Laser Exercise 1

FYSS3552

Problem 1

a

Given an uniform charge distribution inside a sphere of radius R the charge density is computed as:

$$\rho = \frac{Ze}{\frac{4}{3}\pi R^3}$$

From Gauss's law the electric field flux outside a closed surface is:

$$\Phi(E) = \frac{Q}{\epsilon_0}$$

where Q is the charge contained within the surface. Considering the isotropy of the spherical system in exam, the electrical field at distance r from the sphere center is then computed:

$\mathbf{r \leq R}$

$$\begin{aligned} E(r) &= \frac{Q}{4\pi\epsilon_0 r^2} \\ &= \frac{\rho\frac{4}{3}\pi r^3}{4\pi\epsilon_0 r^2} \\ &= \frac{Ze}{4\pi\epsilon_0}\frac{r}{R^3} \end{aligned}$$

$\mathbf{r > R}$

$$\begin{aligned} E(r) &= \frac{Q}{4\pi\epsilon_0 r^2} \\ &= \frac{Ze}{4\pi\epsilon_0 r^2} \end{aligned}$$

The potential difference between two points can be extracted as:

$$\Delta V_{r_1,r_2} = V(r_1) - V(r_2) = -\int_{r_2}^{r_1} E(r)dr$$

At $r > R$, since $V(\infty) = 0$:

$$\begin{aligned} V(r) = V(r) - V(\infty) &= \int_r^{\infty} E(r')dr' \\ &= \int_r^{\infty} \frac{Ze}{4\pi\epsilon_0 r'^2}dr' \\ &= \frac{Ze}{4\pi\epsilon_0}\left[\frac{1}{r'}\right]_{\infty}^{r} \\ &= \frac{Ze}{4\pi\epsilon_0 r} \end{aligned}$$

Similarly for $r \leq R$:

$$\begin{aligned} V(r) &= \int_r^\infty E(r')dr' \\ &= \int_r^R E(r')dr' - \int_R^\infty E(r')dr' \\ &= \int_r^R \frac{Ze}{4\pi\epsilon_0}\frac{r'}{R^3}dr' + \frac{Ze}{4\pi\epsilon_0 R} \\ &= \frac{Ze}{4\pi\epsilon_0 R^3}\left[\frac{1}{2}r'^2\right]_r^R + \frac{Ze}{4\pi\epsilon_0 R} \\ &= \frac{Ze}{4\pi\epsilon_0 R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right) \end{aligned}$$

The potential energy is obtained by multiplying above equations by $-e$, hence:

$\mathbf{r \leq R}$	$\mathbf{r > R}$
$U(r) = -\frac{Ze^2}{4\pi\epsilon_0 R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right)$	$U(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$

b

One wants to show that

$$\Delta E = \frac{4\pi}{10} \mid \Psi(0) \mid^2 \frac{Ze^2}{4\pi\epsilon_0} R^2$$

Using the derived potentials of point (a) and the following equation for the energy perturbation

$$\Delta E = \int_0^\infty \Psi^*(V(r) - V_0(r))\Psi \cdot 4\pi r^2 dr$$

Hence, using the "allowed wavefunction" approximation, $\Psi(0) \sim \Psi(r)$:

$$\Delta E = \mid \Psi(0) \mid^2 \cdot \int_0^\infty (V(r) - V_0(r)) \cdot 4\pi r^2 dr$$

Splitting the integral one has

$$\Delta E = \mid \Psi(0) \mid^2 \left(\int_0^R (V(r) - V_0(r)) \cdot 4\pi r^2 dr + \int_R^\infty (V(r) - V_0(r)) \cdot 4\pi r^2 dr\right)$$

For $r > R$, $V(r) = V_0(r)$ canceling out the second term. Substituting the expressions of the potential energy, the energy perturbation is then

$$\Delta E = -\frac{Ze^2}{4\pi\epsilon_0} \mid \Psi(0) \mid^2 4\pi \left[\int_0^R \frac{3}{2R} \cdot r^2 dr - \int_0^R \frac{r^2}{2R^3} \cdot r^2 dr - \int_0^R \frac{1}{r} \cdot r^2 dr\right]$$

$$\Delta E = -\frac{Ze^2}{4\pi\epsilon_0} \mid \Psi(0) \mid^2 4\pi \left[\frac{3}{2R} \cdot \frac{R^3}{3} - \frac{1}{2R^3} \cdot \frac{R^5}{5} - \frac{R^2}{2}\right]$$

And finally,

$$\Delta E = \frac{Ze^2}{4\pi\epsilon_0} \mid \Psi(0) \mid^2 \frac{4\pi}{10} R^2$$

Problem 2

a

From the wave numbers k in cm^{-1} given for the 2 J states involved of the considered D2 transition, one can give the transition in nm unit, using the wavelength λ :

$$\Delta\lambda = \frac{2\pi}{\Delta k} = \frac{2\pi}{12816.55 \times 10^7} = 780.2412 \text{ nm}$$

One can also give the transition in THz using the frequency ν :

$$\Delta\nu = \frac{\mathrm{c}}{\Delta\lambda} = 384.2305 \text{ THz}$$

b

The lifetime of the considered excited state is $\tau = 26.2$ ns. The spontaneous decay rate A can then be deduced knowing :

$$A = \frac{1}{\tau} = \frac{1}{26.2 \times 10^{-9}} = 3.817 \times 10^7 \text{ s}^{-1}$$

The Einstein coefficient A is a measure of the relative intensity of the spectral line. The natural linewidth of the emitted radiation can be calculated as:

$$\Gamma = \frac{A}{2\pi} \sim 6.078 \text{ MHz}$$

c

The states are further split into hyperfine F states following the coupling of the atomic J spins with the nuclear spin I. The F states are then $\mid I - J \mid \leq F \leq I + J$. Considering first the ground state $S_{1/2}$ of the D2 transition, in case of ^{85}Rb the nuclear spin is $I = 5/2$ which gives $F = [2, 3]$. In case of ^{87}Rb the nuclear spin is $I = 3/2$ which gives $F = [1, 2]$. Considering then the excited state $P_{3/2}$ of the D2 transition, in case of ^{85}Rb the F states are $F = [1, 2, 3, 4]$. In case of ^{87}Rb the F states are $F = [0, 1, 2, 3]$.

The possible electric dipole transitions which are allowed are given by the selection rules which are

$$\Delta F = 0, \pm 1$$

$$F = 0 \not\to F = 0$$

The possible electric dipole transitions are displayed for both ^{85}Rb and ^{87}Rb.

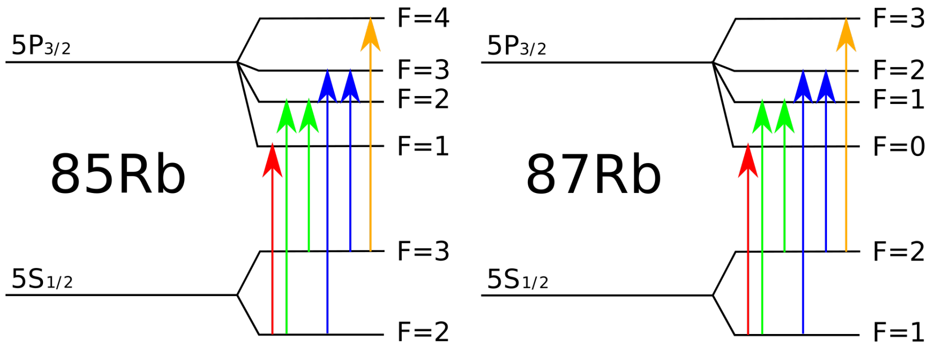

Figure 1: HFS of ^{85}Rb and ^{87}Rb

d

```python
from IPython.display import Markdown
from tabulate import tabulate
A = [1012, 25.002] # MHz
B = [0,25.790] # MHz
I = 5/2
J = [1/2,3/2]

# dictionary containing HF shifts
F_up  = {1:0,2:0,3:0,4:0}
F_low = {2:0,3:0}

table = []
# compute energy shift for each HF component
for f in F_low.keys():

    k = f*(f+1)-I*(I+1)-J[0]*(J[0]+1)
    try:
        B_coeff = (3*0.5*k*(k+1)-2*I*(I+1)*J[0]*(J[0]+1))/(2*I*(2*I-1)*2*J[0]*(2*J[0]-1))
    except:
        B_coeff = 0

    dE = 0.5*A[0]*k + B[0]*B_coeff

    F_low[f] = dE

    table.append([f,dE*1e-3])

Markdown(tabulate(
  table,
  headers=["F", "$\Delta E_{hfs}$ [GHz]"]
))
```

Table 1: Energy shifts with respect to the unperturbed position computed for the ground $S_{1/2}$ state of ^{85}Rb

F	ΔE_{hfs} [GHz]
2	-1.771
3	1.265

```python
table=[]
for f in F_up.keys():

    k = f*(f+1)-I*(I+1)-J[1]*(J[1]+1)
    try:
        B_coeff = (3*0.5*k*(k+1)-2*I*(I+1)*J[1]*(J[1]+1))/(2*I*(2*I-1)*2*J[1]*(2*J[1]-1))
    except:
        B_coeff = 0
```

```python
    dE = 0.5*A[1]*k + B[1]*B_coeff

    F_up[f] = dE
    table.append([f,dE])

Markdown(tabulate(
  table,
  headers=["F", "$\Delta E_{hfs}$ [MHz]"]
))
```

Table 2: Energy shifts with respect to the unperturbed position computed for the excited $P_{3/2}$ state of ^{85}Rb

F	ΔE_{hfs} [MHz]
1	-113.208
2	-83.8355
3	-20.435
4	100.205

Using the HFS shifts presented in previous tables the HFS positions of the allowed transition can be computed as:

$$\gamma = \nu_0 + \Delta E^{P_{3/2}}_{\text{hfs}} - \Delta E^{S_{1/2}}_{\text{hfs}}$$

```python
# allowed transitions
ftof = [
    [2,1],
    [2,2],
    [2,3],
    [3,2],
    [3,3],
    [3,4]
]
table = []
for T in ftof:

    delta = F_up[T[1]]-F_low[T[0]]
    table.append([r"{} $\rightarrow$ {}".format(T[0],T[1]),delta])
Markdown(tabulate(
  table,
  headers=[r"$F_{S_{1/2}} \rightarrow F_{S_{1/2}}$", r"$\gamma - \nu_0$ [MHz]"]
))
```

Table 3: Atomic resonance positions in MHz with respect to the unperturbed resonance frequency ν_0 for the allowed hyperfine transitions of ^{85}Rb

$F_{S_{1/2}} \to F_{S_{1/2}}$	$\gamma - \nu_0$ [MHz]
$2 \to 1$	1657.79
$2 \to 2$	1687.16
$2 \to 3$	1750.57
$3 \to 2$	-1348.84
$3 \to 3$	-1285.43
$3 \to 4$	-1164.8

```python
import satlas2 as sat
import matplotlib.pyplot as plt
import numpy as np

size = 20
plt.rcParams['font.size']=size

#build an hfs model with racah intensities
HFS_model = sat.HFS(I=I, J=J, df=0, fwhml=10,fwhmg=10, A=A, B=B, scale= 1, name='HFS', racah=True)

fig, axs= plt.subplots(figsize=(16,9), dpi=100)

x = np.linspace(-1500, 1800, 1000)

#plot hfs model
axs.plot(x,HFS_model.f(x))

#mark the different transitions
yy=1
for T in ftof:

    delta = F_up[T[1]]-F_low[T[0]]
    label = str(T[0])+"to"+str(T[1])
    if yy == 1:
        yy = 1.15
    else:
        yy = 1
    axs.text(delta,y=yy,horizontalalignment='right',verticalalignment='center',rotation=90,s=label)
    axs.axvline(delta,linestyle='dashed')

axs.set_yticks([])
axs.set_xlabel(r"Frequency- $\nu_0$ [MHz]")
axs.set_ylim(0,1.5)
plt.show()
```

```
/home/andrea/.local/lib/python3.9/site-packages/satlas2/models/hfsModel.py:292: RuntimeWarning: invalid va
  shift = phase * n / d
```

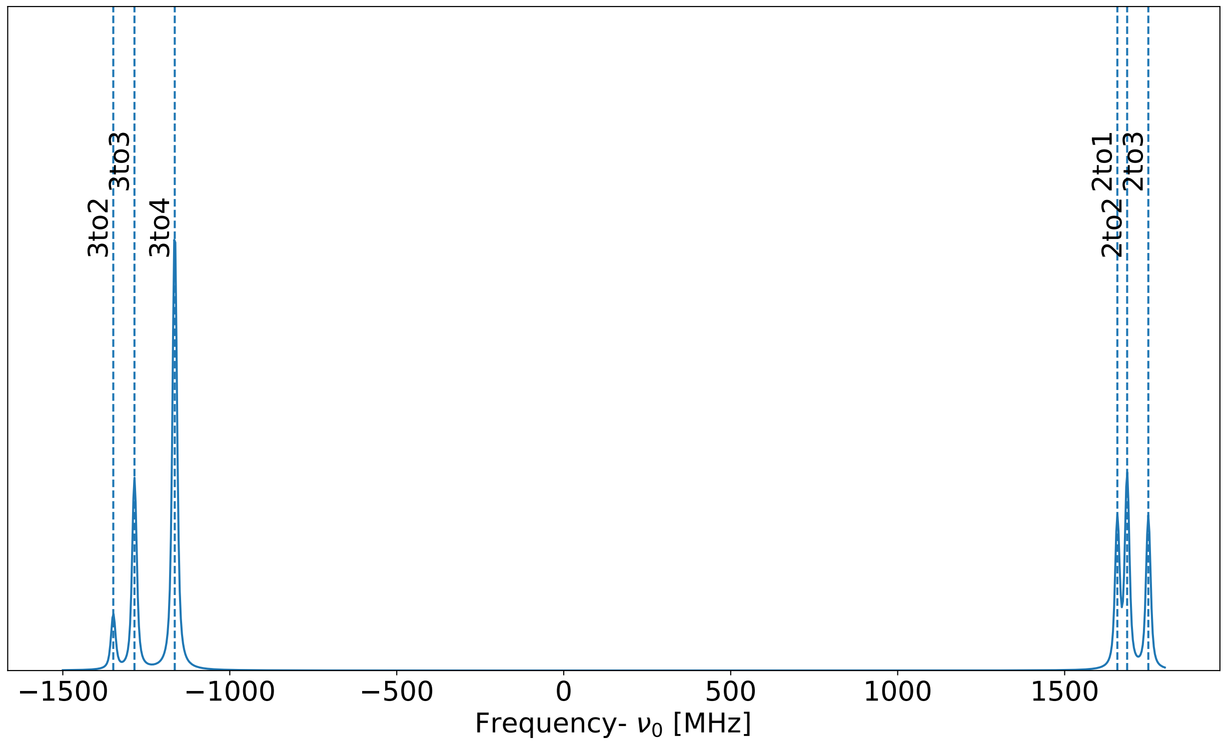

Figure 2: Atomic resonance peak positions in MHz with respect to the unperturbed resonance frequency ν_0 for the allowed hyperfine transitions of ^{85}Rb

Problem 3

a

The Normal Mass Shift NMS in GHz.amu is given by :

$$\text{NMS} = \frac{m_e}{m_u}\nu_0$$

with $\frac{m_e}{m_u}$ is the mass of the electron in amu and $\nu_0 = \frac{c}{\lambda}$ in GHz where the wavelength of the transition is $\lambda = 363.6$ nm. Hence,

$$\text{NMS} = (5.4858 \times 10^{-4}) \times (825.0825 \times 10^{-3}) = 452.5578 \text{ GHz.amu}$$

The Specific Mass Shift SMS in GHz.amu can then be deduced, knowing the Mass Shift MS in GHz.amu, using

$$\text{SMS} = \text{MS} - \text{NMS} = 845 - 425.5578 = 392.4422 \text{ GHz.amu}$$

b

Using the given formula which defines isotopic shift:

$$\delta\nu_i^{A_{ref},A} = \frac{m_A - m_{A_{ref}}}{m_A m_{A_{ref}}} M_i + F_i \delta\langle r^2\rangle^{A_{ref},A}$$

the mean-square charge radii can be computed:

$$\delta\langle r^2\rangle^{A_{ref},A} = \frac{1}{F_i}\left(\delta\nu_i^{A_{ref},A} - \frac{m_A - m_{A_{ref}}}{m_A m_{A_{ref}}} M_i\right)$$

```
isotopes = 102,104,105,106,108,110,112,114,116,118
masses = 101.905602,103.904031,104.905080,105.903480,107.903892,109.905172,111.907330,113.910369,115.914
iso_shifts = 1452.8,958.1,839.7,494.7,0.0,-436.4,-738.0,-962.0,-1080.0,-1164.0
M = 845e3 #MHz.amu
F = -2.9e3 #MHz/fm^2
table = []
delta = []
for iso,mass,iso_shift in zip(isotopes,masses,iso_shifts):
    mass_shift = M*(mass-masses[4])/(mass*masses[4])
    delta.append((iso_shift - mass_shift)/F)
    table.append([iso,mass,iso_shift,mass_shift,delta[-1]])
Markdown(tabulate(
  table,
  headers=['Isotope','Atomic mass [u]', 'Shifts [MHz]','Mass Shift [MHz]',r'$\delta \langle r^2 \rangle
))
```

Table 4: Mean-square charge radii computed for Pd isotopes.

Isotope	Atomic mass [u]	Shifts [MHz]	Mass Shift [MHz]	$\delta\langle r^2\rangle^{108,A}$ [fm^2]
102	101.906	1452.8	-460.945	-0.659912
104	103.904	958.1	-301.462	-0.434332
105	104.905	839.7	-223.858	-0.366744
106	105.903	494.7	-147.921	-0.221593
108	107.904	0	0	-0
110	109.905	-436.4	142.597	0.199654
112	111.907	-738	280.152	0.351087
114	113.91	-962	412.93	0.474114
116	115.914	-1080	541.174	0.559026
118	117.919	-1164	665.111	0.630728

```
size = 20
plt.rcParams['font.size']=size

fig, axs= plt.subplots(figsize=(16,9), dpi=100)

#plot hfs model
axs.plot(isotopes,delta,"ob--")

axs.set_xlabel('A')
axs.set_ylabel(r'$\delta \langle r^2 \rangle^{108,A}$ [fm$^2$]')
```

```
plt.show()
```

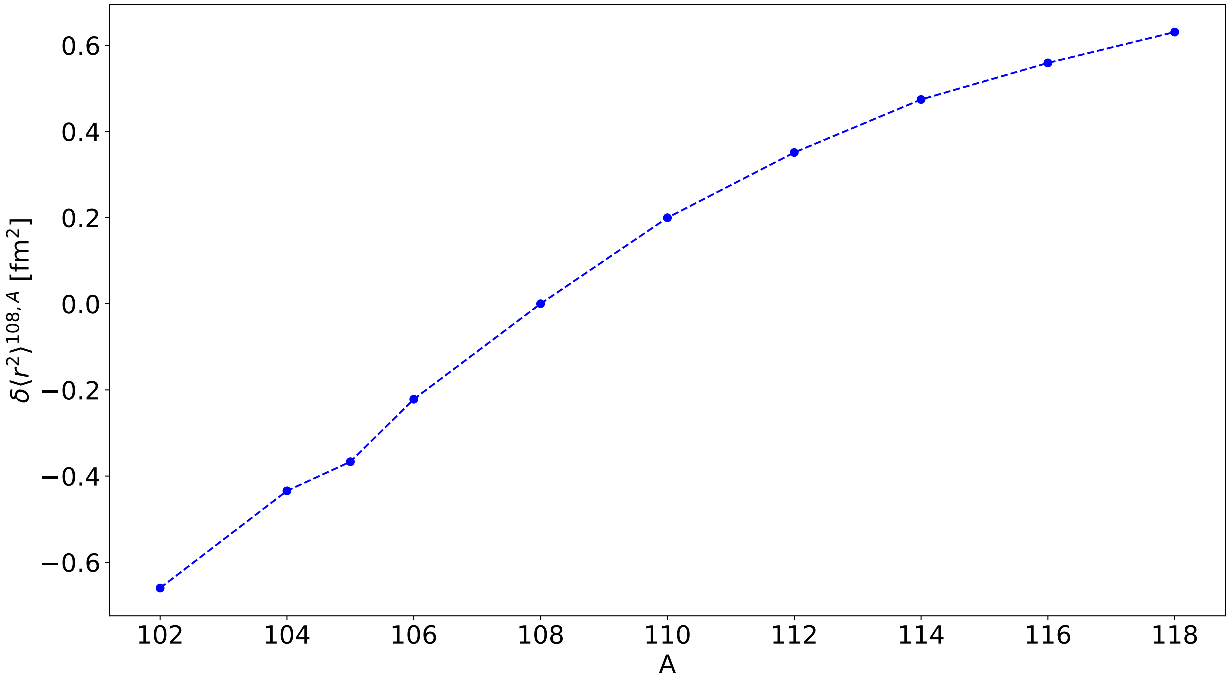

Figure 3: Mean-square charge radii computed for Pd isotopes as a function of neutrons number.

Problem 4

a

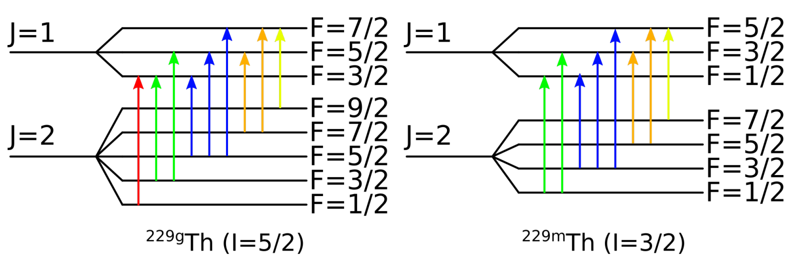

Figure 4: HFS of ^{229g}Th and ^{229m}Th

b

Using the given relations:

$$\frac{A}{A_{ref}} \sim \frac{\mu\ I_{ref}}{\mu_{ref}\ I} \qquad\qquad \frac{B}{B_{ref}} \sim \frac{Q_s}{Q_{s,ref}}$$

the magnetic moment and electric quadrupole moment of the isomeric state can be extracted as:

$$\frac{A_{iso}}{A_{gs}} \sim \frac{\mu_{iso}}{\mu_{gs}} \frac{I_{gs}}{I_{iso}} \qquad \frac{B_{iso}}{B_{gs}} \sim \frac{Q_{s,iso}}{Q_{s,gs}}$$

$$\mu_{iso} \sim \frac{A_{iso}}{A_{gs}} \frac{I_{iso}}{I_{gs}} \mu_{gs} = 0.371\mu_{\mathrm{n}} \qquad Q_{s,iso} \sim \frac{B_{iso}}{B_{gs}} Q_{s,gs} = 1.75\mathrm{eb}$$

The A and B factor of the g.s. and isomeric states where chosen from the 20711 cm^{-1} level.

c

In the case of strongly deformed nuclei the following relation is valid:

$$Q_s = \frac{3K^2 - I(I+1)}{(I+1)(2I+3)} Q_0$$

where K is the projection of the nuclear spin on the symmetry axis. In the states considered in particular K is equal to I.

Finally:

$$Q_0^{^{229g}\mathrm{Th}} = \frac{(I+1)(2I+3)}{3I^2 - I(I+1)} Q_s = \frac{14}{5} Q_s = 8.82\mathrm{eb} \qquad Q_0^{^{229m}\mathrm{Th}} = \frac{(I+1)(2I+3)}{3I^2 - I(I+1)} Q_s = 5Q_s = 8.75\mathrm{eb}$$

The two values are in good agreement, this means that the nuclear charge distribution has a similar shape (prolate) in both the configurations.

d

Assuming a negligible mass shift contribution the mean-square charge radii deviation can be computed as:

$$\delta\langle r^2\rangle^{1,2} \sim \frac{\delta\nu^{1,2}}{F}$$

Knowing the ratio between isomer to isotope shifts, the isomeric mean-square charge radii shift can be computed as:

$$\delta\langle r^2\rangle^{229m,229} = \delta\langle r^2\rangle^{229,232} \frac{\delta\nu^{229m,229}}{\delta\nu^{229,232}} = 0.012\ \mathrm{fm}^2$$