Accompanying $\vec{S}_p$ is: $\boxed{\vec{\mu}_p = g_p \frac{e}{2m_p} \vec{S}_p}$ (41)[+]

[proton mass ≈ 2000 m_e]

[g factor of proton, $g_p = 5.586$ experimentally]

$$\vec{\mu}_p = g_p \left(\frac{e\hbar}{2m_p}\right) \frac{1}{\hbar} \vec{S}_p \equiv g_p \mu_N \frac{1}{\hbar} \vec{S}_p$$

where μ_N = Nuclear Magneton $= \frac{e\hbar}{2m_p} = \underbrace{\left(\frac{e\hbar}{2m_e}\right)}_{\mu_B} \cdot \underbrace{\frac{m_e}{m_p}}_{\sim 1/2000} \approx \underbrace{3.152 \times 10^{-8}\ \text{eV/Tesla}}_{\ll \mu_B}$

(important in MRI)

$\Rightarrow$ expect effects to be tiny!

[+] Remark:

For other nuclei, $\vec{I}$ = total spin AM of nucleus is used since there are many nucleons.

Physical Picture (Rough) Nucleus (proton) ≈ tiny magnet ; electron ≈ tiny magnet

they interact like two magnetic moments

$\vec{\mu}_N$ [proton] ($s = 1/2$) $\qquad$ $\vec{\mu}_{spin}$ [electron] ($s = 1/2$)

$\hat{H}'_{\substack{\text{nucleus-}\\\text{spin}}\,\substack{\text{electron}\\\text{spin}}}$ = Additional interaction energy[+] due to nucleus spin and electron spin

$$= A' \, \vec{S}_p \cdot \vec{S}_e$$

$$= A \left(\frac{\vec{S}_p}{\hbar} \cdot \frac{\vec{S}_e}{\hbar} \right) \qquad (42)$$

A: an energy giving how tiny the interaction is; $\vec{S}_p$: nucleus (proton); $\vec{S}_e$: electron

Note:

- $\frac{\vec{S}}{\hbar}$ is a number

this should be included into the Hamiltonian of the atom (if such accuracy is necessary)

[+] Form is similar to $\hat{H}'_{so} = f(r)\,\vec{S}\cdot\vec{L}$ in spin-orbit interaction. Thus, same technique can be applied to handle $\hat{H}'_{\substack{\text{nucleus-}\\\text{spin}}\,\substack{\text{electron}\\\text{spin}}}$. Here, the interaction is between nucleus <u>spin</u> & electron <u>spin</u> (spin-spin). In $\hat{H}'_{so}$, the nucleus provides $V(r)$ for the electron so that $\hat{H}'_{so} \sim \vec{S}\cdot(\vec{\nabla}V \times \vec{p})$.

- Reminder on two pieces of old physics

• See "$\vec{S}\cdot\vec{L}$", define $\vec{J}=\vec{S}+\vec{L}$ →

Recall: In spin-orbit coupling $\hat{H}_{so}' = f(r)\,\vec{S}\cdot\vec{L}$, the coupled $\vec{S}$ and $\vec{L}$ lead us to consider $\vec{J}=\vec{L}+\vec{S}$ and

$$\vec{S}\cdot\vec{L} = \frac{J^2-L^2-S^2}{2}$$

, and states $|\ell,(s),j,m_j\rangle$ are convenient. Here, we do the same thing.

Now, See $\vec{S}_p\cdot\vec{S}_e$

define $\vec{S}_{total}=\vec{S}_p+\vec{S}_e$

$\vec{S}_p$ ↑ nucleus, $\vec{S}_e$ ↑ electron

Adding two $s=\frac{1}{2}$ angular momenta?

$S=1$ (triplet)

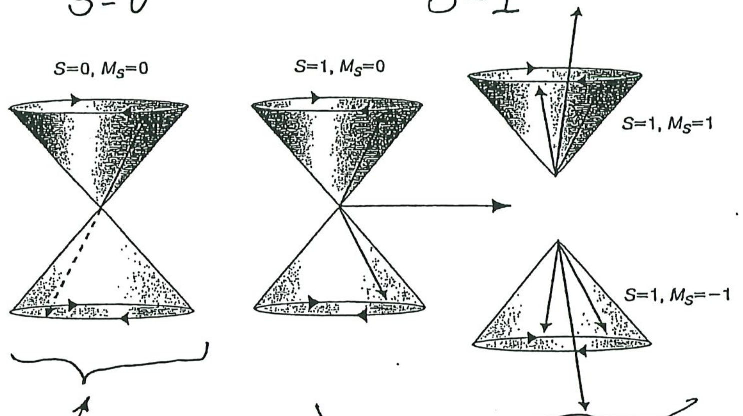
$S=0$ (singlet)

Here, $\vec{S}_1$ is nucleus spin

$\vec{S}_2$ is electron spin

Recall: Adding two spin-½ angular Momenta

$S=0$ $\qquad$ $S=1$



Vector model of the singlet and triplet states. The individual spin angular momentum vectors and their vector sum S (black arrow) are shown for the triplet states. For the singlet state (left image), $|S| = 0$ and $M_S = 0$. The dashed arrow in the left image indicates that the vector on the yellow cone is on the opposite side of the cone from the vector on the blue cone.

Singlet state: Two spin angular momenta tend to be anti-parallel

triplet states: Two spin angular momenta tend to be aligned

Let's see what happens to Hydrogen atom Ground State

$$\hat{H}'_{\text{hyperfine}} = \hat{H}'_{\substack{\text{nucleus-}\\ \text{spin}}\substack{\text{electron}\\ \text{spin}}} = A\left(\frac{\vec{S}_p}{\hbar}\cdot\frac{\vec{S}_e}{\hbar}\right) \propto \vec{S}_p\cdot\vec{S}_e$$

[1s : $n=1$, $l=0$, $\underset{\text{electron}}{s=\tfrac{1}{2}}$, $j=\tfrac{1}{2}$ (due to s, "$l=0$") (2 states $\left(\begin{matrix} m_j=\pm\tfrac{1}{2} \\ \text{OR} \\ m_s=\pm\tfrac{1}{2}\end{matrix}\right)$ of same energy)
(ignore $\hat{H}'_{\text{hyperfine}}$)]

Introduce: $\vec{S}_{\text{total}} = \vec{S}_p + \vec{S}_e$ (spin quantum numbers: $S_p=\tfrac{1}{2}$, $S_e=\tfrac{1}{2}$ both spin-half particles)

$$|\vec{S}_{\text{total}}| = \sqrt{S(S+1)}\,\hbar \qquad S_{\text{total},z} = M_S\hbar$$

with $\begin{cases} S=1,\ M_S=1,0,-1 \ (\text{triplet}) & [\vec{S}_p, \vec{S}_e \text{ tend to align}] \\ S=0,\ M_S=0 \ (\text{singlet}) & [\text{tend to anti-align}] \end{cases}$

$$\vec{S}_p\cdot\vec{S}_e = \frac{S_{\text{total}}^2 - S_p^2 - S_e^2}{2} \text{ takes on } \frac{\left[S(S+1)-\tfrac{3}{4}-\tfrac{3}{4}\right]\hbar^2}{2} \text{ depending on } S$$

could be 0 or 1

1s states (can use $s_e = 1/2$ and m_s OR $j = 1/2$ and m_j)
[doesn't matter because $l = 0$]

<u>Without</u> $\hat{H}'_{\text{hyperfine}}$, can use

$$\Big|\overbrace{s_p, m_{s_p}}^{\text{nucleus' spin}}\,;\ \overset{\text{"}n\text{"}}{1}, \overset{\text{"}l\text{"}}{0}, \overset{\text{"}m_l\text{"}}{0},\ \underbrace{\overset{1/2\ \text{always}}{s_e}, m_s}_{\text{electron spin}}\Big\rangle$$

$s_p = 1/2$ always

<u>Not invoked before</u> [no need, nucleus effect not included]

<u>With</u> $\hat{H}'_{\text{hyperfine}}$, invoke $|S, M_S, s_p, s_e, \overset{\text{"}n\text{"}}{1}, \overset{\text{"}l\text{"}}{0}, \overset{\text{"}m_l\text{"}}{0}\rangle$ is useful

$S = 1, 0$; $s_p = 1/2$; $s_e = 1/2$

<u>Why?</u>

depends on value of quantum number S

$$\hat{H}'_{\text{hyperfine}}|S, \dots\rangle = \left[\frac{S(S+1) - 3/4 - 3/4}{2}\right] A\,|S, \dots\rangle$$

(Key idea)

States of $S=1$: (triplet) $\quad \dfrac{\vec{S}_p}{\hbar}\cdot\dfrac{\vec{S}_e}{\hbar} = \dfrac{2-3/4-3/4}{2} = +1/4$

State of $S=0$: (singlet) $\quad \dfrac{\vec{S}_p}{\hbar}\cdot\dfrac{\vec{S}_e}{\hbar} = \dfrac{0-3/4-3/4}{2} = -3/4$

$\therefore$ 1st order perturbation†:

$$\left.\begin{aligned} E_{hf}(\underbrace{S=1, m_s}_{3\ \text{states}}) &= \frac{A}{4} \\ E_{hf}(S=0, m_s=0) &= \frac{-3A}{4} \end{aligned}\right\}$$

shift in energy due to hyperfine interaction

"A" here is actually same expectation value $\langle A \rangle$, c.f. $\langle f(r) \rangle$ in treating $\hat{H}'_{so}$

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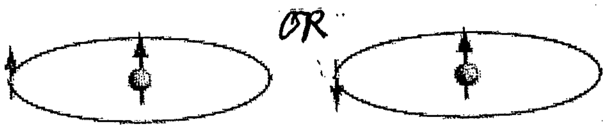
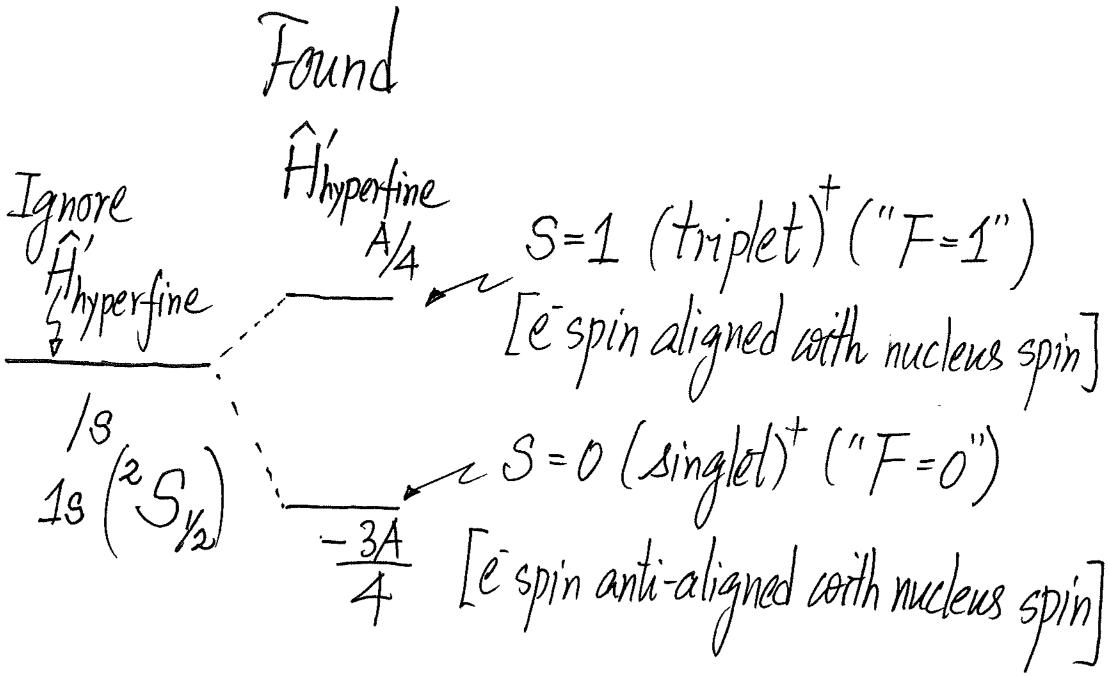
† In most books, the total spin (nucleus + electron) is labelled by the quantum number F. So, $(F=1, m_F)$ are the triplet states and $(F=0, m_F=0)$ is singlet. We avoided new notations for simplicity.

Pictorially With $\hat{H}'_{hyperfine}$

amounts to asking which of the hydrogen 1s state



has a lower energy?



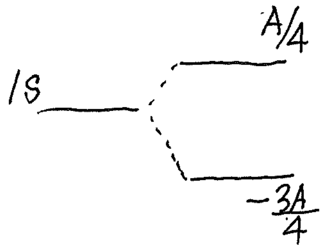
"Hyperfine splitting"

How big is the hyperfine splitting in H-atom?

$^+$ It is the total spin AM (electron's Spin AM + proton's spin AM) that matters! The total Spin AM is characterized by S. So these are allowed energies of the atom as a whole!

For hydrogen 1s with $\hat{H}_{hf}$:

$$\Delta E_{\text{hyperfine}} = A = \frac{4\, g_p \hbar^4}{m_p m_e^2 c^2 a_B^4} \cong \underbrace{5.88 \times 10^{-6}\,\text{eV}}_{\text{Note order of magnitude}}$$



Wrote a nice textbook on Mechanics

Due to works by Goldenberg, Kleppner, Ramsey

1989 Nobel Prize

The corresponding frequency is:

$$\nu = \frac{\Delta E}{h} = \underbrace{1420\text{ MHz}}_{\text{Important! (See below)}}$$

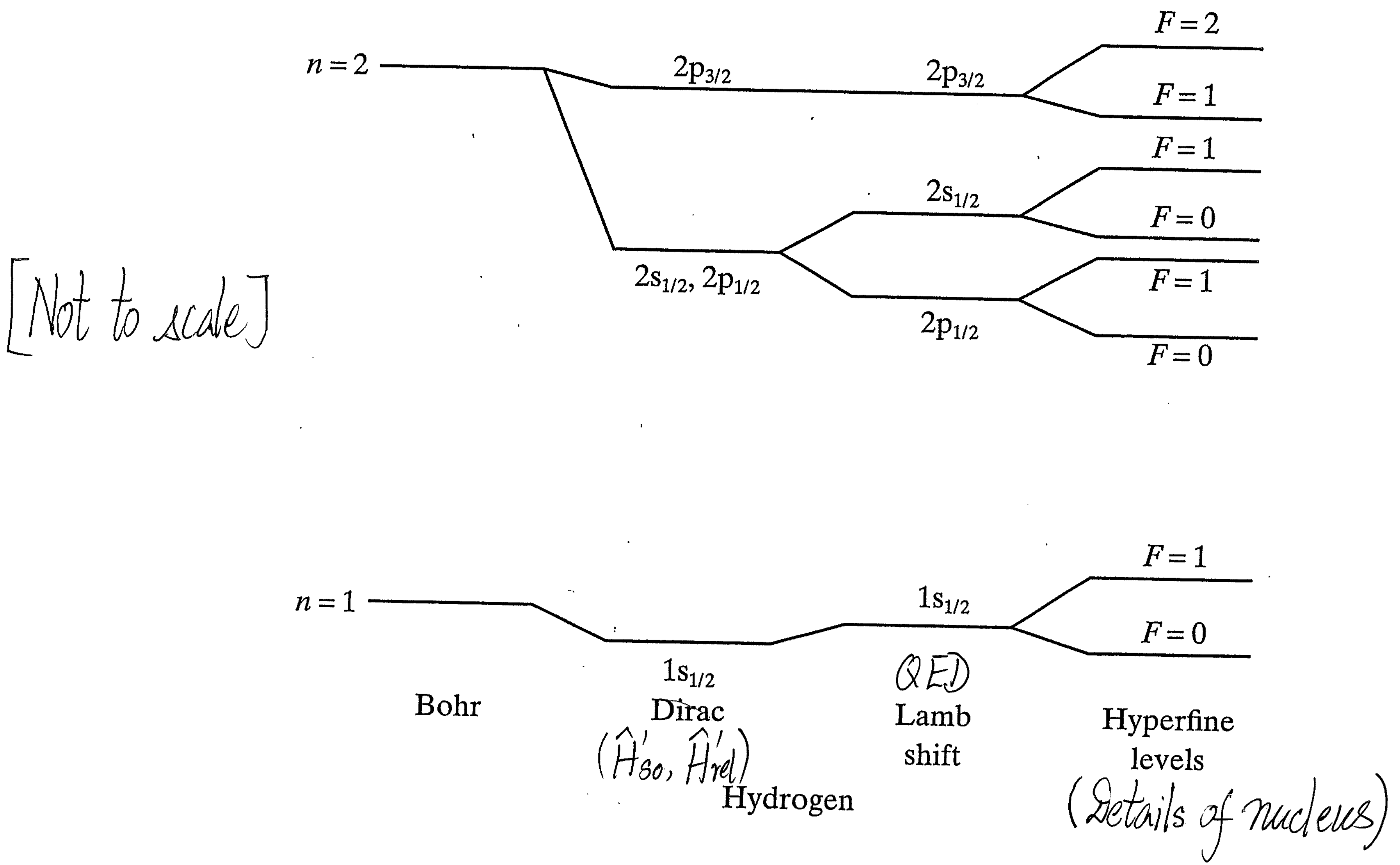
Measured to be 1420 405 751.7667 Hz (very accurately known)

The corresponding wavelength is:

$$\lambda = \frac{c}{\nu} = \underbrace{21.121\text{ cm}}_{\text{or the "21-cm line" of hydrogen}}$$

"21 cm cosmology"

Finally, putting all effects together† (hydrogen atom)



† See Remark on the notation F.

Aside: Standard Notations in describing Hyperfine interaction

Electrons part : $\vec{J}$ — total AM of electrons

Nucleus (many protons/neutrons) : $\vec{I}$ — total AM of nucleons

$$\boxed{\hat{H}'_{\text{hyperfine}} = A\left(\frac{\vec{I}}{\hbar}\cdot\frac{\vec{J}}{\hbar}\right) \propto \vec{I}\cdot\vec{J}}$$

Introduce $\vec{F} = \vec{I} + \vec{J}$ — total AM of nucleus and electrons

F^2 takes on $F(F+1)\hbar^2$

F_z takes on $M_F\hbar$

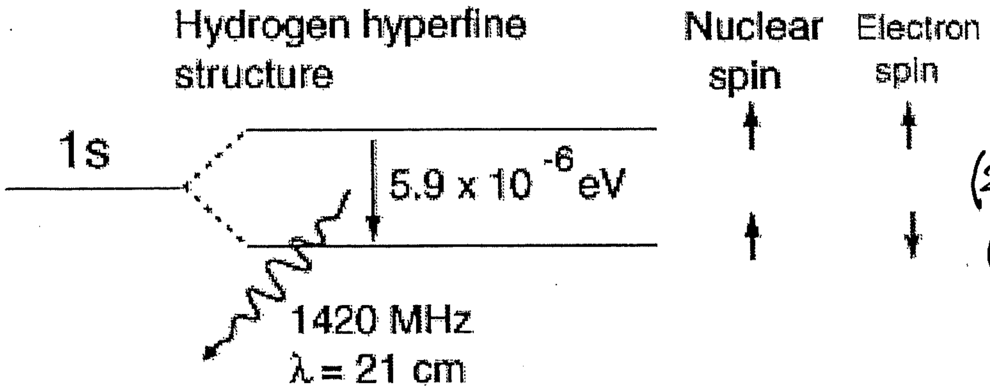
$$\vec{I}\cdot\vec{J} = \frac{F^2 - I^2 - J^2}{2}$$

$$\frac{\vec{I}\cdot\vec{J}}{\hbar^2}|F, M_F\ I, J\rangle$$

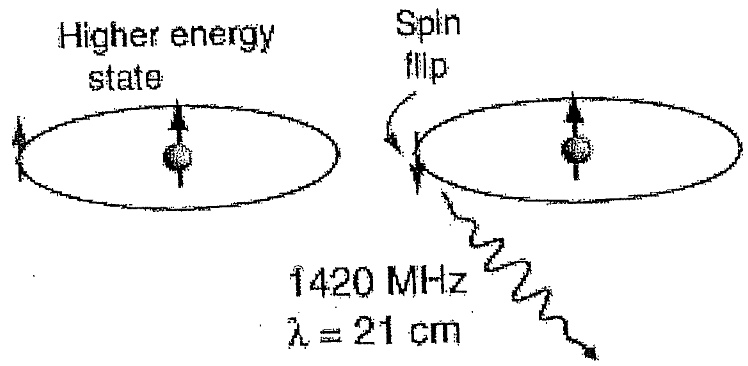
$$= \frac{F(F+1) - I(I+1) - J(J+1)}{2}|F, M_F; I, J\rangle$$

this is how the label F comes about

Radio Astronomy (21 cm Astrophysics)



(21.1 cm, 1420 MHz)
$(\underbrace{\sim 0.07\,K}_{\text{"temperature"}})$



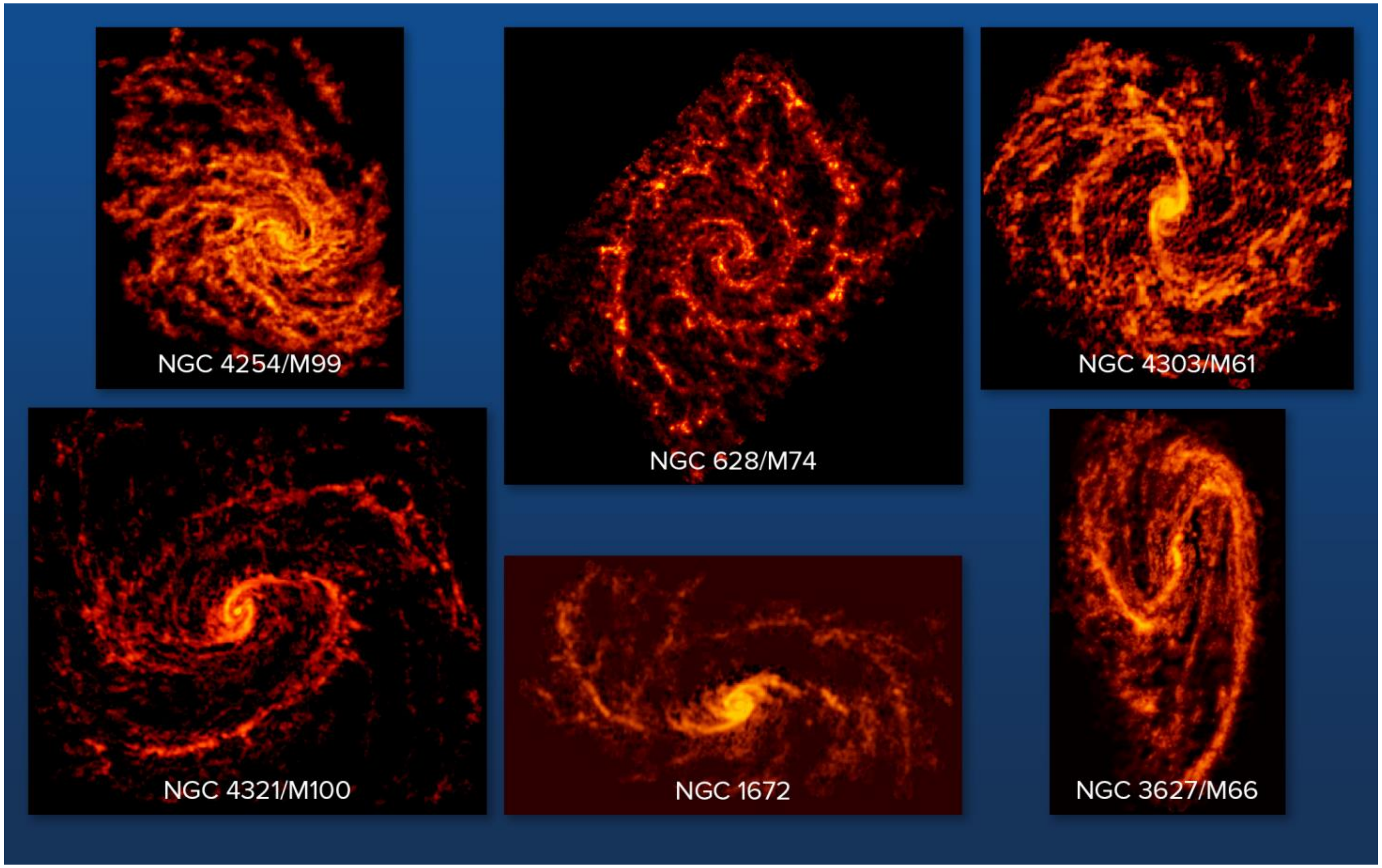
1951 Ewen and Purcell observed 21-cm line from interstellar neutral hydrogen in our galaxy (beginning of radio astronomy). The 21-cm wave can penetrate dust clouds, thus giving a map of hydrogen.

With Doppler's shift on the line, can infer velocity of source (toward us OR away from us), thus beautiful spiral pictures of galaxies.

Cosmic background (~3K) radiation is responsible for excitation across $\Delta E_{\text{hyperfine}}$.

21cm Astronomy/Cosmology

Radio Astronomy maps galaxy pictures by Doppler's effect of neutral Hydrogen atom (HI) hyperfine



NSF (US) National Radio Astronomy Observatory https://public.nrao.edu/gallery/phangs-alma-survey-sample-galaxies/

FAST (*F*ive-hundred-meter *A*perture *S*pherical radio *T*elescope)

FAST in China (貴州洼坑) completed construction in 2016. It is the most powerful radio telescope.

See http://fast.bao.ac.cn/ for its design and scientific goals.

In September 2016, FAST was completed. Science (the magazine) carried a featured article introducing the new concepts in the telescope's design. See the article entitled "The Biggest Ear" at http://science.sciencemag.org/content/353/6307/1488 (accessible via CUHK sites).

21-cm line is also a way to study the baby universe (first billion years of the universe). See 2019 Nature article: https://www.nature.com/articles/d41586-019-02417-7

For a professional discussion on what 21-cm physics can do for 21st century cosmology, read the review article

J.R. Pritchard and A. Loeb, *21 cm cosmology in the 21st century*, Reports on Progress in Physics **75** (2012) 086901

http://iopscience.iop.org/article/10.1088/0034-4885/75/8/086901/pdf (from CUHK sites)

Remark: Other effects of Nucleus

- Finite mass (use reduced mass)
- Isotope (spectrum of H-atom vs D-atom)

  nucleus has $1p + 1n$

- Proton is not a point particle (as $U(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$ assumed)
  - How big is a proton? (a fundamental question in nuclear physics)

R (radius)

proton

$+e$ charge

$$U(r) = \begin{cases} \dfrac{e^2}{4\pi\varepsilon_0 (2R)}\left(\dfrac{r^2}{R^2} - 3\right), & r \le R \\[2ex] \dfrac{-e^2}{4\pi\varepsilon_0 R}, & r > R \end{cases}$$

How will this alter e.g. $2p \to 1s$ transition?

Can high-precision spectroscopy (H-atom) help determine the size of a proton?

Final Remarks

- Hydrogen spectrum and high-precision spectroscopy are driving forces of advancements in many branches of physics
  - proton size
  - antimatter vs matter

    can measure anti-hydrogen's spectrum
  - Where does proton's (neutron's) spin come from?

    (something (quarks) inside)

Further Reading on Hyperfine Structure (Quantum Mechanics)

A more thorough treatment of Hyperstructure and Effects due to the nucleus for hydrogen atom can be found in

B.H. Bransden & C.J. Joachain, *Physics of atoms and molecules*

[first-order perturbation theory works]