Hyperfine splitting

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In atomic physics, **hyperfine structure** is the different effects leading to small shifts and splittings in the energy levels of atoms, molecules and ions. The name is a reference to the *fine structure* which results from the interaction between the magnetic moments associated with electron spin and the electrons' orbital angular momentum. Hyperfine structure, with energy shifts is typically orders of magnitude smaller than the fine structure, results from the interactions of the nucleus (or nuclei, in molecules) with internally generated electric and magnetic fields.

In atoms, hyperfine structure occurs due to the energy of the nuclear magnetic dipole moment in the magnetic field generated by the electrons, and the energy of the nuclear electric quadrupole moment in the electric field gradient due to the distribution of charge within the atom. Molecular hyperfine structure is generally dominated by these two effects, but also includes the energy associated with the interaction between the magnetic moments associated with different magnetic nuclei in a molecule, as well as between the nuclear magnetic moments and the magnetic field generated by the rotation of the molecule.

http://en.wikipedia.org/wiki/Hyperfine_structure

$$\hat{\boldsymbol{\mu}}_e = -\frac{g_e \mu_B}{\hbar}\hat{\boldsymbol{S}}_e \approx -\frac{2\mu_B}{\hbar}\hat{\boldsymbol{S}}_e, \quad \text{(the magnetic moment of electron)}$$

$$\hat{\boldsymbol{\mu}}_p = \frac{g_p \mu_N}{\hbar}\hat{\boldsymbol{S}}_p. \quad \text{(the magnetic moment of proton).}$$

where g_e (=2.0023193043618) is the electron g-factor for electron and g_p (=5.58569) is the nuclear g-factor for proton with mass m_p.

$$\mu_B = \frac{e\hbar}{2m_e c}, \qquad \mu_N = \frac{e\hbar}{2m_p c}$$

The magnetic field generated by a magnetic moment of the proton is given by

$$\boldsymbol{B} = \frac{1}{r^5}[3(\boldsymbol{\mu}_p \cdot \boldsymbol{r})\boldsymbol{r} - \boldsymbol{\mu}_p r^2] + \frac{8\pi}{3}\boldsymbol{\mu}_p \delta(\boldsymbol{r})$$

(see J.D. Jackson, Classical Electrodynamics, 2nd edition (John Wiley & Sons, 1975) p.184.

So the Hamiltonian of the electron, in the magnetic field due to the proton's magnetic moment is

$$\begin{aligned}\hat{H}_{hf} &= -\hat{\boldsymbol{\mu}}_e \cdot \boldsymbol{B} \\ &= \frac{2g_p\mu_B\mu_N}{\hbar^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e\cdot\hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e|\hat{\boldsymbol{r}}|^2] + \frac{8\pi}{3}\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e\delta(\hat{\boldsymbol{r}})\} \\ &= \frac{g_p e^2}{2m_e m_p c^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e\cdot\hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e|\hat{\boldsymbol{r}}|^2] + \frac{8\pi}{3}\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e\delta(\hat{\boldsymbol{r}})\}\end{aligned}$$

The ground state of the hydrogen (n = 1, l =0) is very special since $|\psi_{1,0,0}(\boldsymbol{r})|^2$ is not zero at the origin. The ground state is also a non-degenerate state. The first-order correction to the energy is the expectation value of the perturbing Hamiltonian;

$$\begin{aligned}E_{hf}{}^{(1)} &= \langle n=1, l=0, m=0|\frac{g_p e^2}{2m_e m_p c^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e\cdot\hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e|\hat{\boldsymbol{r}}|^2]\}|n=1, l=0, m=0\rangle \\ &+ \frac{4\pi g_p e^2}{3m_e m_p c^2}\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e\langle n=1, l=0, m=0|\delta(\hat{\boldsymbol{r}})|n=1, l=0, m=0\rangle\end{aligned}$$

In the ground state (with l = 0) the wave function is spherically symmetric, and the first expectation value vanishes. Then we get

$$E_{hf}{}^{(1)} = \frac{4\pi g_p e^2}{3m_e m_p c^2}\hat{\boldsymbol{S}}_p\cdot\hat{\boldsymbol{S}}_e|\psi_{1,0,0}(\boldsymbol{r}=0)|^2,$$

where

$$|\psi_{1,0,0}(\boldsymbol{r}=0)|^2 = \frac{1}{\pi a_B{}^3}$$

This is a contact-type (or Fermi-type) interaction. This has non-zero only when the electron is at the position of proton. The interaction energy is proportional to the probability $|\psi_{1,0,0}(\boldsymbol{r}=0)|^2$ of the electron being at the position of the proton.

We redefine this interaction as the perturbing Hamiltonian

$$\hat{H}_1 = \frac{g_p e^2\hbar^2}{3m_e m_p a_B{}^3 c^2}\hat{\boldsymbol{\sigma}}_p\cdot\hat{\boldsymbol{\sigma}}_e = \frac{g_p\hbar^4}{3m_p m_e{}^2 c^2 a_B{}^4}\hat{\boldsymbol{\sigma}}_p\cdot\hat{\boldsymbol{\sigma}}_e$$

in the ground state, where

$$a_B = \frac{\hbar^2}{m_e e^2}, \qquad \alpha = \frac{e^2}{\hbar c}$$

Here we introduce the Dirac spin exchange operator

$$\hat{P}_{ep} = \frac{1}{2}(\hat{1} + \hat{\boldsymbol{\sigma}}_p \cdot \hat{\boldsymbol{\sigma}}_e).$$

There are four states which are the combination of the spin states of electron and proton;

$|++\rangle$: electron spin up and proton spin up

$|+-\rangle$: electron spin up and proton spin down

$|-+\rangle$: electron spin down and proton spin up

$|--\rangle$: electron spin down and proton spin down

Note that

$$\hat{P}_{ep}|++\rangle = |++\rangle, \ \hat{P}_{ep}|+-\rangle = |-+\rangle,$$

$$\hat{P}_{ep}|-+\rangle = |+-\rangle, \ \hat{P}_{ep}|--\rangle = |++\rangle.$$

The spin-spin coupling is rewritten as

$$\hat{H}_1 = E_0(2\hat{P}_{ep} - \hat{1}),$$

where

$$E_0 = \frac{g\hbar^4}{3m_p m_e^2 c^2 a_B^4}.$$

Then we have

$$\hat{H}_1|++\rangle = E_0(2\hat{P}_{ep} - \hat{1})|++\rangle = E_0|++\rangle$$

$|++\rangle$ is the eigenket of $\hat{H}_1$ with the energy eigenvalue E_0.

$$\hat{H}_1|--\rangle = E_0(2\hat{P}_{ep} - \hat{1})|--\rangle = E_0|--\rangle$$

$|--\rangle$ is the eigenket of $\hat{H}_1$ with the energy eigenvalue E_0.

$$E_2 = E_0 \qquad |++\rangle$$

$$E_2 = E_0 \qquad |--\rangle$$

$$\hat{H}_1|+-\rangle = E_0(2\hat{P}_{ep} - \hat{1})|+-\rangle = E_0(2|-+\rangle - |+-\rangle)$$

$$\hat{H}_1|-+\rangle = E_0(2\hat{P}_{ep} - \hat{1})|-+\rangle = E_0(2|+-\rangle - |-+\rangle)$$

$$\hat{H}_1 = E_0\begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}$$

The eigenvalue problem:

$$E_2 = E_0 \qquad \frac{1}{\sqrt{2}}[|+-\rangle + |-+\rangle]$$

$$E_1 = -3E_0 \qquad \frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle]$$

The hyperfine splitting in the ground state of hydrogen.

$$\Delta E = 4E_0 = \frac{4g\hbar^4}{3m_p m_e{}^2 c^2 a_B{}^4} = 5.87746\ (\mu\text{eV}).$$

The frequency:

$$\nu = \frac{4E_0}{h} = 1421.16\ \text{MHz}.$$

The wavelength:

$$\lambda = \frac{c}{\nu} = 21.0948 \text{ cm.}$$

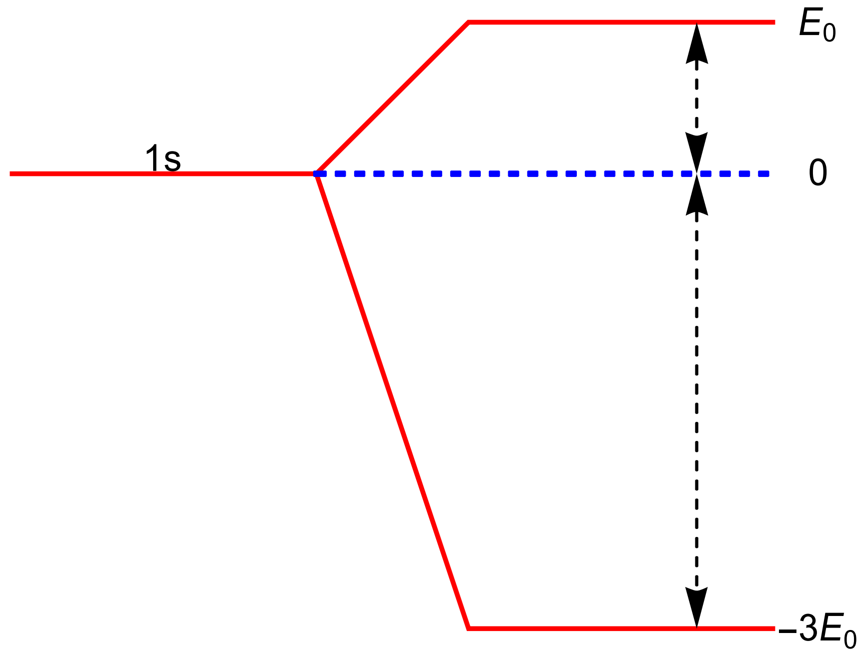


Fig. Hyperfine splitting in the ground state of hydrogen. Triplet state with energy E_0 ($|++\rangle$, $\frac{1}{\sqrt{2}}[|+-\rangle + |-+\rangle]$, $|--\rangle$ and the singlet with the energy $(-3E_0)$ ($\frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle]$

((**Mathematica**))

```
Clear["Global`*"];

rule1 = {c → 2.99792 × 10^10, ℏ → 1.054571628 10^-27,
    me → 9.10938215 10^-28, mp → 1.672621637 × 10^-24,
    qe → 4.8032068 × 10^-10, eV → 1.602176487 × 10^-12,
    keV → 1.602176487 × 10^-9, MeV → 1.602176487 × 10^-6,
    rB → 0.52917720859 × 10^-8};
```

$$E1 = \frac{4\, g\, \hbar^4}{3\, mp\, me^2\, c^2\, rB^4\, eV} \;//.\; rule1 \;/.\; g \to 5.58569$$

5.87746×10^{-6}

$$f = \frac{4\, g\, \hbar^4}{3\, mp\, me^2\, c^2\, rB^4\, (2\, \pi\, \hbar)} \;//.\; rule1 \;/.\; g \to 5.58569$$

1.42116×10^{9}

```
λ = c / f /. rule1
```

21.0948

2. HI 21 cm

Hydrogen is the most abundant element in the interstellar medium (ISM), but the symmetric H_2 molecule has no permanent dipole moment and hence does not emit a detectable spectral line at radio frequencies. Neutral hydrogen (HI) atoms are abundant and ubiquitous in low-density regions of the ISM. They are detectable in the $\lambda = 21.0948$ cm ($\nu = 1421.16$ MHz) hyperfine line. Two energy levels result from the magnetic interaction between the quantized electron and proton spins.

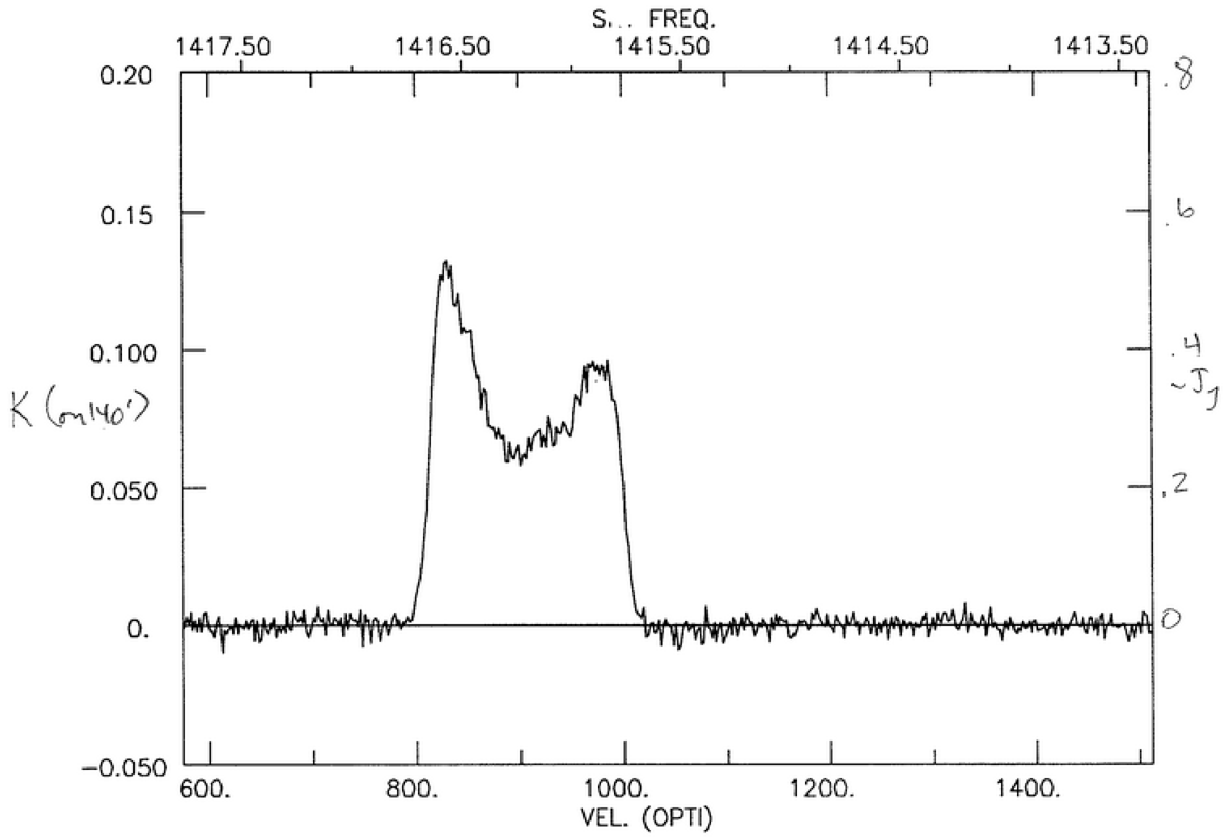


Fig. This integrated HI spectrum of UGC 11707 obtained with the 140-foot telescope shows the typical two-horned profile of a spiral galaxy (red-shift; the observed frequency shifts to the lower frequency side from 1420 MHz to 1416 MHz).

For UGC 11707, the line center frequency is $f = 1416.2$ MHz. According to the Doppler effect, the observed frequency is given by

$$f = f_0(\frac{c - v_t}{c})$$

in the non-relativistic limit. Then the recessional velocity v_t is obtained as

$$v_t = c(1 - \frac{f}{f_0}) = 3 \text{ x } 10^5 \text{ km/s } (1 - \frac{1416.2MHz}{1420.4MHz}) = 890 \text{ km/s.}$$

The distance D is obtained as

$$D = \frac{v_t}{H_0} = \frac{890(km/s)}{67.80(km/s)Mpc^{-1}} = 13.3(Mpc)$$

Note that c is the velocity of light and H_0 is the Hubble constant, and D is the distance from the Earth.

H_0 = 67.80 km/s Mpc^{-1}.

1 pc = 3.26 light year (pc: parsec)

1 Mpc = 3.26 x 10^{6} light year
=3.08567758 x 10^{22} m (Mega parsec)

1 year = 3.1556926 x 10^{7} s.

The time taken after the Big Ban can be calculated as

$$\frac{1}{H_0} = \frac{Mpc}{67.80(km/s)} = \frac{3.08567758\times10^{22}}{67.80\times10^{3}\times3.15569\times10^{7}} = 14.42 \text{ billion year}$$

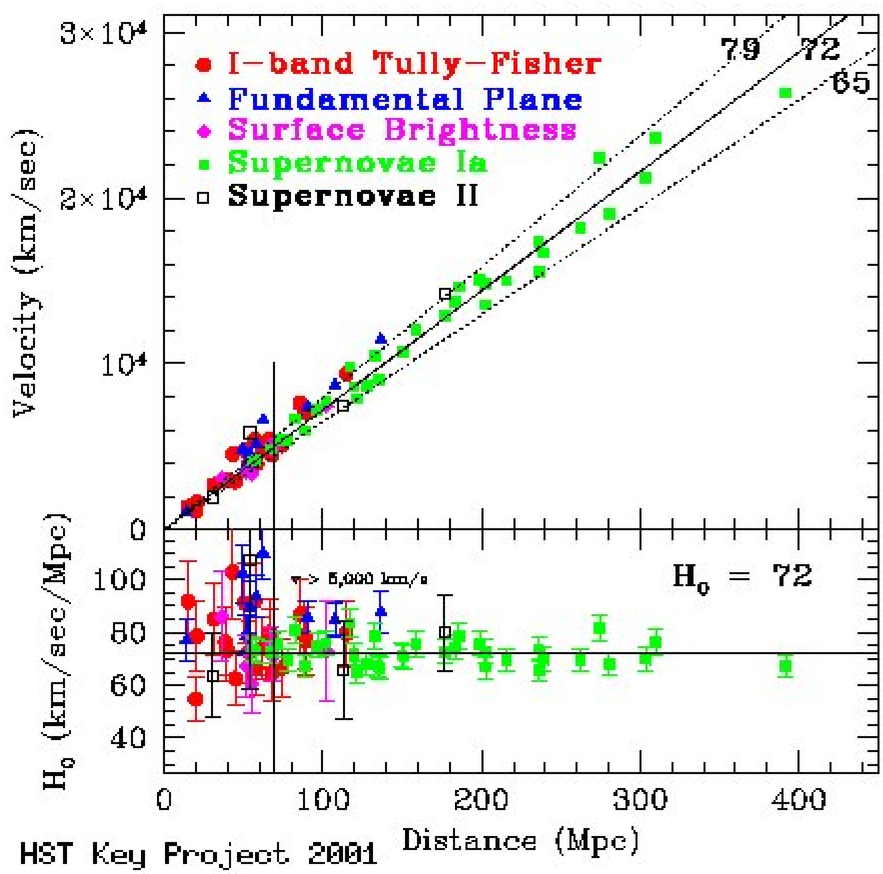


Fig. Hubble diagram from the Hubble Space Telescope Key Project (Freedman et al. 2001) using five different measures of distance. Bottom pane shows H0 vs distance with horizontal equal to the best fit value of 72 km/s Mpc^{-1}. The recessional velocity v of stars moving away from the Earth is proportional to the distance D from the Earth; $v = H_0 D$. H_0 is the Hubble's constant.

REFERENCES

D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, 1995).

J.D. Jackson, *Classical Electrodynamics*, 2nd edition (John Wiley & Sons, 1975) p.184.

S. Dodelson, Modern Cosmology (Academic Press, 2003).

D.H. McIntyre, *Quantum Mechanics A Paradigms Approach* (Pearson Education, 2012). p.361.

APPENDIX-I Magnetic field arising from magnetic moment

We consider the distribuition of the magnetic field $\boldsymbol{B}$ due to the magnetic moment $\boldsymbol{\mu}_p$ at the origin, whose direction is along the z axis. The vector potential $\boldsymbol{A}$ due to the magnetic dipole moment $\boldsymbol{\mu}$ can be described by

$$\boldsymbol{A} = \frac{\boldsymbol{\mu}_p \times \boldsymbol{r}}{r^3} = -\boldsymbol{\mu}_p \times \nabla \frac{1}{r}, \qquad (9)$$

where $\nabla \frac{1}{r} = -\frac{\boldsymbol{r}}{r^3}$

The magnetic field $\boldsymbol{B}$ is obtained as

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}, \qquad (10)$$

So we have $\boldsymbol{B}$ (except for $\boldsymbol{r} = 0$) as

$$\begin{aligned} \boldsymbol{B} &= -\nabla \times (\boldsymbol{\mu}_p \times \nabla \frac{1}{r}) \\ &= (\boldsymbol{\mu}_p \cdot \nabla)\nabla \frac{1}{r} - \boldsymbol{\mu}_p \nabla^2 \frac{1}{r}. \\ &= \frac{3\boldsymbol{r}(\boldsymbol{\mu}_p \cdot \boldsymbol{r}) - r^2 \boldsymbol{\mu}_p}{r^5} \end{aligned} \qquad (11)$$

Note that

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\boldsymbol{r}) \to 0 .$$

$$(\boldsymbol{\mu}_p \cdot \nabla)\nabla \frac{1}{r} = \frac{3\boldsymbol{r}(\boldsymbol{\mu}_p \cdot \boldsymbol{r}) - r^2 \boldsymbol{\mu}_p}{r^5} .$$

The expression for the magnetic field including $\boldsymbol{r} = 0$ is given by

$$\boldsymbol{B} = \frac{3\boldsymbol{r}(\boldsymbol{\mu}_p \cdot \boldsymbol{r}) - r^2 \boldsymbol{\mu}_p}{r^5} + \frac{8\pi}{3}\boldsymbol{\mu}_p \delta(\boldsymbol{r}) .$$

[see J.D. Jackson, Classical Electrodynamics, 2nd edition (John Wiley & Sons, 1975) p.184]. The Hamiltonian of the magnetic moment of electron in the presence of magnetic field arising from the proton, is given by

$$H = -\boldsymbol{\mu}_e \cdot \boldsymbol{B} = \frac{-3(\boldsymbol{\mu}_e \cdot \boldsymbol{r}\cdot)(\boldsymbol{\mu}_p \cdot \boldsymbol{r}) + r^2(\boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p)}{r^5} + \frac{8\pi}{3}\boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p \delta(\boldsymbol{r})$$

The delta function term enters the expression for the hyperfine structure of atomic s states.

APPENDIX-II Proof of the integral which is zero

$$I = \langle n = 1, l = 0, m = 0 | \{ \frac{1}{|\boldsymbol{r}|^5} [3(\boldsymbol{S}_p \cdot \boldsymbol{r})(\boldsymbol{S}_e \cdot \boldsymbol{S}) - \boldsymbol{S}_p \cdot \boldsymbol{S}_e |\boldsymbol{r}|^2]\} | n = 1, l = 0, m = 0 \rangle = 0 .$$

$$I = \iiint r^2 \sin\theta d\theta d\phi |\psi_{100}(\boldsymbol{r})|^2 \frac{1}{|\boldsymbol{r}|^5} [3(\boldsymbol{S}_p \cdot \boldsymbol{r})(\boldsymbol{S}_e \cdot \boldsymbol{r}) - \boldsymbol{S}_p \cdot \boldsymbol{S}_e |\boldsymbol{r}|^2]\} ,$$

where we use

$$x = r\sin\theta\cos\phi , \qquad y = r\sin\theta\sin\phi , \qquad z = r\cos\theta$$

$$\psi_{100}(\mathbf{r}) = R_{10}(r) Y_0^0(\theta,\phi) = \frac{2}{a_B^{3/2}} e^{-r/a} \sqrt{\frac{1}{4\pi}} .$$

((**Mathematica**)) We show the proof of $I = 0$ by using the Mathematica

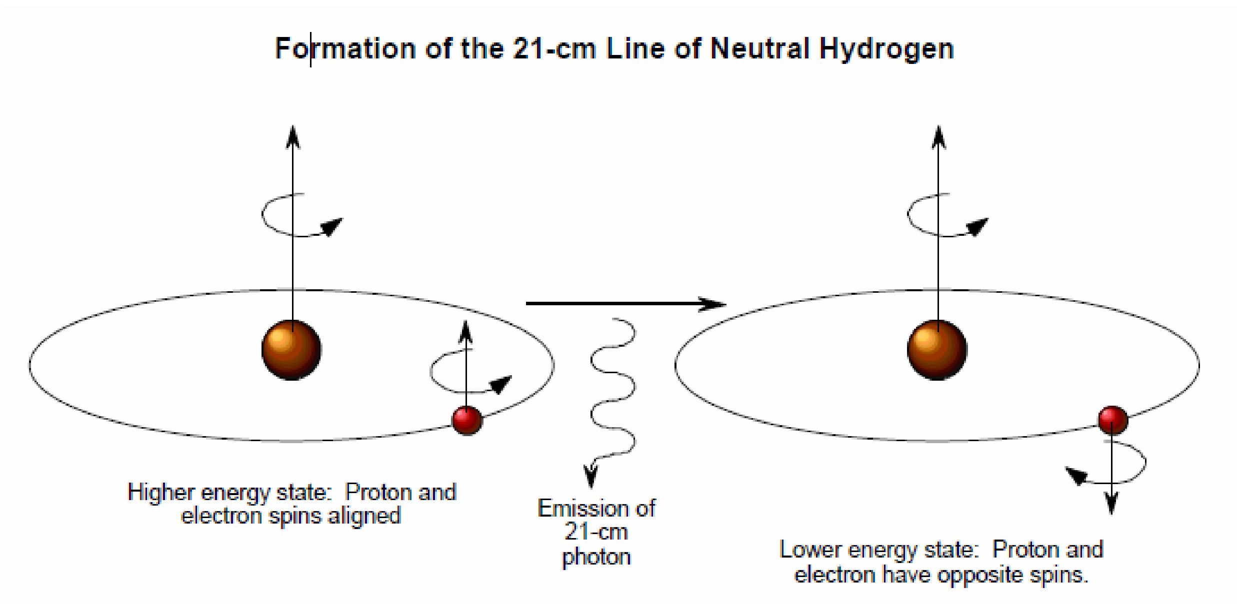
```
Clear["Global`*"]; ψ1 = Sqrt[1/(4 π) 2/a^(3/2)] Exp[-r/a];

F1 =
  (1/r^5 (3 (Se1 x + Se2 y + Se3 z)
        (Sp1 x + Sp2 y + Sp3 z)) -
      1/r^3 (Se1 Sp1 + Se2 Sp2 + Se3 Sp3)) r^2
    Sin[θ] ψ1^2 /. {x → r Sin[θ] Cos[ϕ],
    y → r Sin[θ] Sin[ϕ], z → r Cos[θ]} //
  FullSimplify;

Integrate[Integrate[Integrate[F1, {ϕ, 0, 2 π}],
   {θ, 0, π}], {r, 0, ∞}] // Simplify

0
```

APPENDIX-III



In the case of neutral (not ionized) hydrogen atoms, in their lower energy (ground) state, the proton and the electron spin in opposite directions. If the hydrogen atom acquires a slight amount of energy by colliding with another atom or electron, the spins of the proton and electron in the hydrogen atom can align, leaving the atom in a slightly excited state. If the atom then loses that amount of energy, it returns to its ground state. The amount of energy lost is that associated with a photon of 21.11 cm wavelength (frequency 1428 MHz).

Hydrogen is the key element in the universe. Since it is the main constituent of interstellar gas, we often characterize a region of interstellar space as to whether its hydrogen is neutral, in which case we call it an H I region, or ionized, in which case we call it an H II region. Some researchers involved in the search for extra-terrestrial intelligence have reasoned that another intelligent species might use this universal 21-cm wavelength line emission by neutral hydrogen to encode a message; thus these searchers have tuned their antennas specifically to detect modulations to this wavelength. But, perhaps more usefully, observations of this wavelength have given us much information about the interstellar medium and locations and extent of cold interstellar gas.

The hydrogen in our galaxy has been mapped by the observation of the 21-cm wavelength line of hydrogen gas. At 1420 MHz, this radiation from hydrogen penetrates the dust clouds and gives us a more complete map of the hydrogen than that of the stars themselves since their visible light won't penetrate the dust clouds.

The 1420 MHz radiation comes from the transition between the two levels of the hydrogen 1s ground state, slightly split by the interaction between the electron spin and the nuclear spin. The splitting is known as hyperfine structure. Because of the quantum properties of of radiation, hydrogen in its lower state will absorb 1420 MHz and the observation of 1420 MHz in emission implies a prior excitation to the upper state.

```
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   rB → 0.52917720859 × 10^-8};

E1 = (4 g ℏ^4)/(3 mp me^2 c^2 rB^4 eV) //. rule1 /. g → 5.58569
```

5.87746×10^{-6}

```
f = (4 g ℏ^4)/(3 mp me^2 c^2 rB^4 (2 π ℏ)) //. rule1 /. g → 5.58569
```

1.42116×10^{9}

```
λ = c / f /. rule1
```

21.0948

```
Graphics[{Red, Thick, Line[{{0, 0}, {2, 0}}],
  Line[{{2, 0}, {3, 1}, {5, 1}}],
  Line[{{2, 0}, {3, -3}, {5, -3}}], Blue, Thick,
  Dashed, Line[{{2, 0}, {5, 0}}],
  Arrowheads[{-0.05, 0.05}], Black, Thin,
  Arrow[{{4.5, 1}, {4.5, 0}}],
  Arrow[{{4.5, 0}, {4.5, -3}}],
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  Text[Style["0", Black, 15], {5.3, 0}],
  Text[Style["-3E₀", Black, 15], {5.3, -3}],
  Text[Style["1s", Black, 15], {1.0, 0.1}]}]
```