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

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

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

where g (=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

$$\hat{H}_{hf} = -\hat{\boldsymbol{\mu}}_e \cdot \boldsymbol{B}$$

$$= \frac{2g\mu_B\mu_N}{\hbar^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e \cdot \hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e |\hat{\boldsymbol{r}}|^2] + \frac{8\pi}{3}\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e \delta(\hat{\boldsymbol{r}})\}$$

$$= \frac{ge^2}{2m_e m_p c^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e \cdot \hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e |\hat{\boldsymbol{r}}|^2] + \frac{8\pi}{3}\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e \delta(\hat{\boldsymbol{r}})\}$$

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;

$$E_{hf}^{(1)} = \langle n=1, l=0, m=0 | \frac{ge^2}{2m_e m_p c^2}\{\frac{1}{|\hat{\boldsymbol{r}}|^5}[3(\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{r}})(\hat{\boldsymbol{S}}_e \cdot \hat{\boldsymbol{r}}) - \hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e |\hat{\boldsymbol{r}}|^2]\} | n=1, l=0, m=0 \rangle$$

$$+ \frac{4\pi g e^2}{3m_e m_p c^2}\hat{\boldsymbol{S}}_p \cdot \hat{\boldsymbol{S}}_e \langle n=1, l=0, m=0 | \delta(\hat{\boldsymbol{r}}) | n=1, l=0, m=0 \rangle$$

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

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

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

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

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;

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

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

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

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

Note that

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

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

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

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

$\left|++\right\rangle$ 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.

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

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

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

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.

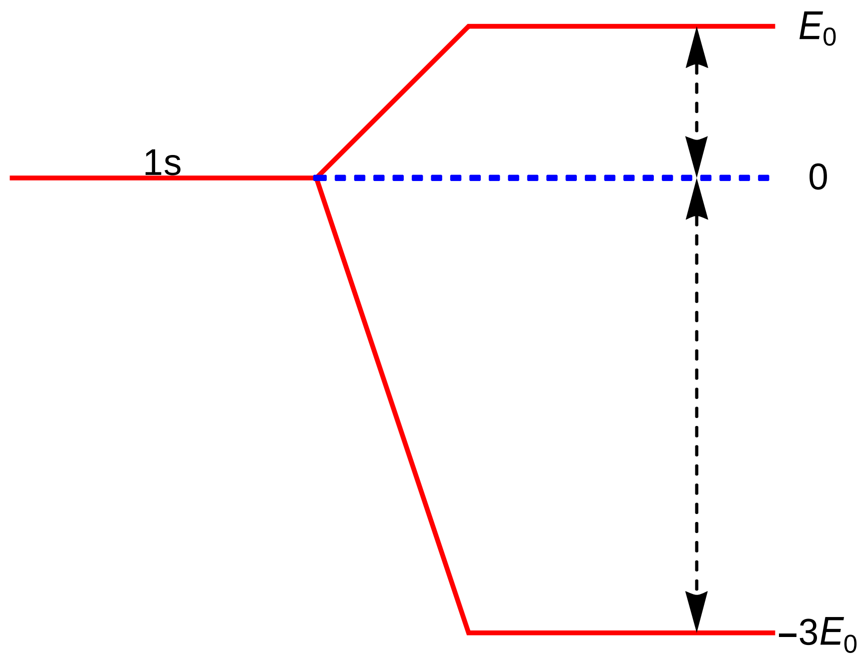
$$\Delta E = 4E_0 = \frac{4g\hbar^4}{3m_p {m_e}^2 c^2 {a_B}^4} = 5.87746\ (\mu\text{eV}).$$

The frequency:

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

The wavelength:

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



((**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};
```

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

5.87746×10^{-6}

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

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.

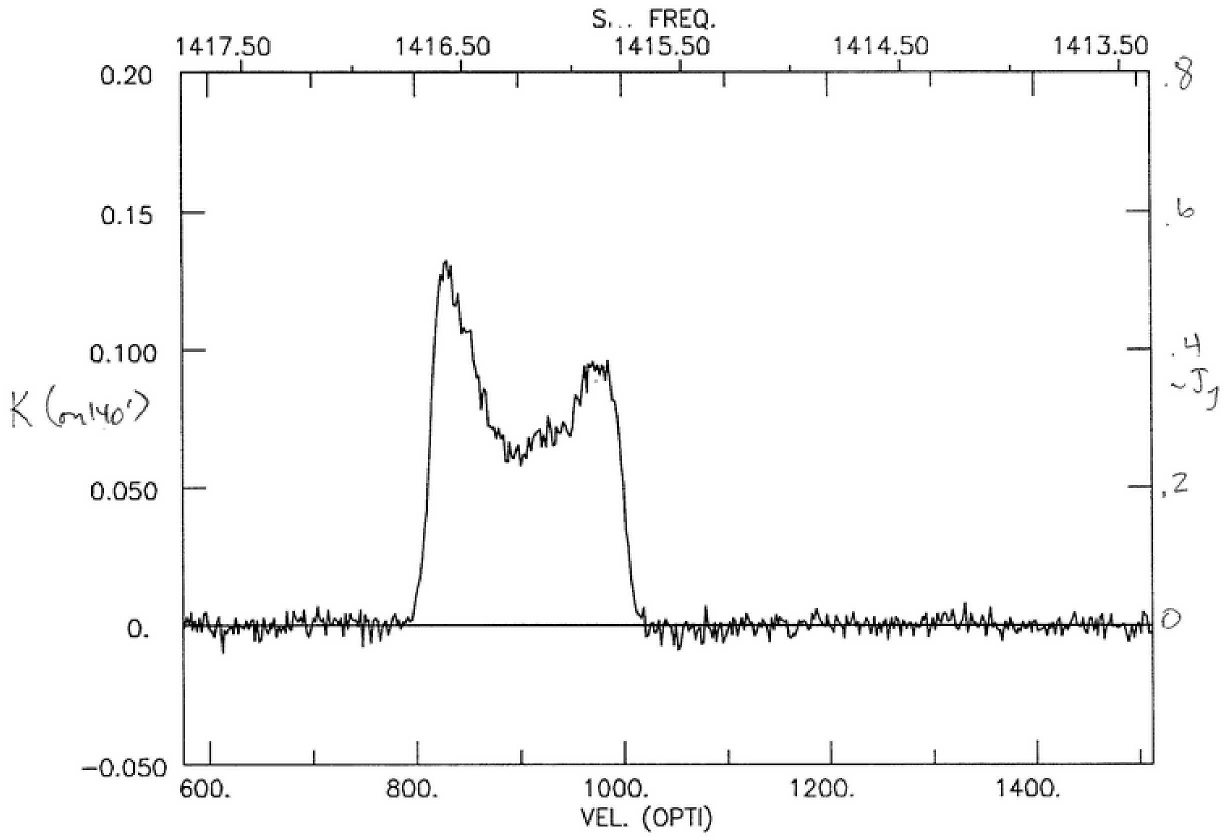


Fig. This integrated HI spectrum of UGC 11707 obtained with the 140-foot telescope shows the typical two-horned profile of a spiral galaxy (red-shift; the observed frequency shifts to the lower frequency side from 1420 MHz to 1416 MHz).

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

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

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

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

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

$$\frac{1}{H_0} = \frac{Mpc}{67.80(km/s)} = \frac{3.08567758 \times 10^{22}}{67.80 \times 10^3 \times 3.15569 \times 10^7} = 14.42 \text{ billion year}$$

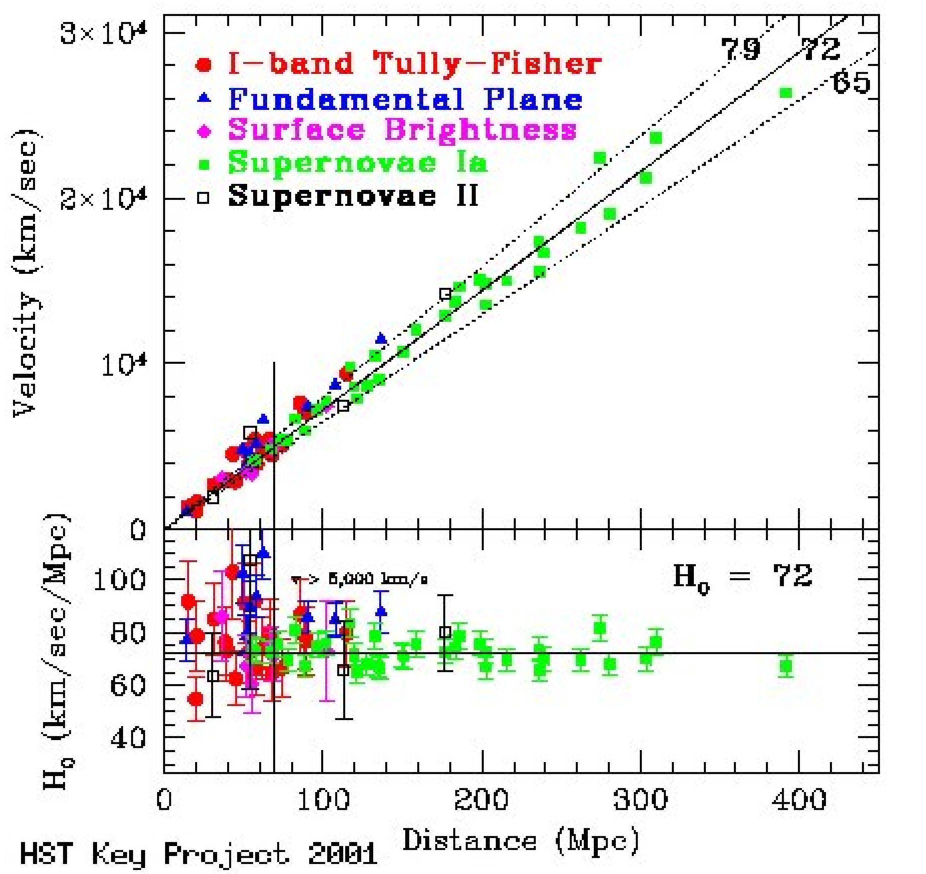


Fig. Hubble diagram from the Hubble Space Telescope Key Project (Freedman et al. 2001) using five different measures of distance. Bottom pane shows H0 vs distance with horizontal equal to the best fit value of 72 km/s Mpc^{-1}. The recessional velocity v of stars moving away from the Earth is proportional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

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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

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

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

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

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}, \tag{10}$$

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

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

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
```