Calculation of the vector potential for a confined current density

If the current density $J(r)$ is confined in space, the vector potential in the Coulomb gauge can be calculated from

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

(1)
Simple example of current density from a rotating charged sphere

Consider the following example corresponding to a rotating charged sphere of radius \(a\), with \(\rho_0\) denoting the uniform charge density within the sphere and \(\omega\) denoting the angular rotation of the sphere:

\[
J(r') = \begin{cases} 
\rho_0 \omega \times r' & \text{for } r' \leq a \\
0 & \text{otherwise}
\end{cases}
\]  

(2)

In order to evaluate the vector potential (12) for this problem, we can make use of the expansion:

\[
\frac{1}{|r - r'|} = \sum_{lm} \frac{4\pi}{2l + 1} \frac{r^l_{l+1}}{r'} Y_{lm}(\hat{r}) Y_{lm}(\hat{r}').
\]  

(3)

Noting that

\[
r' = r' \sqrt{\frac{4\pi}{3}} \left( Y_{1-1}(\hat{r}') \frac{\hat{x} + i\hat{y}}{\sqrt{2}} + Y_{11}(\hat{r}') \frac{-\hat{x} + i\hat{y}}{\sqrt{2}} + Y_{10}(\hat{r}') \hat{z} \right),
\]  

(4)

we see that the angular integral in Eq. (12) can be simplified with the use of the identity:

\[
\int d\Omega' \sum_m Y_{lm}(\hat{r}) Y_{lm}(\hat{r}') r' = \frac{r'}{r} r \delta_{l1}.
\]  

(5)
Simple example of current density from a rotating charged sphere – continued

Therefore the vector potential for this system is:

\[
A(r) = \frac{\mu_0 \rho_0 \omega}{3r} \int_0^a \frac{d r'}{r'^2} r'^3 \frac{r <}{r'^2},
\]

which can be evaluated as:

\[
A(r) = \begin{cases} 
\frac{\mu_0 \rho_0}{3} \omega \times r \left( \frac{a^2}{2} - \frac{3r^2}{10} \right) & \text{for } r \leq a \\
\frac{\mu_0 \rho_0}{3} \omega \times r \frac{a^5}{5r^3} & \text{for } r \geq a
\end{cases}
\]

\[
B(r) = \nabla \times A(r) = \begin{cases} 
\frac{\mu_0 \rho_0}{3} \left[ \omega \left( a^2 - \frac{6}{5}r^2 \right) + \frac{3}{5} r (\omega \cdot r) \right] & \text{for } r \leq a \\
\frac{\mu_0 \rho_0}{3} \left[ -\omega \frac{a^5}{5r^3} + \frac{3a^5}{5r^5} r (\omega \cdot r) \right] & \text{for } r \geq a
\end{cases}
\]
Another example – current associated with an electron in a spherical atom

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 $\psi_{nlm_l}(r)$, where the azimuthal quantum number $m_l$ is associated with a factor of the form $e^{im_l\phi}$. For such a wavefunction the quantum mechanical current density operator can be evaluated:

$$J(r) = \frac{-e\hbar}{2m_e i} \left( \psi^*_{nlm_l} \nabla \psi_{nlm_l} - \psi_{nlm_l} \nabla \psi^*_{nlm_l} \right). \quad (9)$$

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

$$J(r) = \frac{-e\hbar}{2m_e i r \sin \theta} \left( \psi^*_{nlm_l} \frac{\partial}{\partial \phi} \psi_{nlm_l} - \psi_{nlm_l} \frac{\partial}{\partial \phi} \psi^*_{nlm_l} \right) \hat{\phi} = \frac{-e\hbar m_l \hat{\phi}}{m_e r \sin \theta} |\psi_{nlm_l}|^2. \quad (10)$$

where $m_e$ denotes the electron mass and $e$ denotes the magnitude of the electron charge.
Current associated with an electron in a spherical atom – continued

\[ J(r) = \frac{-e\hbar m_l}{m_e r \sin \theta} |\psi_{nlm_l}(r)|^2 \cdot \frac{-e\hbar m_l \hat{z} \times r}{m_e r^2 \sin^2 \theta} |\psi_{nlm_l}(r)|^2. \]  \hspace{1cm} (11)

\[ A(r) = \frac{\mu_0}{4\pi} \left( \frac{-e\hbar m_l}{m_e} \right) \int d^3 r' \frac{\hat{z} \times r'}{|r - r'|} \frac{|\psi_{nlm_l}(r')|^2}{r'^2 \sin^2 \theta'}. \]  \hspace{1cm} (12)

Note that for some atomic wavefunctions, \( \psi_{nlm_l}(r') \), the evaluation of the vector potential \( A(r) \) simplifies.
Current associated with an electron in a spherical atom – continued

For example, consider the \(|nlm = 211\rangle\) state of a H atom:

\[
\psi_{211}(r) = -\sqrt{\frac{1}{64\pi a^3}} \frac{r}{a} e^{-r/(2a)} \sin \theta e^{i\phi},
\]  

(13)

and

\[
J(r') = -\frac{e\hbar}{64me \pi a^5} e^{-r' / a} \hat{z} \times r',
\]  

(14)

where \(a\) here denotes the Bohr radius. Using arguments similar to those above, we find that

\[
A(r) = -\frac{e\hbar\mu_0}{192m_e \pi a^5 r} \int_0^\infty dr' r'^3 e^{-r' / a} \frac{r < r^2}{r^2}.
\]  

(15)

This expression can be integrated to give:

\[
A(r) = -\frac{e\hbar\mu_0}{8m_e \pi r^3} \left[ 1 - e^{-r / a} \left( 1 + \frac{r}{a} + \frac{r^2}{2a^2} + \frac{r^3}{8a^3} \right) \right].
\]  

(16)
Current associated with an electron in a spherical atom – continued

Previous result:

\[
A(r) = \frac{-e\hbar\mu_0 \hat{\mathbf{z}} \times \mathbf{r}}{8m_e \pi r^3} \left[ 1 - e^{-r/a} \left( 1 + \frac{r}{a} + \frac{r^2}{2a^2} + \frac{r^3}{8a^3} \right) \right].
\] (17)

Note that for \( r \to \infty \):

\[
A(r) = \frac{-e\hbar\mu_0 \hat{\mathbf{z}} \times \mathbf{r}}{8m_e \pi r^3} = \frac{\mu_0}{4\pi} \left( -\frac{e\hbar}{2m_e} \right) \hat{\mathbf{z}} \times \mathbf{r} = \frac{\mu_0}{4\pi} \frac{\mathbf{m} \times \mathbf{r}}{r^3},
\] (18)

where

\[
\mathbf{m} = \left( -\frac{e\hbar}{2m_e} \right) \hat{\mathbf{z}}.
\] (19)

More generally:

\[
\mathbf{m} = \frac{1}{2} \int d^3 r' \, \mathbf{r}' \times \mathbf{J}(\mathbf{r}').
\] (20)
Current associated with an electron in a spherical atom – continued

Note that the general form of the current density for a spherical atom is given by:

$$J(r) = \frac{-e\hbar m_l}{m_e r \sin \theta} |\psi_{nlm_l}(r)|^2 = \frac{-e\hbar m_l}{m_e} \frac{\hat{\mathbf{z}} \times \hat{\mathbf{r}}}{r \sin^2 \theta} |\psi_{nlm_l}(r)|^2. \quad (21)$$

In this case, the general form of the magnetic dipole moment is given by

$$\mathbf{m} = \frac{1}{2} \int d^3r' \ r' \times \mathbf{J}(r') = -\frac{e\hbar m_l}{2m_e} \hat{\mathbf{z}} \int d^3r' |\psi_{nlm_l}(r')|^2 = -\frac{e\hbar}{2m_e} m_l \hat{\mathbf{z}}. \quad (22)$$
Systematic multipole analysis of vector potential for a general confined current density \( J(r) \) (assuming \( \nabla \cdot J(r) = 0 \)).

\[
A(r) = \frac{\mu_0}{4\pi} \int d^3r' \frac{J(r')}{|r - r'|}. \tag{23}
\]

For field point \( r \) outside of extent of current density:

\[
\frac{1}{|r - r'|} = \frac{1}{r} + \frac{r \cdot r'}{r^3} \ldots. \tag{24}
\]

\[
A(r) \approx \frac{\mu_0}{4\pi} \left( \frac{1}{r} \int d^3r' J(r') + \frac{r}{r^3} \cdot \int d^3r' r' J(r') \ldots. \right) \tag{25}
\]

Note that

\[
\int d^3r' J(r') = 0 \tag{26}
\]

\[
\mathbf{r} \cdot \int d^3r' r' J(r') = -\frac{1}{2} \mathbf{r} \times \int d^3r' r' \times J(r') \equiv \mathbf{m} \times \mathbf{r}. \tag{27}
\]
Magnetic dipolar field

The magnetic dipole moment is defined by

\[ m = \frac{1}{2} \int d^3 r' r' \times J(r'), \quad (28) \]

with the corresponding potential

\[ A(r) = \frac{\mu_0}{4\pi} \frac{m \times \hat{r}}{r^2}, \quad (29) \]

and magnetostatic field

\[ B_m(r) = \frac{\mu_0}{4\pi} \left\{ \frac{3\hat{r}(m \cdot \hat{r}) - m}{r^3} + \frac{8\pi}{3} m \delta^3(r) \right\}. \quad (30) \]
Magnetic dipolar field – continued

Some details:

\[ \nabla \times (s \mathbf{V}) = \nabla s \times \mathbf{V} + s \nabla \times \mathbf{V}. \] (31)

\[ \nabla \times (\mathbf{V}_1 \times \mathbf{V}_2) = \mathbf{V}_1(\nabla \cdot \mathbf{V}_2) - \mathbf{V}_2(\nabla \cdot \mathbf{V}_1) + (\mathbf{V}_2 \cdot \nabla)\mathbf{V}_1 - (\mathbf{V}_1 \cdot \nabla)\mathbf{V}_2. \] (32)

For \( r > 0 \):

\[ \nabla \times \left( \frac{\mathbf{m} \times \mathbf{r}}{r^3} \right) = \frac{3r(\mathbf{m} \cdot \mathbf{r}) - r^2 \mathbf{m}}{r^5}. \] (33)
Justification for the $\delta$ function contribution at the origin of the magnetic dipole

Note: This derivation is very similar to the analogous electrostatic case.

The evaluation of the field at the origin of the dipole is poorly defined, but we make the following approximation.

$$B(r \approx 0) \approx \left( \int_{\text{sphere}} B(r) d^3r \right) \delta^3(r). \quad (34)$$

First we note that

$$\int_{r \leq R} B(r) d^3r = R^2 \int_{r=R} \hat{r} \times A(r) d\Omega. \quad (35)$$

This result follows from the divergence theorem:

$$\int_{\text{vol}} \nabla \cdot \mathbf{V} d^3r = \int_{\text{surface}} \mathbf{V} \cdot d\mathbf{A}. \quad (36)$$
Singular contribution to dipolar field – continued

The divergence theorem can be used to prove Eq. (35) for each cartesian coordinate of $\nabla \times \mathbf{A}$ since $\nabla \times \mathbf{A} = \hat{x} (\hat{x} \cdot (\nabla \times \mathbf{A})) + \hat{y} (\hat{y} \cdot (\nabla \times \mathbf{A})) + \hat{z} (\hat{z} \cdot (\nabla \times \mathbf{A}))$. Note that $\hat{x} \cdot (\nabla \times \mathbf{A}) = -\nabla \cdot (\hat{x} \times \mathbf{A})$ and that we can use the Divergence theorem with $\mathcal{V} \equiv \hat{x} \times \mathbf{A}(\mathbf{r})$ for the $x-$ component for example:

$$\int_{\text{vol}} \nabla \cdot (\hat{x} \times \mathbf{A}) d^3r = \int_{\text{surface}} (\hat{x} \times \mathbf{A}) \cdot \hat{r} dA = \int_{\text{surface}} (\mathbf{A} \times \hat{r}) \cdot \hat{x} dA. \quad (37)$$

Therefore,

$$\int_{r \leq R} (\nabla \times \mathbf{A}) d^3r = - \int_{r = R} (\mathbf{A} \times \hat{r}) \cdot (\hat{x} \hat{x} + \hat{y} \hat{y} + \hat{z} \hat{z}) dA = R^2 \int_{r = R} (\hat{r} \times \mathbf{A}) d\Omega \quad (38)$$

which is identical to Eq. (35). We can use the identity (as in electrostatic case),

$$\int d\Omega \frac{\hat{r}}{|\mathbf{r} - \mathbf{r}'|} = \frac{4\pi}{3} \begin{cases} r \leq R \\ r^2 \geq \end{cases} \hat{r}'. \quad (39)$$
Singular contribution to dipolar field – continued

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

\[ \mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3 r \frac{\mathbf{J}(\mathbf{r'})}{|\mathbf{r} - \mathbf{r'}|}, \tag{40} \]

the integral over \( \Omega \) in Eq. 35 becomes

\[ R^2 \int_{r=R} (\hat{\mathbf{r}} \times \mathbf{A}) d\Omega = \frac{4\pi}{3} \frac{\mu_0}{4\pi} \int d^3 r' \frac{r_<}{r_>^2} \hat{\mathbf{r'}} \times \mathbf{J}(\mathbf{r'}). \tag{41} \]

If the sphere \( R \) contains the entire current distribution, then \( r_> = R \) and \( r_< = r' \) so that (41) becomes

\[ R^2 \int_{r=R} (\hat{\mathbf{r}} \times \mathbf{A}) d\Omega = \frac{4\pi}{3} \frac{\mu_0}{4\pi} \int d^3 r' \mathbf{r'} \times \mathbf{J}(\mathbf{r'}) = \frac{8\pi}{3} \frac{\mu_0}{4\pi} \mathbf{m}, \tag{42} \]

which thus justifies the delta-function contribution in Eq. 30 and results so-called “Fermi contact” contribution in the “hyperfine” interaction.
Magnetic field due to electrons in the vicinity of a nucleus

Contribution due to “orbital” magnetism in a spherical atom

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:

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

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

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

The vector potential for this current density can be written

$$
\mathbf{A}(\mathbf{r}) = -\frac{\mu_0}{4\pi} \frac{e\hbar}{m_e} m_l \int d^3r' \frac{\hat{z} \times \mathbf{r}'}{\left| \mathbf{r} - \mathbf{r}' \right|} \frac{\left| \psi_{nlm_l}(\mathbf{r}') \right|^2}{r'^2 \sin^2 \theta'}
$$
Contribution due to “orbital” magnetism in a spherical atom – continued

We want to evaluate the magnetic field \( B = \nabla \times A \) in the vicinity of the nucleus \((r \rightarrow 0)\). Taking the curl of the Eq. 45, we obtain

\[
B_o(r) = \frac{\mu_0}{4\pi} \frac{e\hbar}{m_e} m_l \int d^3r' \frac{(r - r') \times (\hat{z} \times r')}{|r - r'|^3} \frac{\psi_{nlml}(r')}{r'^2 \sin^2 \theta'} \quad (46)
\]

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

\[
B_o(0) = -\frac{\mu_0}{4\pi} \frac{e\hbar}{m_e} m_l \int d^3r' \frac{r' \times (\hat{z} \times r')}{r'^3} \frac{|\psi_{nlml}(r')|^2}{r'^2 \sin^2 \theta'} \quad (47)
\]
Contribution due to “orbital” magnetism in a spherical atom – continued

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

(48)

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

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

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

(49)

and

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

(50)
“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.

$$\mathcal{H}_{HF} = -\mu_N \cdot (B_{\mu e} + B_o(0)).$$  \hspace{1cm} (51)

$$\mathcal{H}_{HF} = -\frac{\mu_0}{4\pi} \left( \frac{3(\mu_N \cdot \hat{r})(\mu_e \cdot \hat{r}) - \mu_N \cdot \mu_e}{r^3} + \frac{8\pi}{3} \mu_N \cdot \mu_e \delta^3(r) + \frac{e}{m_e} \left\langle \frac{L \cdot \mu_N}{r^3} \right\rangle \right).$$  \hspace{1cm} (52)