Notes for Lecture #17

Derivation of the hyperfine interaction

Magnetic dipole field

These notes are very similar to the notes for Lecture #12 on the electric dipole field.

The magnetic dipole moment is defined by

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

(1)

with the corresponding potential

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

(2)

and magnetostatic field

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

(3)

The first terms come from 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 \( \mathbf{B}(r) \) about zero. (For this purpose, we are supposing that the dipole \( \mathbf{m} \) is located at \( r = 0 \).) In this case we will approximate

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

(4)

First we note that

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

(5)

This result follows from the divergence theorem:

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

(6)

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

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

(7)
Therefore,
\[
\int_{r \leq R} (\nabla \times \mathbf{A}) d^3 r = - \int_{r = R} (\mathbf{A} \times \mathbf{f}) \cdot (\hat{x} \hat{x} + \hat{y} \hat{y} + \hat{z} \hat{z}) dA = R^2 \int_{r = R} (\hat{f} \times \mathbf{A}) d\Omega
\]
(8)
which is identical to Eq. (5). We can use the identity (as in Lecture Notes 12),
\[
\int d\Omega \frac{\hat{f}}{|\mathbf{r} - \mathbf{r}'|} = \frac{4\pi}{3} \frac{r_{<}}{r_g^2} \hat{r}'.
\]
(9)
Now, expressing the vector potential in terms of the current density:
\[
\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3 \mathbf{r}' \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},
\]
(10)
the integral over \( \Omega \) in Eq. 5 becomes
\[
R^2 \int_{r = R} (\hat{f} \times \mathbf{A}) d\Omega = \frac{4\pi R^2}{3} \frac{\mu_0}{4\pi} \int d^3 r' \frac{r_{<}}{r_g^2} \hat{r}' \times \mathbf{J}(\mathbf{r}').
\]
(11)
If the sphere \( R \) contains the entire current distribution, then \( r_{>} = R \) and \( r_{<} = r' \) so that (11) becomes
\[
R^2 \int_{r = R} (\hat{f} \times \mathbf{A}) d\Omega = \frac{4\pi}{3} \frac{\mu_0}{4\pi} \int d^3 r' \hat{r}' \times \mathbf{J}(\mathbf{r}') \equiv \frac{8\pi}{3} \frac{\mu_0}{4\pi} \mathbf{m},
\]
(12)
which thus justifies the so-called “Fermi contact” term in Eq. 3.

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

In Lecture notes #15, we showed that the current density associated with an electron in a bound state of an atom as described by a quantum mechanical wavefunction \( \psi_{nlm_i}(\mathbf{r}) \) can be written:
\[
\mathbf{J}(\mathbf{r}) = -\frac{e\hbar m_0 \hat{\phi}}{m_e r \sin \theta} |\psi_{nlm_i}(\mathbf{r})|^2.
\]
(13)
In the following, it will be convenient to represent the azimuthal unit vector \( \hat{\phi} \) in terms of cartesian coordinates:
\[
\hat{\phi} = -\sin \phi \hat{x} + \cos \phi \hat{y} = \frac{\hat{z} \times \mathbf{r}}{r \sin \theta}.
\]
(14)
The vector potential for this current density can be written
\[
\mathbf{A}(\mathbf{r}) = -\frac{\mu_0 e\hbar}{4\pi m_e m_i} \int d^3 r' \frac{\hat{z} \times \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \frac{|\psi_{nlm_i}(\mathbf{r}')|^2}{r'^2 \sin^2 \theta'}
\]
(15)
We want to evaluate the magnetic field \( \mathbf{B} = \nabla \times \mathbf{A} \) in the vicinity of the nucleus \( (\mathbf{r} \to 0) \). Taking the curl of the Eq. 15, we obtain
\[
\mathbf{B}(\mathbf{r}) = \frac{\mu_0 e\hbar}{4\pi m_e} m_i \int d^3 r' \frac{(\mathbf{r} - \mathbf{r}') \times (\hat{z} \times \mathbf{r}') |\psi_{nlm_i}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|^3} \frac{1}{r'^2 \sin^2 \theta'}
\]
(16)
Evaluating this expression with \( r \to 0 \), we obtain

\[
B(0) = -\frac{\mu_0}{4\pi m_e} \frac{e\hbar}{m_i} \int d^3r' \frac{r' \times \left( \hat{z} \times r' \right) |\psi_{niml}(r')|^2}{r'^2 \sin^2 \theta'}
\]  

(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

\[
B(0) = -\frac{\mu_0 e\hbar m_i}{4\pi m_e} \int d^3r' \frac{\hat{z} r'^2 \sin^2 \theta' |\psi_{niml}(r')|^2}{r'^2 \sin^2 \theta'}
\]  

(18)

and

\[
B(0) = -\frac{\mu_0 e\hbar m_i}{4\pi m_e} \int d^3r' |\psi_{niml}|^2 \frac{1}{r'^3} \equiv -\frac{\mu_0 e}{4\pi m_e} L_z \hat{z} \left\langle \frac{1}{r'^3} \right\rangle.
\]  

(19)