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Notes for Lecture #16

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

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

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

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

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 $\nabla\times\mathbf{A} = \hat{\mathbf{x}}\,(\hat{\mathbf{x}}\cdot(\nabla\times\mathbf{A})) + \hat{\mathbf{y}}\,(\hat{\mathbf{y}}\cdot(\nabla\times\mathbf{A})) + \hat{\mathbf{z}}\,(\hat{\mathbf{z}}\cdot(\nabla\times\mathbf{A}))$. 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,

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

which is identical to Eq. (5). We can use the identity (as in Lecture Notes 16),

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

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 so-called "Fermi contact" term in Eq. 3.

Magnetic field due to electrons in the vicinity of a nucleus

In Lecturenotes #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 $\psi_{nlm_l}(\mathbf{r})$ 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 ($\mathbf{r}\to 0$). Taking the curl of the Eq. 15, we obtain

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

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

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

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

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

and

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