Notes for Lecture #17

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

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

with the corresponding potential

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

and magnetostatic field

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

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

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

First we note that

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

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 \( \nabla \times A \) since \( \nabla \times A = \hat{x} \left( \hat{x} \cdot (\nabla \times A) \right) + \hat{y} \left( \hat{y} \cdot (\nabla \times A) \right) + \hat{z} \left( \hat{z} \cdot (\nabla \times A) \right). \) Note that \( \hat{x} \cdot (\nabla \times A) = \)
\[-\nabla \cdot (\hat{x} \times \mathbf{A})\] and that we can use the Divergence theorem with \(V \equiv \hat{x} \times \mathbf{A}(\mathbf{r})\) for the \(x\)-component for example:

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

Therefore,

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

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

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

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

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

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

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

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

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

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

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

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

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

The vector potential for this current density can be written

\[
\mathbf{A}(\mathbf{r}) = -\frac{\mu_0 e \hbar}{4\pi m_e} \int d^3r' \frac{\hat{z} \times \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} \frac{|\psi_{nlm_l}(\mathbf{r}')|^2}{r'^2 \sin^2 \theta'} \tag{15}
\]
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

\[
B_0(r) = \frac{\mu_0 e h}{4\pi m_e} m_l \int d^3r' \frac{(r - r') \times (\hat{z} \times r') |\psi_{nlm_l}(r')|^2}{|r - r'|^3}.
\]

(16)

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

\[
B_0(0) = -\frac{\mu_0 e h}{4\pi m_e} m_l \int d^3r' \frac{r' \times (\hat{z} \times r') |\psi_{nlm_l}(r')|^2}{r'^3 \sin^2 \theta'}.
\]

(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

\[
B_0(0) = \frac{\mu_0 e h}{4\pi m_e} m_l \int d^3r' \frac{\hat{z} r'^{2} \sin^2 \theta' |\psi_{nlm_l}(r')|^2}{r'^3 \sin^2 \theta'}.
\]

(18)

and

\[
B_0(0) = -\frac{\mu_0 e h m_l \hat{z}}{4\pi m_e} \int d^3r' |\psi_{nlm_l}|^2 \frac{1}{r'^3} = -\frac{\mu_0 e}{4\pi m_e} L_z \hat{z} \left\langle \frac{1}{r'^3} \right\rangle.
\]

(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.

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

(20)

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

(21)