February 26, 2008

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

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

with the corresponding potential

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

and magnetostatic field

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

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 $\mathbf{r} = \mathbf{0}$.) In this case we will approximate

$$\mathbf{B}(\mathbf{r}\approx\mathbf{0}) \approx \left(\int_{\text{sphere}} \mathbf{B}(\mathbf{r})\mathbf{d^3r}\right)\delta^{\mathbf{3}}(\mathbf{r}). \tag{4}$$

First we note that

$$\int_{r\leq R}\mathbf{B}(\mathbf{r})d^3r = R^2\int_{r=R}\hat{\mathbf{r}}\times\mathbf{A}(\mathbf{r})\,d\Omega. \tag{5}$$

This result follows from the divergence theorm:

$$\int_{\text{vol}}\nabla\cdot\mathcal{V}\mathbf{d^3r} = \int_{\text{surface}}\mathcal{V}\cdot\mathbf{dA}. \tag{6}$$

In our case, this theorem can be used to prove Eq. (5) for each cartesian coordinate of $\nabla\times\mathbf{A}$ since $\nabla\times\mathbf{A} = \hat{\mathbf{x}}\left(\hat{\mathbf{x}}\cdot(\nabla\times\mathbf{A})\right) + \hat{\mathbf{y}}\left(\hat{\mathbf{y}}\cdot(\nabla\times\mathbf{A})\right) + \hat{\mathbf{z}}\left(\hat{\mathbf{z}}\cdot(\nabla\times\mathbf{A})\right)$. Note that $\hat{\mathbf{x}}\cdot(\nabla\times\mathbf{A}) =$

$-\nabla \cdot (\hat{\mathbf{x}} \times \mathbf{A})$ and that we can use the Divergence theorem with $\mathcal{V} \equiv \hat{\mathbf{x}} \times \mathbf{A}(\mathbf{r})$ for the $x-$ component for example:

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

Therefore,

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

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

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

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 Ω in Eq. 5 becomes

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

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

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

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:

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

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

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

The vector potential for this current density can be written

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

We want to evaluate the magnetic field $B = \nabla \times A$ in the vicinity of the nucleus ($\mathbf{r} \rightarrow 0$). Taking the curl of the Eq. 15, we obtain

$$\mathbf{B_o}(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{e\hbar}{m_e}\, m_l \int d^3r' \frac{(\mathbf{r}-\mathbf{r}') \times (\hat{\mathbf{z}} \times \mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^{\mathbf{3}}} \frac{|\psi_{nlm_l}(\mathbf{r}')|^2}{r'^2 \sin^2\theta'} \tag{16}$$

Evaluating this expression with ($\mathbf{r} \rightarrow 0$), we obtain

$$\mathbf{B_o}(\mathbf{0}) = -\frac{\mu_0}{4\pi}\frac{e\hbar}{m_e}\, m_l \int d^3r' \frac{\mathbf{r}' \times (\hat{\mathbf{z}} \times \mathbf{r}')}{r'^3} \frac{|\psi_{nlm_l}(\mathbf{r}')|^2}{r'^2 \sin^2\theta'} \tag{17}$$

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

In evaluating the integration over the azimuthal variable ϕ', the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ components vanish which reduces to

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

and

$$\mathbf{B_o}(\mathbf{0}) = -\frac{\mu_0 e\hbar m_l \hat{\mathbf{z}}}{4\pi m_e} \int d^3r' \, |\psi_{nlm_l}|^2 \, \frac{1}{r'^3} \equiv -\frac{\mu_0 e}{4\pi m_e} L_z \hat{\mathbf{z}} \left\langle \frac{1}{r'^3} \right\rangle . \tag{19}$$

“Hyperfine” interaction

The so-called “hyperfine” interaction results from the magnetic dipole moment of a nucleus $\mu_{\mathbf{N}}$ responding to the magnetic field formed by the magnetic dipole of the electron spin ($\mu_{\mathbf{e}}$) as well as the electron orbital current contribution.

$$\mathcal{H}_{\mathrm{HF}} = -\mu_{\mathbf{N}} \cdot (\mathbf{B}_{\mu_e} + \mathbf{B}_o(0)) . \tag{20}$$

$$\mathcal{H}_{\mathrm{HF}} = -\frac{\mu_0}{4\pi}\left(\frac{3(\mu_{\mathbf{N}} \cdot \hat{\mathbf{r}})(\mu_{\mathbf{e}} \cdot \hat{\mathbf{r}}) - \mu_{\mathbf{N}} \cdot \mu_{\mathbf{e}}}{r^3} + \frac{8\pi}{3}\mu_{\mathbf{N}} \cdot \mu_{\mathbf{e}} \delta^3(\mathbf{r}) + \frac{e}{m_e}\left\langle \frac{\mathbf{L} \cdot \mu_{\mathbf{N}}}{r^3} \right\rangle \right) . \tag{21}$$