Notes for Lecture #19

Derivation of the hyperfine interaction

Magnetic dipole field

These notes are very similar to the notes on the electric dipole field.

The magnetic dipole moment is defined by

\[ \mathbf{m} = \frac{1}{2} \int d^3r' \mathbf{r}' \times J(\mathbf{r}'), \]  

with the corresponding potential

\[ \mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \frac{\mathbf{m} \times \mathbf{r}}{r^2}, \]  

and magnetostatic field

\[ \mathbf{B}_m(\mathbf{r}) = \frac{\mu_0}{4\pi} \left\{ \frac{3\mathbf{r}(\mathbf{r} \cdot \hat{\mathbf{r}}) - \mathbf{m}}{r^3} + \frac{8\pi}{3} \mathbf{m} \delta^3(\mathbf{r}) \right\}. \]  

The first terms come form evaluating \( \nabla \times \mathbf{A} \) in Eq. 2. The last term of the field expression follows from the following derivation. We note that Eq. (3) is poorly defined as \( r \to 0 \), and consider the value of a small integral of \( \mathbf{B}(\mathbf{r}) \) about zero. (For this purpose, we are supposing that the dipole \( \mathbf{m} \) is located at \( \mathbf{r} = 0 \).) In this case we will approximate

\[ \mathbf{B}(\mathbf{r} \approx 0) \approx \left( \int_{\text{sphere}} \mathbf{B}(\mathbf{r}) d^3r \right) \delta^3(\mathbf{r}). \]  

First we note that

\[ \int_{r \leq R} \mathbf{B}(\mathbf{r}) d^3r = R^2 \int_{r=R} \hat{\mathbf{r}} \times \mathbf{A}(\mathbf{r}) \ d\Omega. \]  

This result follows from the divergence theorem:

\[ \int_{\text{vol}} \nabla \cdot \mathbf{V} d^3r = \int_{\text{surface}} \mathbf{V} \cdot d\mathbf{A}. \]  

In our case, this theorem can be used to prove Eq. (5) for each cartesian coordinate of \( \nabla \times \mathbf{A} \) since \( \nabla \times \mathbf{A} = \hat{x} (\hat{x} \cdot (\nabla \times \mathbf{A})) + \hat{y} (\hat{y} \cdot (\nabla \times \mathbf{A})) + \hat{z} (\hat{z} \cdot (\nabla \times \mathbf{A})). \) Note that \( \hat{x} \cdot (\nabla \times \mathbf{A}) = \hat{y} \cdot (\nabla \times \mathbf{A}) = \hat{z} \cdot (\nabla \times \mathbf{A}) = 0 \).
\(-\nabla \cdot (\mathbf{\hat{x}} \times \mathbf{A})\) and that we can use the Divergence theorem with \(V \equiv \mathbf{\hat{x}} \times \mathbf{A}(r)\) for the \(x\)-component for example:

\[
\int_{\text{vol}} \nabla \cdot (\mathbf{\hat{x}} \times \mathbf{A}) d^3r = \int_{\text{surface}} (\mathbf{\hat{x}} \times \mathbf{A}) \cdot \mathbf{n} dA = \int_{\text{surface}} (\mathbf{A} \times \mathbf{\hat{r}}) \cdot \mathbf{\hat{x}} dA.
\] (7)

Therefore,

\[
\int_{r \leq R} (\nabla \times \mathbf{A}) d^3r = -\int_{r = R} (\mathbf{A} \times \mathbf{\hat{r}}) \cdot (\mathbf{\hat{x}} \mathbf{\hat{x}} + \mathbf{\hat{y}} \mathbf{\hat{y}} + \mathbf{\hat{z}} \mathbf{\hat{z}}) dA = R^2 \int_{r = R} (\mathbf{\hat{r}} \times \mathbf{A}) d\Omega
\] (8)

which is identical to Eq. (5). We can use the identity (as in Lecture Notes 15),

\[
\int d\Omega \frac{\mathbf{\hat{r}}}{|r - r'|} = \frac{4\pi r_<}{3 r_>^2} \mathbf{\hat{r}}'.
\] (9)

Now, expressing the vector potential in terms of the current density:

\[
\mathbf{A}(r) = \frac{\mu_0}{4\pi} \int d^3r' \frac{\mathbf{J}(r')}{|r - r'|},
\] (10)

the integral over \(\Omega\) in Eq. 5 becomes

\[
R^2 \int_{r = R} (\mathbf{\hat{r}} \times \mathbf{A}) d\Omega = \frac{4\pi R^2}{3} \frac{\mu_0}{4\pi} \int d^3r' \frac{r_<}{r_>^2} \mathbf{\hat{r}}' \times \mathbf{J}(r').
\] (11)

If the sphere \(R\) contains the entire current distribution, then \(r_> = R\) and \(r_< = r'\) so that (11) becomes

\[
R^2 \int_{r = R} (\mathbf{\hat{r}} \times \mathbf{A}) d\Omega = \frac{4\pi \mu_0}{3} \frac{\mu_0}{4\pi} \int d^3r' \mathbf{r}' \times \mathbf{J}(r') \equiv \frac{8\pi \mu_0}{3} \frac{\mu_0}{4\pi} \mathbf{m},
\] (12)

which thus justifies the delta-function contribution in Eq. 3 and results so-called “Fermi contact” contribution in the “hyperfine” interaction.

**Magnetic field due to electrons in the vicinity of a nucleus**

In Lecture Notes #14, we showed that the current density associated with an electron in a bound state of an atom as described by a quantum mechanical wavefunction \(\psi_{nlm_l}(r)\) can be written:

\[
\mathbf{J}(r) = -\frac{e\hbar m_l}{m_e r \sin \theta} |\psi_{nlm_l}(r)|^2.
\] (13)

In the following, it will be convenient to represent the azimuthal unit vector \(\mathbf{\hat{\phi}}\) in terms of cartesian coordinates:

\[
\mathbf{\hat{\phi}} = -\sin \phi \mathbf{\hat{x}} + \cos \phi \mathbf{\hat{y}} = \frac{\mathbf{\hat{z}} \times \mathbf{r}}{r \sin \theta}.
\] (14)

The vector potential for this current density can be written

\[
\mathbf{A}(r) = -\frac{\mu_0 e\hbar}{4\pi m_e m_l} \int d^3r' \frac{\mathbf{\hat{z}} \times \mathbf{r}'}{|r - r'|} \frac{|\psi_{nlm_l}(r')|^2}{r'^2 \sin^2 \theta'}
\] (15)
We want to evaluate the magnetic field \( B = \nabla \times A \) in the vicinity of the nucleus \((r \to 0)\). Taking the curl of the Eq. 15, we obtain

\[
B_o(r) = \frac{\mu_0 e \hbar}{4\pi m_e} m_l \int d^3 r' \frac{(r - r') \times (\hat{z} \times r') |\psi_{nlm_l}(r')|^2}{|r - r'|^3} \quad (16)
\]

Evaluating this expression with \((r \to 0)\), we obtain

\[
B_o(0) = -\frac{\mu_0 e \hbar}{4\pi m_e} m_l \int d^3 r' \frac{\hat{z} r'^2 \sin^2 \theta'}{r'^3} \quad (17)
\]

Expanding the cross product and expressing the result in spherical polar coordinates, we obtain in the numerator \( \hat{r}' \times (\hat{z} \times \hat{r}') = \hat{z} (1 - \cos^2 \theta') - \hat{x} \cos \theta' \sin \theta' \cos \phi' - \hat{y} \cos \theta' \sin \theta' \sin \phi' \).

In evaluating the integration over the azimuthal variable \( \phi' \), the \( \hat{x} \) and \( \hat{y} \) components vanish which reduces to

\[
B_o(0) = -\frac{\mu_0 e \hbar}{4\pi m_e} m_l \int d^3 r' \frac{\hat{z} r'^2 \sin^2 \theta'}{r'^3} |\psi_{nlm_l}(r')|^2 \quad (18)
\]

and

\[
B_o(0) = -\frac{\mu_0 e \hbar m_l}{4\pi m_e} \int d^3 r' |\psi_{nlm_l}|^2 \frac{1}{r'^3} = -\frac{\mu_0 e}{4\pi m_e} L_z \langle \frac{1}{r'^3} \rangle. \quad (19)
\]

"Hyperfine" interaction

The so-called "hyperfine" interaction results from the magnetic dipole moment of a nucleus \( \mu_N \) responding to the magnetic field formed by the magnetic dipole of the electron spin \( (\mu_e) \) as well as the electron orbital current contribution.

\[
\mathcal{H}_{HF} = -\mu_N \cdot (B_{\mu_e} + B_o(0)). \quad (20)
\]

\[
\mathcal{H}_{HF} = -\frac{\mu_0}{4\pi} \left( 3(\mu_N \cdot \hat{r})(\mu_e \cdot \hat{r}) - \mu_N \cdot \mu_e \right) + \frac{8\pi}{3} \mu_N \cdot \mu_e \delta^3(r) + \frac{e}{m_e} \left( \frac{\mathbf{L} \cdot \mu_N}{r^3} \right). \quad (21)
\]