February 22, 2001

Notes for Lecture #17

Derivation of the hyperfine interaction

Magnetic dipole field

These notes are very similar to the notes for Lecture #13 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

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

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

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3r \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \tag{9}$$

we can use the identity,

$$\int d\Omega \frac{\hat{\mathbf{r}}}{|\mathbf{r} - \mathbf{r}'|} = \frac{4\pi}{3} \frac{r_<}{r_>^2} \hat{\mathbf{r}}'. \tag{10}$$

Therefore,

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

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

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

Magnetic field due to electrons in the vicinity of a nucleus

According to the Biot-Savart law (or the curl of Eq. 9), the magnetic field produced by a current density $\mathbf{J}(\mathbf{r}')$ is given by:

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3r' \frac{\mathbf{J}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \tag{13}$$

In this case, we assume that the current density is due to an electron in a bound atomic state with quantum numbers $|nlm_l\rangle$, as described by a wavefunction $\psi_{nlm_l}(\mathbf{r})$, where the azimuthal quantum number m_l is associated with a factor of the form $\mathrm{e}^{im_l\phi}$. For such a wavefunction the quantum mechanical current density operator can be evaluated:

$$\mathbf{J}(\mathbf{r}') = \frac{-e\hbar}{2mi} \left(\psi^*_{nlm_l} \nabla' \psi_{nlm_l} - \psi_{nlm_l} \nabla' \psi^*_{nlm_l} \right). \tag{14}$$

Since the only complex part of this wavefunction is associated with the azimuthal quantum number, this can be written:

$$\mathbf{J}(\mathbf{r}') = \frac{-e\hbar}{2mir' \sin\theta'} \left(\psi^*_{nlm_l} \frac{\partial}{\partial\phi'} \psi_{nlm_l} - \psi_{nlm_l} \frac{\partial}{\partial\phi'} \psi^*_{nlm_l} \right) \hat{\phi}' = \frac{-e\hbar m_l \hat{\phi}'}{mr' \sin\theta'} \left|\psi_{nlm_l}\right|^2. \tag{15}$$

We need to use this current density in the Biot-Savart law and evaluate the field at the nucleus ($\mathbf{r} = \mathbf{0}$). The vector cross product in the numerator can be evaluated in spherical polar coordinates as:

$$\hat{\phi}' \times (-\mathbf{r}') = r' \left(-\hat{\mathbf{x}} \cos\theta' \cos\phi' - \hat{\mathbf{y}} \cos\theta' \sin\phi' + \hat{\mathbf{z}} \sin\theta' \right) \tag{16}$$

Thus the magnetic field evaluated at the nucleus is given by the integral:

$$\mathbf{B}(\mathbf{0}) = -\frac{\mu_0 e\hbar m_l}{4\pi m} \int d^3r' \, |\psi_{nlm_l}|^2 \, \frac{r' \left(-\hat{\mathbf{x}}\cos\theta' \cos\phi' - \hat{\mathbf{y}}\cos\theta' \sin\phi' + \hat{\mathbf{z}}\sin\theta'\right)}{r' \sin\theta' \, r'^3} . \tag{17}$$

In evaluating the integration over the azimuthal variable ϕ', the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ components vanish leaving the simple result:

$$\mathbf{B}(\mathbf{0}) = -\frac{\mu_0 e\hbar m_l \hat{\mathbf{z}}}{4\pi m} \int d^3r' \, |\psi_{nlm_l}|^2 \, \frac{1}{r'^3} \equiv -\frac{\mu_0 e}{4\pi m} L_z \hat{\mathbf{z}} \left\langle \frac{1}{r'^3} \right\rangle . \tag{18}$$