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Course: **8.421 - AMO I**
Problem set: **#5**
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1. Magnetic field of a magnetic dipole

(a) From the identity

$$\partial_i\partial_j\left(\frac{1}{r}\right) = -\partial_i\left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) = -\partial_i\left(\frac{x_j}{r^3}\right) = \frac{3\hat{\boldsymbol{r}}_i\hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3} - \frac{4\pi}{3}\delta_{ij}\delta^3(\boldsymbol{r}),$$

we simply contract to get

$$\begin{aligned}
\nabla^2\left(\frac{1}{r}\right) &= \sum_{i=1}^{3}\partial_i\partial_i\left(\frac{1}{r}\right) \\
&= \sum_{i=1}^{3}\frac{3\hat{\boldsymbol{r}}_i\hat{\boldsymbol{r}}_i - \delta_{ii}}{r^3} - \frac{4\pi}{3}\delta_{ii}\delta^3(\boldsymbol{r}) \\
&= \sum_{i=1}^{3}\frac{3\hat{\boldsymbol{r}}_i\hat{\boldsymbol{r}}_i - 1}{r^3} - \frac{4\pi}{3}\delta^3(\boldsymbol{r}) \\
&= \frac{3(x^2+y^2+z^2)/r^2 - 3}{r^3} - 4\pi\delta^3(\boldsymbol{r}) \\
&= \frac{3r^2/r^2 - 3}{r^3} - 4\pi\delta^3(\boldsymbol{r}) \\
&= -4\pi\delta^3(\boldsymbol{r})
\end{aligned}$$

as desired. Note that here $\delta_{ii} = 1$ is a matrix element since we are not using Einstein summation convention here. We will use it in the next part of the problem, however.

(b) Let the vector potential for a magnetic dipole be given

$$\boldsymbol{A}^{\text{dip}}(\boldsymbol{r}) = \frac{\boldsymbol{m}\times\hat{\boldsymbol{r}}}{r^2}.$$

For ease of computation, we may rewrite this using the Levi-Civita symbol and Einstein summation convention:

$$\boldsymbol{A}_i^{\text{dip}}(\boldsymbol{r}) = \frac{1}{r^2}\epsilon_{ijk}\boldsymbol{m}_j\hat{\boldsymbol{r}}_k$$

The magnetic field of a magnetic dipole is thus given by taking the curl of $\boldsymbol{A}_{\text{dip}}$, by definition:

$$\begin{aligned}
\boldsymbol{B}_a^{\text{dip}}(\boldsymbol{r}) &= [\boldsymbol{\nabla}\times\boldsymbol{A}^{\text{dip}}(\boldsymbol{r})]_a \\
&= \epsilon_{abc}\partial_b\boldsymbol{A}_c^{\text{dip}}(\boldsymbol{r}) \\
&= \epsilon_{abc}\partial_b\left(\frac{1}{r^2}\epsilon_{cjk}\boldsymbol{m}_j\hat{\boldsymbol{r}}_k\right) \\
&= \epsilon_{abc}\epsilon_{cjk}\boldsymbol{m}_j\partial_b\left(\frac{\hat{\boldsymbol{r}}_k}{r^2}\right).
\end{aligned}$$

Using the identity given in the problem statement and the fact that

$$\epsilon_{abc}\epsilon_{cjk} = \epsilon_{cab}\epsilon_{cjk} = \delta_{aj}\delta_{bk} - \delta_{ak}\delta_{bj}$$

we have

$$
\begin{aligned}
\boldsymbol{B}_a^{\text{dip}}(\boldsymbol{r}) &= -(\delta_{aj}\delta_{bk} - \delta_{ak}\delta_{bj})\,\boldsymbol{m}_j \partial_b \partial_k \left(\frac{1}{r}\right) \\
&= -(\delta_{aj}\delta_{bk} - \delta_{ak}\delta_{bj})\,\boldsymbol{m}_j \left(\frac{3\hat{\boldsymbol{r}}_b \hat{\boldsymbol{r}}_k - \delta_{bk}}{r^3} - \frac{4\pi}{3}\delta_{bk}\delta^3(\boldsymbol{r})\right) \\
&= -\delta_{aj}\delta_{bk}\boldsymbol{m}_j \left(\frac{3\hat{\boldsymbol{r}}_b \hat{\boldsymbol{r}}_k - \delta_{bk}}{r^3} - \frac{4\pi}{3}\delta_{bk}\delta^3(\boldsymbol{r})\right) + \delta_{ak}\delta_{bj}\boldsymbol{m}_j \left(\frac{3\hat{\boldsymbol{r}}_b \hat{\boldsymbol{r}}_k - \delta_{bk}}{r^3} - \frac{4\pi}{3}\delta_{bk}\delta^3(\boldsymbol{r})\right) \\
&= -\boldsymbol{m}_a \left(\cancel{\frac{3\hat{\boldsymbol{r}}_b \hat{\boldsymbol{r}}_b - \delta_{bb}}{r^3}} - \frac{4\pi}{3}\delta_{bb}\delta^3(\boldsymbol{r})\right) + \boldsymbol{m}_b \left(\frac{3\hat{\boldsymbol{r}}_b \hat{\boldsymbol{r}}_a - \delta_{ba}}{r^3} - \frac{4\pi}{3}\delta_{ba}\delta^3(\boldsymbol{r})\right) \\
&= \boldsymbol{m}_a 4\pi\delta^3(\boldsymbol{r}) + \frac{3(\boldsymbol{m}_b \hat{\boldsymbol{r}}_b)\hat{\boldsymbol{r}}_a - \boldsymbol{m}_a}{r^3} - \frac{4\pi}{3}\boldsymbol{m}_a\delta^3(\boldsymbol{r}) \\
&= \frac{3(\boldsymbol{m}\cdot\hat{\boldsymbol{r}})\hat{\boldsymbol{r}}_a - \boldsymbol{m}_a}{r^3} + \frac{8\pi}{3}\boldsymbol{m}_a\delta^3(\boldsymbol{r}),
\end{aligned}
$$

where we have used the contraction identity $\delta_{ii} = 3$. Putting back into vector form, we find

$$
\boldsymbol{B}^{\text{dip}}(\boldsymbol{r}) = \frac{3(\boldsymbol{m}\cdot\hat{\boldsymbol{r}})\hat{\boldsymbol{r}} - \boldsymbol{m}}{r^3} + \frac{8\pi}{3}\boldsymbol{m}\delta^3(\boldsymbol{r})
$$

as desired.

(c) It remains to prove the provided identity:

$$
\partial_i \partial_j \left(\frac{1}{r}\right) = -\partial_i \left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) = -\partial_i \left(\frac{x_j}{r^3}\right) = \frac{3\hat{\boldsymbol{r}}_i \hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3} - \frac{4\pi}{3}\delta_{ij}\delta^3(\boldsymbol{r}),
$$

The first two equalities are straightforward to show, but I will show the proofs here anyway as the technique carries over to proving the third equality (which is the one we really care about):

$$
\begin{aligned}
\partial_i \partial_j \left(\frac{1}{r}\right) &= \partial_i \partial_j \frac{1}{\left(\sum_{a=1}^3 x_a^2\right)^{1/2}} \\
&= -\partial_i \left[\frac{1}{2\left(\sum_{a=1}^3 x_a^2\right)^{3/2}} \partial_j \left(\sum_{a=1}^{3} x_a\right)\right] \\
&= -\partial_i \left[\frac{1}{2r^3} \sum_{a=1}^{3} 2x_a \delta_{ja}\right] \\
&= -\partial_i \left(\frac{x_j}{r^3}\right) \\
&= -\partial_i \left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right).
\end{aligned}
$$

where we have used $x_j = r\hat{\boldsymbol{r}}_j$. Now we focus on the last equality. We will consider two cases. For $r \neq 0$, we may prove the identity above but ignoring the δ-function piece:

$$
\partial_i \partial_j \left(\frac{1}{r}\right) = -\partial_i \left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) = -\partial_i \left(\frac{x_j}{r^3}\right) = \frac{3\hat{\boldsymbol{r}}_i \hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3}.
$$

To prove this, we simply calculate away:

$$
\begin{aligned}
\partial_i \partial_j \left(\frac{1}{r}\right) &= -\partial_i \left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) \\
&= -\partial_i \left(\frac{x_j}{r^3}\right) \\
&= \frac{-\partial_i x_j}{r^3} - x_j \partial_i \frac{1}{r^3} \\
&= -\frac{\delta_{ij}}{r^3} - x_j \partial_i \frac{1}{\left(\sum_{a=1}^3 x_a^2\right)^{3/2}} \\
&= -\frac{\delta_{ij}}{r^3} + \frac{3}{2} \frac{x_j}{r^5} \partial_i \left(\sum_{a=1}^3 x_a^2\right) \\
&= -\frac{\delta_{ij}}{r^3} + \frac{3}{2} \frac{x_j}{r^5} \left(\sum_{a=1}^3 2 x_a \delta_{ia}\right) \\
&= -\frac{\delta_{ij}}{r^3} + \frac{3 x_i x_j}{r^5} \\
&= \frac{3 \hat{\boldsymbol{r}}_i \hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3}.
\end{aligned}
$$

And we're done.

Now consider the case where r can be 0. We will to calculate $\partial_i \partial_j (1/r)$ via integration rather than taking derivatives. To this end, we make use of Gauss-Ostrogradsky theorem for volume integral of a gradient field:

$$\int_V \boldsymbol{\nabla} \psi \, dV = \int_{\partial V} \psi \boldsymbol{n} \, da.$$

In index notation, this is

$$\int_V \partial_i \psi \, dV = \int_{\partial V} \psi \boldsymbol{n}_i \, da.$$

Let $\psi = \hat{\boldsymbol{r}}_j / r^2$ and the volume V to be that of a sphere centered at the origin with radius ϵ. We have that

$$
\begin{aligned}
I_{ij} &= \int_V \partial_i \left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) dV \\
&= \int_{\partial V} \frac{\hat{\boldsymbol{r}}_j \hat{\boldsymbol{r}}_i}{r^2} \, da \\
&= \int_{\partial V, r=\epsilon} \frac{\hat{\boldsymbol{r}}_j \hat{\boldsymbol{r}}_i}{r^2} r^2 \sin\theta \, dr d\theta d\phi \\
&= \int_{\partial V, r=\epsilon} \frac{x_i x_j}{r^2} \sin\theta \, dr d\theta d\phi.
\end{aligned}
$$

At this point one may argue that due to spherical symmetry, only the diagonal terms $i = j$ are nonzero and are equal to a third of the trace. It then suffices to find the trace using the usual form of the Gauss-Ostrogradsky theorem. Here, I will present an explicit calculation of the (tensor) elements by expressing x_i in spherical coordinates.

$$
\begin{aligned}
x &= \epsilon \sin\theta \cos\phi \\
y &= \epsilon \sin\theta \cos\phi \\
z &= \epsilon \cos\theta.
\end{aligned}
$$

Using Mathematica (this is really not necessary since we can tell which integrand is odd/even... but for completeness I will just show everything explicitly):

$$I_{xx} = I_{yy} = I_{zz} = \frac{4\pi}{3}$$
$$I_{xy} = I_{yx} = I_{xz} = I_{zx} = I_{yz} = I_{zy} = 0.$$

With this, we're done. Putting everything together, we find that

$$I_{ij} = \frac{4\pi}{3}\delta_{ij}.$$

Using the same technique[1] (or in view of Gauss-Ostrogradsky theorem), we can also show that

$$\int_V \frac{3\hat{\boldsymbol{r}}_i\hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3}\,dV = 0.$$

Therefore the condition that

$$-\int_V \partial_i\partial_j\frac{1}{r} = \int_V \partial_i\left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right)dV = \frac{4\pi}{3}\delta_{ij} \quad \text{if } 0 \in V$$

is only satisfied if $\partial_i\partial_j(1/r)$ has a Dirac δ-function piece in addition to the usual "dipole" piece which doesn't contribute to the integral over $V \ni 0$:

$$\partial_i\partial_j\left(\frac{1}{r}\right) = -\partial_i\left(\frac{\hat{\boldsymbol{r}}_j}{r^2}\right) = -\partial_i\left(\frac{x_j}{r^3}\right) = \frac{3\hat{\boldsymbol{r}}_i\hat{\boldsymbol{r}}_j - \delta_{ij}}{r^3} - \frac{4\pi}{3}\delta_{ij}\delta^3(\boldsymbol{r}).$$

We have thus proved the identity.

Mathematica code:

```
(*Ixx*)
Integrate[
r*Cos[p]*Sin[t]*r*Cos[p]*Sin[t]*r^2/r^4*Sin[t], {t, 0, Pi}, {p, 0,
2 Pi}]

Out[19]= (4 \[Pi])/3

(*Iyy*)
Integrate[
r*Cos[p]*Sin[t]*r*Cos[p]*Sin[t]*r^2*Sin[t]/r^4, {t, 0, Pi}, {p, 0,
2 Pi}]

Out[17]= (4 \[Pi])/3

(*Izz*)
Integrate[
r^2 Cos[t]^2*r^2*Sin[t]/r^4, {t, 0, Pi}, {p, 0, 2 Pi}]

Out[23]= (4 \[Pi])/3

(*Ixy*)
Integrate[
r*Cos[p]*Sin[t]*r*Sin[p]*Sin[t]*r^2/r^4*Sin[t], {t, 0, Pi}, {p, 0,
2 Pi}]

Out[29]= 0

(*Iyz*)
Integrate[
r*Cos[t]*r*Sin[p]*Sin[t]*r^2/r^4*Sin[t], {t, 0, Pi}, {p, 0, 2 Pi}]

Out[30]= 0
```

[1] This integral diverges and therefore requires *regularization* in the sense that integration over the angular variables is carried out first, giving zero, rendering the radial integration unnecessary. The Mathematica code in the box has only integration over θ, ϕ.

```
(*Ixz*)
Integrate[
r*Cos[t]*r*Sin[p]*Cos[t]*r^2/r^4*Sin[t], {t, 0, Pi}, {p, 0, 2 Pi}]

Out[31]= 0





(*Dipole stuff... regularization is needed, i.e. I won't do \
the integral over r. Suffices to integrate over angles*)

(*xx*)
Integrate[(3*Cos[p]*Sin[t]*Cos[p]*Sin[t] - 1)/r*Sin[t], {t,
0, Pi}, {p, 0, 2 Pi}]

Out[36]= 0

(*yy*)
Integrate[(3*Sin[p]*Sin[t]*Sin[p]*Sin[t] - 1)/r*Sin[t], {t,
0, Pi}, {p, 0, 2 Pi}]

Out[39]= 0

(*zz*)
Integrate[(3*Cos[t] Cos[t] - 1)/r*Sin[t], {t, 0, Pi}, {p, 0,
2 Pi}]

Out[40]= 0

(*xy*)
Integrate[(3*Cos[p]*Sin[t]*Sin[p]*Sin[t])/r*Sin[t], {t, 0,
Pi}, {p, 0, 2 Pi}]

Out[44]= 0

(*yz*)
Integrate[(3*Cos[t]*Sin[t]*Sin[p])/r*Sin[t], {t, 0, Pi}, {p,
0, 2 Pi}]

Out[45]= 0

(*xz*)
Integrate[(3*Cos[t]*Cos[p]*Sin[t])/r*Sin[t], {t, 0, Pi}, {p,
0, 2 Pi}]

Out[47]= 0
```

2. Atoms in magnetic fields: the Breit-Rabi formula

(a)

(b)

(c)

(d)

(e)

(f)

3. Atomic g factors

Before starting this problem, let us write down the formula for g_F:

$$\begin{aligned} g_F &= \frac{g_J}{2}\frac{F(F+1)+J(J+1)-I(I+1)}{F(F+1)} \\ &= \frac{1}{2}\frac{F(F+1)+J(J+1)-I(I+1)}{F(F+1)}\left(1+\frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\right) \end{aligned}$$

where we have taken $g_E = 2$ and neglected $g_I \ll g_J$. Inserting this into Mathematica gives us a nice routine to find the Landé g-factor for given $(F, I, J, L, S = 1/2)$. For this problem, we're looking at sodium with $I = 3/2$. $S = 1/2$ as usual.

(a)

$$^2P_{1/2}, F = 1 \qquad g_F = -1/6$$
$$^2P_{1/2}, F = 2 \qquad g_F = +1/6$$

(b)

$$^2P_{3/2}, F = 0 \qquad g_F = \text{n/a}$$
$$^2P_{3/2}, F = 1 \qquad g_F = +2/3$$
$$^2P_{3/2}, F = 2 \qquad g_F = +2/3$$
$$^2P_{3/2}, F = 3 \qquad g_F = +2/3$$

(c)

$$^2S_{1/2}, F = 1 \qquad g_F = -1/2$$
$$^2S_{1/2}, F = 2 \qquad g_F = +1/2$$

For the stretched states, we simply have $F = I + J = I + L + S$. The Landé g-factor by definition is given by the projection of J on F multiplied by g_J, which is by definition (plus the condition that J is maximal) is just the ratio $(J + 2S)/J$. As a result, we have that the Landé g-factor g_F for the stretched states is given by

$$g_F = \frac{J}{F} g_J = \frac{J}{F} \frac{L + 2S}{J} = \frac{L + 2S}{F}.$$

With this, we can find that for the stretched state $^2P_{3/2}, F = 3$,

$$g_F = \frac{1 + 2(1/2)}{3} = \frac{2}{3} \qquad \checkmark$$

Similarly, we may find for the state $^2S_{1/2}, F = 2$:

$$g_F = \frac{0 + 2(1/2)}{2} = \frac{1}{2} \qquad \checkmark$$

Mathematica code:

```
In[48]:= (*g-factors*)
In[50]:= gJ[J_,S_,L_]:=1+(J*(J+1)+S(S+1)-L(L+1))/(2*J*(J+1));
In[51]:= gF[F_,I_,J_,L_,S_]:=gJ[J,S,L]/2*(F*(F+1)+J(J+1)-I*(I+1))/(F*(F+1))
(*F=1,I=3/2,J=1/2,L=1,S=1/2*)
In[53]:= gF[1,3/2,1/2,1,1/2]
Out[53]= -(1/6)
(*F=2,I=3/2,J=1/2,L=1,S=1/2*)
In[54]:= gF[2,3/2,1/2,1,1/2]
Out[54]= 1/6
In[55]:= (*F=0,I=3/2,J=3/2,L=1,S=1/2*)
In[63]:= (*Indeterminate*)
In[57]:= (*F=1,I=3/2,J=3/2,L=1,S=1/2*)
In[58]:= gF[1,3/2,3/2,1,1/2]
Out[58]= 2/3
In[59]:= (*F=2,I=3/2,J=3/2,L=1,S=1/2*)
In[60]:= gF[2,3/2,3/2,1,1/2]
Out[60]= 2/3
In[61]:= (*F=3,I=3/2,J=3/2,L=1,S=1/2*)
In[62]:= gF[3,3/2,3/2,1,1/2]
Out[62]= 2/3
In[64]:= (*F=1,I=3/2,J=1/2,L=0,S=1/2*)
In[65]:= gF[1,3/2,1/2,0,1/2]
Out[65]= -(1/2)
In[66]:= (*F=2,I=3/2,J=1/2,L=0,S=1/2*)
In[67]:= gF[2,3/2,1/2,0,1/2]
Out[67]= 1/2
```