Solutions to End-of-Chapter Exercises
Chapter 2

Fundamental constants & properties of nuclei

$c = 2.997 \times 10^{8}$ m s^{-1}
$e = 1.602 \times 10^{-19}$ C
$k = 1.381 \times 10^{-23}$ J K^{-1}
$h = 6.626 \times 10^{-34}$ J s

Mass

Electron = $9.109\,390 \times 10^{-31}$ kg
Proton = $1.672\,622 \times 10^{-27}$ kg

$\mu_0 = 4\pi \times 10^{-7}$ J s^{2} C^{-2} m^{-1} (= T^{2} J^{-1} m^{3})
$\mu_B = 9.274 \times 10^{-24}$ J T^{-1}
$\mu_N = 5.050\,784 \times 10^{-27}$ J T^{-1}
$g_e = 2.0023\,193$ (electron g factor)
$g_p = 5.585\,694\,7$ (proton g factor)
$\gamma_e = 1.761 \times 10^{11}$ s^{-1} T^{-1}

Properties for other common nuclei

	g_N	ν_N / MHz	γ / 10^{7} s^{-1} T^{-1}
^{1}H	5.5857	14.9021	26.752
^{2}H	0.8574	2.2876	4.107
^{13}C	1.4048	3.7479	6.728
^{14}N	0.4038	1.0772	1.934
^{31}P	2.2632	6.0380	10.839

ν_L (in units of MHz) for $B = 0.35$ T

Exercise 2.1) Calculate the g value of the resonance due to the unknown radical in Fig. 2.4. Assume a microwave frequency of 9.5 GHz and $g_{\text{DPPH}} = 2.0036$.

ANSWER
From the resonance equation given in eqn 2.9:

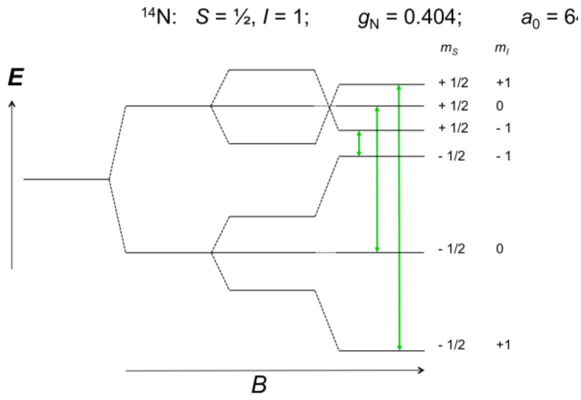
$$g = \frac{(6.626 \times 10^{-34}\ \text{Js}) \times (9.5 \times 10^{9}\ \text{s}^{-1})}{(9.274 \times 10^{-24} \text{JT}^{-1}) \times (3387 \times 10^{-4}\ \text{T})} = 2.0040$$

Or using the reference expression $g = g_{\text{ref}} B_{\text{ref}} / B$ (see margin notes, page 10):

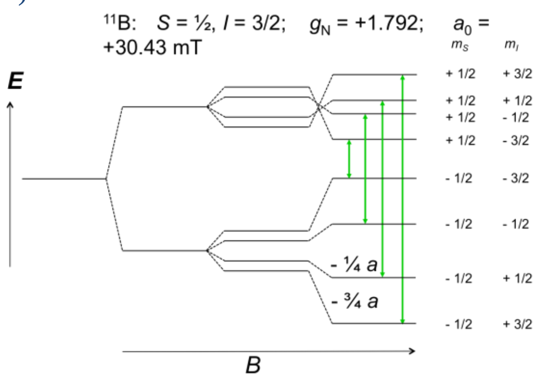
$$g = \frac{(2.0037) \times (338.745\ \text{mT})}{(338.700\ \text{mT})} = 2.0040$$

Exercise 2.2) Draw the energy level diagram for an unpaired electron interacting with a single nucleus of i) ^{14}N, ii) ^{11}B, and iii) ^{15}N. Assume the magnitude of the hyperfine interaction is much larger than the energy associated with the nuclear Zeeman interaction (i.e., $|a| >> g_N \mu_N B \cdot m_I$).

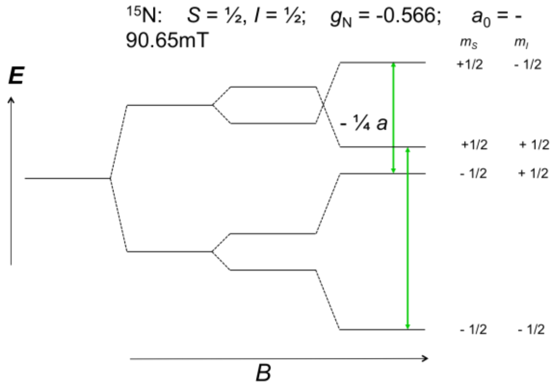
ANSWER
i)



ii)



iii)



Exercise 2.3) In a magnetic field of 335 mT, calculate the polarization parameters for the operating temperatures of 4, 50 and 298 K.

ANSWER
From the polarization expression given in eqn 2.25, where $B = 0.335$ Tesla:

$$\text{At 4K, } P = \frac{h\gamma B}{4\pi kT} = \frac{(6.626\times 10^{-34}\text{ Js})\times(1.761\times 10^{11}\text{ s}^{-1}\text{T}^{-1})\times(0.335\text{ T})}{4\pi\times(1.381\times 10^{-23}\text{ JK}^{-1})\times(4\text{ K})} = 0.056$$

$$\text{At 50K, } P = \frac{h\gamma B}{4\pi kT} = \frac{(6.626\times 10^{-34}\text{ Js})\times(1.761\times 10^{11}\text{ s}^{-1}\text{T}^{-1})\times(0.335\text{ T})}{4\pi\times(1.381\times 10^{-23}\text{ JK}^{-1})\times(50\text{ K})} = 0.0045$$

$$\text{At 298K, } P = \frac{h\gamma B}{4\pi kT} = \frac{(6.626\times 10^{-34}\text{ Js})\times(1.761\times 10^{11}\text{ s}^{-1}\text{T}^{-1})\times(0.335\text{ T})}{4\pi\times(1.381\times 10^{-23}\text{ JK}^{-1})\times(298\text{ K})} = 0.000756$$

Exercise 2.4) The isotropic hyperfine coupling of a ^{1}H atom is 50.69 mT. For an observed hyperfine coupling of 7.1 mT, calculate the electron spin density on a ^{1}H nucleus.

ANSWER

Electron spin density $= \frac{a_{\text{expt}}}{a_0}\times 100 = \frac{7.1\text{ mT}}{50.69\text{ mT}}\times 100 = 14\%$

Exercise 2.5) Using the classical expression for a magnetic moment ($\mu = IA$, where I is the effective current and A is the area of a circular orbit), show that the orbital magnetic moment of an electron can be described by:

$$\mu_L = \frac{e\hbar}{2m_e}\sqrt{l(l+1)}$$

ANSWER:

The orbital motion of an electron can be treated classically as a current loop of radius r. Thus the current around the loop (I) is the charge of the electron (e) divided by the time period for one cycle, $T = 2\pi r / v$ (where v is the linear speed of the electron) and $A = \pi r^2$. The magnitude of the resultant magnetic moment is thus given by:

$$\mu = IA = \frac{e}{2\pi r/_{\text{v}}}\times \pi r^2 = \frac{evr}{2}$$

Since orbital angular momentum is defined as $L = mvr$ (for an electron $m = m_e$) we can write:

$$\mu_L = \frac{e}{2m_e} m_e \text{v} r = \frac{e}{2m_e} L$$

If the quantization of the angular momentum is taken into consideration, then

$\mu_L = \frac{e}{2m_e} L = \frac{e}{2m_e}\sqrt{l(l+1)}\hbar = \mu_B\sqrt{l(l+1)}$ (remember this has units of $\hbar$) where

$$\mu_B = \frac{e\hbar}{2m_e}$$