Abstract

The magnetic field generated by an electron bound in a spherically symmetric potential is calculated for eigenstates of the orbital and total angular momentum. General expressions are presented for the current density in such states and the magnetic field is calculated through the vector potential, which is obtained from the current density by direct integration. The method is applied to the hydrogen atom, for which we reproduce and extend known results.

I. Introduction

Recently, Gough [1] has presented calculations of the magnetic field produced by a hydrogen atom in various angular-momentum eigenstates. The calculations were done by solution of the differential equation for the various multipole components of the vector potential. The purpose of this paper is to present a method for similar calculations, where the field is calculated by a direct integration from the current density. The multipole expansion of the latter involves only the angular part of the wave functions and we shall show results valid for angular-momentum eigenstates irrespective of the radial part. Our method involves some manipulations of spherical harmonics, which may
appear tedious, but provide a welcome opportunity to develop skills, which are of use in other applications of quantum mechanics. In particular, we gain some insight in the systematics of occurrence of various multipole comportment of the magnetic field, using identities known from the derivation of selection rules in spectroscopy.

The magnetic field generated by electrons occupying states in partially field shells is of interest in magnetism. Magnetic neutron scattering is mainly due to the interaction of the neutrons’s spin with the magnetic field. The magnetic form factor [2] is said to be given by the Fourier transform of the magnetization density of an atom. However, to avoid ambiguities involved in the definition of the magnetization density of an atom, it is important to bear in mind that it is the $B$ field due to unpaired electrons that is being measured. Of course, the electronic states in a magnetic material are different from the ones bound to free atoms. Nevertheless, the study of the latter is useful to clarify the concepts and methods involved in the calculation of magnetic form factors. In view of their relevance to magnetic materials, we shall discuss $d$ and $f$ states in particular.

II The vector potential

The vector potential $A$ satisfies the Poisson equation

$$\nabla^2 A = -\mu_0 j$$

(1)

with the current density $j$ as source. In reference [1], this differential equation has been solved for the dipole and octupole components of the azimuthal current density. Each Cartesian component of eq. (1) is of the form familiar from electrostatics as one relating the potential to charge density. Accordingly, the solution can be written in the integral form

$$A_i(r) = \frac{\mu_0}{4\pi} \int_{V'} \frac{j_i(r')dV'}{R},$$

(2)

where $i$ stands for $x,y$ and $z$, and $R = |r - r'|$. The factor $\frac{1}{R}$ can be expanded [3] as

$$\frac{1}{R} = \frac{1}{r} \sum_{l=0}^{\infty} \left(\frac{r'}{r}\right)^l P_l(\cos \alpha)$$

(3)
for $r > r'$, where $P_l$ is a Legendre polynomial of degree $l$. This equation is also valid for $r' > r$ after interchanging $r$ with $r'$. The nature of the angular-momentum eigenstates to be studied in the coming sections makes it convenient to work with spherical components. In particular, it will be seen that the current density has no $r$ or $\theta$ components and therefore, since $\text{div}j$ must vanish, it does not depend on $\phi$, i.e., $j = j(r, \theta) \hat{\phi}$. Consequently, the Cartesian components take the form

$$j_x = -j(r, \theta) \sin \phi; \quad (4)$$

$$j_y = j(r, \theta) \cos \phi. \quad (5)$$

Substituting eqs. (3) to (5) into eq. (2) then gives the Cartesian components of the vector potential,

$$A_x = -\frac{\mu_0}{4\pi} \left[ \int \int \int_{r'=0}^r (j(r', \theta')) \sin \phi' \frac{1}{r'} \sum_{l=0}^{\infty} \left( \frac{r'}{r} \right)^l P_l(\cos \alpha) dV' \right.$$

$$+ \int \int \int_{r'=r}^\infty (j(r', \theta')) \sin \phi' \frac{1}{r'} \sum_{l=0}^{\infty} \left( \frac{r'}{r} \right)^l P_l(\cos \alpha) dV' \biggr]$$

$$A_y = \frac{\mu_0}{4\pi} \left[ \int \int \int_{r'=0}^r (j(r', \theta')) \cos \phi' \frac{1}{r'} \sum_{l=0}^{\infty} \left( \frac{r'}{r} \right)^l P_l(\cos \alpha) dV' \right.$$

$$+ \int \int \int_{r'=r}^\infty (j(r', \theta')) \cos \phi' \frac{1}{r'} \sum_{l=0}^{\infty} \left( \frac{r'}{r} \right)^l P_l(\cos \alpha) dV' \biggr]$$

The function $P_l(\cos \alpha)$ can be expanded [3] as

$$P_l(\cos \alpha) = P_l(\cos \theta)P_l(\cos \theta') + 2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\cos \theta)P_l^m(\cos \theta') \times \cos m(\phi - \phi') \ldots \ldots (8)$$

where the $P_l^m$ are associated Legendre functions. We shall decompose the current density into multipole components as

$$j = \sum_{l=1,3,\ldots} j_l(r) P_l^1(\cos \theta), \ldots \ldots (9)$$
where \( j_1(r), j_3(r), \ldots \) are the dipole, octupole, 32-pole,... component of the current density, which enables the use of the orthogonality of the associated Legendre functions,

\[
\int_0^\pi P_p^m(\cos \theta') P_q^m(\cos \theta') \sin \theta' d\theta' = \frac{2}{2q + 1} \frac{(q + m)!}{(q - m)!} \delta_{p,q}
\]  \(10\)

together with the integrals

\[
\int_0^{2\pi} \cos m(\phi - \phi') \sin \phi' d\phi' = \pi \sin \phi \delta_{m,1}
\]  \(11\)

and

\[
\int_0^{2\pi} \cos m(\phi - \phi') \cos \phi' d\phi' = \pi \cos \phi \delta_{m,1}.
\]  \(12\)

The latter ensure that the expansion (9) is limited to \( m = 1 \). It is easily shown that for the dipole component the result is

\[
A_{x1} = -\frac{\mu_0}{3} \sin \phi P_1^1(\cos \theta) \left[ \frac{1}{r^2} \int_{r' = 0}^r j_1(r') r^3 dr' + r \int_{r' = r}^\infty j_1(r') dr' \right]
\]  \(13\)

\[
A_{y1} = \frac{\mu_0}{3} \cos \phi P_1^1(\cos \theta) \left[ \frac{1}{r^2} \int_{r' = 0}^r j_1(r') r^3 dr' + r \int_{r' = r}^\infty j_1(r') dr' \right]
\]  \(14\)

The dipole component of the vector potential is then of the form \( \mathbf{A}_1 = A_1(r) P_1^1(\cos \theta) \hat{\phi} \), where

\[
A_1 = \frac{\mu_0}{3} \left[ \frac{1}{r^2} \int_{r' = 0}^r j_1(r') r^3 dr' + r \int_{r' = r}^\infty j_1(r') dr' \right].
\]  \(15\)

Following the same procedure, we find the further coefficients in the multipole expansion of the vector potential,

\[
\mathbf{A} = \sum_{l=1,3,\ldots} A_l(r) P^l_1(\cos \theta) \hat{\phi},
\]  \(16\)

to be given by

\[
A_l = \frac{\mu_0}{2l + 1} \left[ \frac{1}{r^{l+1}} \int_{r' = 0}^r j_l(r') r^{l+2} dr' + r^l \int_{r' = r}^\infty \frac{j_l(r')}{r^{l-1}} dr' \right].
\]  \(17\)
III Current density in eigenstates of the angular momentum $L$ and the spin operator $S_z$

III.I Multipole expansion of the orbital current density in angular momentum eigenstates

The orbital current density generated by an electron in the $|n, l, m>\$ angular-momentum eigenstate has been given by Gough [1] as

$$j^o_\phi = -2\mu_B|\psi_{nlm}|^2 \frac{m}{r \sin \theta}, \quad (18)$$

where $\mu_B$ is the Bohr magneton and $\phi$ refers to the azimuthal component, the other components being zero, $j^o_r = j^o_\theta = 0$, and

$$\psi_{nlm} = R_{nl}(r)Y^m_l(\theta, \phi) \quad (19)$$

is the normalized wave function. The function $j^o_\phi$ can be factorized into radial and angular parts,

$$j^o_\phi = -2\mu_B \frac{R^2_{nl}}{r} m Y^m_l \frac{m Y^m_l}{\sin \theta}$$

$$= -2\mu_B \frac{R^2_{nl}(r)}{r} f_{lm}(\theta) \quad (20)$$

where we have defined $f_{lm}(\theta) = (-1)^m Y_l^m - \frac{m Y^m_l}{\sin \theta}$. It is clear within the formalism used in the previous section, that the various multipole components of the current density give rise to the corresponding components of the vector potential. Therefore, it will be convenient to carry out the angular integrals for each multipole separately. To this end, in the present section we shall carry out the multipole expansion of the angular part of functions of the form (20). In doing so, we encounter the compartments

$$\sin \theta = P^1_1(\cos \theta) \quad (dipole) ; \quad (21)$$

$$4 \cos^2 \theta \sin \theta - \sin^3 \theta = \frac{2}{3} P^1_3(\cos \theta) \quad (octupole) ; \quad (22)$$
\begin{align*}
8 \cos^4 \theta \sin \theta &- 12 \cos^2 \theta \sin^3 \theta + \sin^5 \theta = \frac{8}{15} P_5^1(\cos \theta) \ (32 - pole) ; \\
\text{which we identify with the appropriate Legendre functions of } \cos \theta. \text{ To find the desired expansion coefficients for the angular part, first the identity } [4]
\end{align*}

\begin{align*}
\frac{m Y^m_l}{\sin \theta} &= -\frac{1}{2} \left\{ \begin{array}{c}
\sqrt{\frac{2l+1}{2l-1}} \left[ (l-m-1)(l-m) e^{-i \phi} Y^{m+1}_{l-1} \\
+ \sqrt{(l+m-1)(l+m)} e^{i \phi} Y^{m-1}_{l-1} \right] \\
\end{array} \right. \\
\text{will be used and subsequently the expansion}
\end{align*}

\begin{align*}
Y^m_{l_1} Y^m_{l_2} &= \sum_{LM} \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}} C^{L0}_{l_10l_20} C^{LM}_{l_1m_1l_2m_2} Y^M_L ,
\end{align*}

where the Clebsch-Gordan coefficients obey the following rules:

\begin{align*}
C^{L0}_{l_10l_20} &= 0 \ , \text{ unless } l_1 + l_2 + L \text{ is even} ; \\
C^{LM}_{l_1m_1l_2m_2} &= 0 \ , \text{ unless } |l_1 - l_2| \leq L \leq l_1 + l_2 \text{ and } m_1 + m_2 = M. 
\end{align*}

Collecting terms, we find

\begin{align*}
f_{lm}(\theta) &= (-1)^m \frac{(2l+1)}{8\pi} \sum_{L=1,3,5, \ldots}^{L=2l-1} C^{L0}_{l_10l_20} \left\{ \begin{array}{c}
\sqrt{\frac{(l-m-1)(l-m)}{L(L+1)}} C^{L1}_{l_1-1m_1+1l-1} \\
- \sqrt{\frac{(l+m-1)(l+m)}{L(L+1)}} C^{L1}_{l_1-1m_1+l-m} \end{array} \right] P^1_L(\cos \theta) , \\
\end{align*}

where we have used the defining equations

\begin{align*}
Y^m_l &= (-1)^m \left[ \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{\frac{1}{2}} P^m_l(\cos \theta) e^{im \phi} \\
\text{and}
\end{align*}

\begin{align*}
P^{-m}_l(\cos \theta) &= (-1)^m \frac{(l-m)!}{(l+m)!} P^m_l(\cos \theta) .
\end{align*}
Equation (28), together with the rules (26) and (27) reveals some regularities in the occurrence of various multipole components. First, it is clear that only the $M = 1$ components appear and secondly, $L = 1, 3, \ldots, 2l - 1$. This is in accordance with the findings of Gough, in particular that in the $|2, 1, 1>$ state only the function (21) appears, whereas in $|3, 2, 1>$ and $|3, 2, 2>$ the functions (21) and (22). It is important to note that this regularity was seen to follow from the angular dependence of $j_\phi$ only. This implies that the result will hold for any $p, d, f,$ etc. states, irrespective of the radial function $R(r)$.

Substitution of the Clebsch-Gordan expressions leads to Table 1.

Table 1. The coefficients of the $\alpha_{lm}^L$ in the multipole expansion of the orbital current density, see equation (2.52)

| $L$ | $l$ | $m$ | 1 | 3 | 5 |
|-----|-----|-----|---|---|---|
| 3   | 1   | $\frac{3}{8}$ | $\frac{7}{24}$ | $\frac{5}{24}$ |
| 2   | $\frac{6}{8}$ | $\frac{7}{24}$ | $-\frac{1}{24}$ |
| 3   | $\frac{9}{8}$ | $-\frac{7}{24}$ | $\frac{1}{24}$ |
| 2   | 1   | $\frac{3}{8}$ | $\frac{2}{8}$ |
| 2   | $\frac{6}{8}$ | $-\frac{1}{8}$ |
| 1   | 1   | $\frac{3}{8}$ |

Again we find that some of the results of reference [1] are quite general: $p$ states in general give rise to pure dipole fields, $d$ states generate an octupole field as well, which is opposite in sign and stronger by a factor of two for $m_l = 1$ than for $m_l = 2$, etc. These and similar regularities found in Table 2 follow from the fact that the $L$-th order multipole component of the current
density operator is an irreducible tensor operator of rank \( L \).

III.II Multipole expansion of the spin current density for the eigenfunctions of the spin operator \( S_z \)

The current density associated with the electron spin for eigenfunctions of the spin operator \( S_z \) has been given in reference [1] as

\[
\hat{j}_\phi^s = \hat{j}_r^s = 0; \\
\hat{j}_\phi^s = 2m_s \mu_B (\sin \theta \frac{d}{dr} + \cos \theta \frac{d}{d\theta}) \Psi \Psi^*,
\]

where

\[
\Psi \Psi^* = R^{m}_l Y^m_l Y^m_l.
\]

As in the previous section (III.I), eq. (25) will be used to expand \( Y^m_l Y^m_l \) as

\[
Y^m_l Y^m_l = (-1)^m \sum_{l} \frac{(2l + 1)}{\sqrt{4\pi (2L + 1)}} C^{L0}_{l00} C^{L0}_{ml-m} Y^0_L(\theta, \phi).
\]

and eq. (29) will give

\[
Y^0_L = \frac{(2L+1)}{4\pi} P_L(\cos \theta) \text{ where } P_L = P^0_L; \text{ consequently,}
\]

\[
Y^m_l Y^m_l = (-1)^m \sum_{L} \frac{(2l + 1)}{4\pi} C^{L0}_{l00} C^{L0}_{ml-m} P_L(\cos \theta).
\]

To get the multipole expansion of the spin current density given in eq. (31), we need to express \( \sin \theta P_L \) and \( \cos \theta \frac{d}{d\theta} P_L \) as linear combinations of Legendre functions. For the former, the identity [3],

\[
\sin \theta P^m_l = \frac{1}{2l + 1} (P^{m+1}_{l+1} - P^{m+1}_{l-1})
\]

will be used, as a result,

\[
\sin \theta P_L = \frac{1}{2L + 1} (P^1_{L+1} - P^1_{L-1}).
\]

For the latter, the definition of the \( M = 1 \) associate Legendre polynomial,

\[
\frac{d}{d\theta} P_L(\cos \theta) = -P^1_L,
\]
will be used and subsequently the identity [5]

\[ \cos \theta P_l^m = \frac{1}{2L + 1} \{(l - m + 1)P_{l+1}^m + (l + m)P_{l-1}^m\}, \quad (38) \]

which gives

\[ \cos \theta P_L^1 = \frac{1}{2L + 1} \{LP_{L+1}^1 + (L + 1)P_{L-1}^1\}, \quad (39) \]

Combining eqs. (37) and (39) we find

\[ \cos \theta \frac{dP_L}{d\theta} = -\frac{1}{2L + 1} \{LP_{L+1}^1 + (L + 1)P_{L-1}^1\}. \quad (40) \]

Substitution of eq. (34) into eq. (32) and then (32) into eq. (31) with the help of eqs. (36) and (40) gives

\[ j_s^s(r, \theta) = (-1)^m \mu_B \frac{(2l + 1)}{4\pi} \sum_{L=0,2,...}^{L=2l} \frac{1}{2L + 1} C_{l010}^{L0} C_{lm1m}^{L0} \]

\[ \times \left\{ \left( \frac{\partial R_{nl}^2}{\partial r} - \frac{LR_{nl}^2}{r} \right) P_{L+1}^1 - \left( \frac{\partial R_{nl}^2}{\partial r} + (L + 1) \frac{R_{nl}^2}{r} \right) P_{L-1}^1 \right\}. \quad (41) \]

By shifting the value of the summation index \( L \), and noticing that \( P_{-1}^1 = 0 \), the above equation can be rewritten as,

\[ j_s^s(r, \theta) = (-1)^m 2m_s \mu_B \frac{(2l + 1)}{4\pi} \left\{ \sum_{L=1,3,...}^{L=2l+1} \frac{1}{2L - 1} C_{l010}^{L-10} C_{lm1m}^{L-10} \left( \frac{\partial R_{nl}^2}{\partial r} \right) \right. \]

\[ - (L - 1) \frac{R_{nl}^2}{r} P_{L+1}^1 - \sum_{L=1,3,...}^{L=2l-1} \frac{1}{2L + 3} C_{l010}^{L+10} C_{lm1m}^{L+10} \left( \frac{\partial R_{nl}^2}{\partial r} \right) \]

\[ + (L + 2) \frac{R_{nl}^2}{r} P_{L-1}^1 \right\}. \quad (42) \]

Here again we can recognize a feature of Gough’s results as being the consequence of a general rule: the highest multipole component of the magnetic field associated with spin currents is of order \( 2l + 1 \). That is, \( s \) states generate only dipole fields, \( p \) states dipole plus octupole, ect. As we find different linear combination of \( \frac{\partial}{\partial r} R_{nl}^2 \) and \( \frac{R_{nl}^2}{r} \) in the different multipole components, no general expressions can be given for the ratio of different components. This feature is inherent in the expression (31), which shows that the spin-current density, unlike the orbital one, eq.(20), cannot be written as a single product of an \( r \)-dependent and an angle-dependent factor.
IV Current density in eigenstates of the total angular momentum

The eigenfunctions of the total angular momentum being superpositions of the two eigenfunctions of $S_z$, the calculation of the expectation values of the current densities involves two-component spinors. As in the previous case, we find that the spin current density is not factorized in radial and angular parts. However, it turns out that the total current density can be written as a single product of $r$- and $\theta$-dependent functions. Therefore, we shall derive this expression first, in section IV.I, and turn to the problem of the multipole expansion of the radial part in section IV.II.

IV.I The factorization of the total current density

The eigenfunctions of the total angular momentum are of the form

$$\Psi = \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{pmatrix},$$

(43)

where

$$\psi_\uparrow(j = l - \frac{1}{2}, m_j = m + \frac{1}{2}) = R_{nl} \sqrt{\frac{l-m}{2l+1}} Y^m_l;$$
$$\psi_\downarrow(j = l - \frac{1}{2}, m_j = m + \frac{1}{2}) = -R_{nl} \sqrt{\frac{l+m+1}{2l+1}} Y^{m+1}_l;$$

(44)

for the low-lying spin-orbit coupled state and

$$\psi_\uparrow(j = l + \frac{1}{2}, m_j = m + \frac{1}{2}) = R_{nl} \sqrt{\frac{l+m+1}{2l+1}} Y^m_l;$$
$$\psi_\downarrow(j = l - \frac{1}{2}, m_j = m + \frac{1}{2}) = R_{nl} \sqrt{\frac{l-m}{2l+1}} Y^{m+1}_l$$

(45)

for higher-lying state. The current density operators applicable to wavefunctions of this form are represented as $2 \times 2$ matrices:

$$j^o = \frac{e\hbar}{2m_e} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*)$$

(46)

where $\nabla$ stands for \( \begin{pmatrix} \nabla & 0 \\ 0 & \nabla \end{pmatrix} \), and

$$j^s = -\mu_B \nabla \times <\sigma>, \quad (47)$$
where $\sigma$ stands for the Pauli matrices,

$$
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
$$

which can be transformed to spherical components using the transformation matrix

$$
\begin{pmatrix} \sigma_r \\ \sigma_\theta \\ \sigma_\phi \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \\ \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}
$$

(49)
giving

$$
\sigma_r = \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}; \quad \sigma_\theta = \begin{pmatrix} -\sin \theta & \cos \theta e^{-i\phi} \\ \cos \theta e^{i\phi} & \sin \theta \end{pmatrix};
\sigma_\phi = \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix}.
$$

(50)

As a consequence of the diagonal form of the operator (46), the orbital current density is found to be the sum of the currents generated by the separate spin components, given by eq. (20):

$$
\mathbf{j}^o = -\frac{2eB}{r \sin \theta} (m \psi^*_+ \psi_+ + (m + 1) \psi^*_- \psi_-) \hat{\phi}.
$$

(51)

Substitution of the spinor components (44) gives

$$
\mathbf{j}^o_{j=\frac{l-1}{2}} = -\frac{2eB}{r} \frac{R(r)^2_{nl}}{r^2} \frac{1}{(2l+1)} \left\{ (l - m)|Y^m_l|^2 \frac{m}{\sin \theta} - 2 \sin \theta \sqrt{(l - m)(l + m + 1)} Y^m_l \psi^*_l \psi_l e^{-i\phi} \right\}
$$

(52)

The evaluation of the spin current density is a bit more elaborate as it requires the three components of the spin density. Taking the expectation values of the matrices (50) using again the spinor components (44), we find

$$
< \sigma_r > = R^2_{nl} \frac{1}{2l+1} \left\{ \cos \theta \left[ (l - m)|Y^m_l|^2 - (l + m + 1)|Y^{m+1}_l|^2 \right] - 2 \sin \theta \sqrt{(l - m)(l + m + 1)} Y^m_l Y^{m+1}_l e^{-i\phi} \right\};
$$

(53)

$$
< \sigma_\theta > = R^2_{nl} \frac{1}{2l+1} \left\{ -\sin \theta \left[ (l - m)|Y^m_l|^2 - (l + m + 1)|Y^{m+1}_l|^2 \right] - 2 \cos \theta \sqrt{(l - m)(l + m + 1)} Y^m_l Y^{m+1}_l e^{-i\phi} \right\};
$$

(54)
\[ <\sigma_\phi> = 0, \]  
where we have made use of the fact that \( Y_l^m Y_l^{m+1} e^{-i\phi} = Y_l^m Y_l^{m+1} e^{i\phi} \) is real. As \(<\sigma_\phi>\) vanishes and \(<\sigma_r>\) and \(<\sigma_\theta>\) are independent of \(\phi\), eq.(47) will provide only a \(\phi\) component, which depends only on \(r\) and \(\theta\):

\[
j^s = -\frac{\mu_B}{r} \left[ \frac{\partial}{\partial r} (r <\sigma_\theta>) - \frac{\partial}{\partial \theta} <\sigma_r> \right] \hat{\phi}. \tag{56}
\]

To evaluate this quantity, we require the derivative

\[
\frac{\partial}{\partial \theta} <\sigma_r> = <\sigma_\theta> + R_{nl}^2 \frac{1}{2l+1} \left\{ \cos \theta [(l - m) \frac{\partial}{\partial \theta} |Y_l^m|^2 \right. \\
- (l + m + 1) \frac{\partial}{\partial \theta} |Y_l^{m+1}|^2 \right. \\
\left. \left. - 2 \sin \theta \sqrt{(l - m)(l + m + 1)} Y_l^m Y_l^{m+1} Y_l^{m+1} e^{-i\phi} \right\} \right. \\
- R_{nl}^2 \left\{ \cos \theta [(l - m) \frac{\partial}{\partial \theta} |Y_l^m|^2 \right. \\
- (l + m + 1) \frac{\partial}{\partial \theta} |Y_l^{m+1}|^2 \right. \\
\left. \left. \left. - 2 \sin \theta \sqrt{(l - m)(l + m + 1)} Y_l^m Y_l^{m+1} Y_l^{m+1} e^{-i\phi} \right\} \hat{\phi}. \tag{57}
\]

Substituting this expression and eq.(54) into eq.(56), we find

\[
j_{j_l = l - \frac{1}{2}}^s = -\frac{\mu_B}{r(2l+1)} \left( \frac{\partial R_{nl}^2}{\partial r} \right) \left\{ \frac{\partial}{\partial r} (r <\sigma_\theta>) \right. \\
\left. \left. - \sin \theta [(l - m) |Y_l^m|^2 \right. \\
\left. - (l + m + 1) |Y_l^{m+1}|^2 \right. \\
\left. \left. - 2 \cos \theta \sqrt{(l - m)(l + m + 1)} Y_l^m Y_l^{m+1} Y_l^{m+1} e^{-i\phi} \right\} \hat{\phi}. \tag{58}
\]

To eliminate the derivatives from the second pair of braces, we make repeated use of the identities [4]

\[
\frac{\partial}{\partial \theta} Y_l^m = m \cot \theta Y_l^m + \sqrt{(l - m)(l + m + 1)} Y_l^{m+1} e^{-i\phi} \tag{59}
\]

and we find that the awkward terms containing \(\frac{1}{\sin \theta}\) in eq.(52) can be combined with \(\frac{\cos^2 \theta}{\sin \theta}\) terms, so that the seemingly disparate angular functions appearing in \(j^o\) and \(j^s\) provide the desired factorized from for \(j = j^o + j^s\):

\[
j_{j_l = l - \frac{1}{2}} = \frac{\mu_B}{2l+1} \left( \frac{\partial R_{nl}^2}{\partial r} + 2(l + 1) \frac{R_{nl}^2}{r} \right) \left\{ \sin \theta [(l - m) |Y_l^m|^2 \right. \\
\left. \left. - (l + m + 1) |Y_l^{m+1}|^2 \right. \\
\left. \left. \left. - 2 \cos \theta \sqrt{(l - m)(l + m + 1)} Y_l^m Y_l^{m+1} Y_l^{m+1} e^{-i\phi} \right\} \hat{\phi.} \tag{60}
\]
This indeed is a product of a radial and an angular function, the former being independent of \( m \). Similarly, for the case \( j = l + \frac{1}{2} \) we find

\[
\mathbf{j}_{j = l + \frac{1}{2}} = \frac{\mu_B}{2l + 1} \left[ \frac{\partial R^2_{nl}}{\partial r} - 2l \frac{R^2_{nl}}{r} \right] \left\{ \sin \theta [(l + m + 1)|Y^m_l|^2 - (l - m)|Y^{m+1}_l|^2] - 2 \cos \theta \sqrt{(l - m)(l + m + 1)} Y^m_l Y^{m+1}_l e^{-i\phi} \right\} \mathbf{\hat{\phi}}.
\]

(61)

**IV.II Multipole expansion of angular part.**

To find the multipole components of the total current density, as given in eqs.(60) and (61), we again use eqs.(25) and (29). These readily yield eq.(34) and

\[
Y^m_l Y^{m+1}_l e^{-i\phi} = \frac{(-1)^{m+1}}{4\pi} \sum_{L=1,3,\ldots} \frac{2l + 1}{\sqrt{L(L+1)}} \sum_{L=1,3,\ldots} \frac{1}{L(2L-1)} C^{L-1}_m \{ (l - m)[L - 2(l + m + 1)] C^L_{l+m+1} - (l + m + 1)[L + 2(l - m)] C^L_{l-m} \} P_L^1 \mathbf{\hat{\phi}}.
\]

To come to our final result, we require eqs.(36) and (39) and the identity [4]

\[
\sqrt{L(L+1)} C^{L+1}_m = \sqrt{(l-m)(l+m+1)} (C^{L}_l - (m+1) l + C^{L}_l - m l m) .
\]

(62)

As before, some shifting of summation indices is necessary, in order to group terms according to the order of the Legendre function they belong to and this results in:

\[
\mathbf{j}_{j = l + \frac{1}{2}, m_j} = \mu_B \frac{(-1)^{m+1}}{4\pi} \left[ \frac{\partial R^2_{nl}}{\partial r} + 2(l + 1) \frac{R^2_{nl}}{r} \right] \left[ \sum_{L=1,3,\ldots} \frac{1}{L(2L-1)} C^{L-1}_m \{ (l - m)[L - 2(l + m + 1)] C^L_{l+m+1} - (l + m + 1)[L + 2(l - m)] C^L_{l-m} \} P_L^1 \mathbf{\hat{\phi}} - 2(l + m + 1) C^{L-1}_m \{ (l - m)[L - 2(l + m + 1)] C^L_{l+m+1} - (l + m + 1)[L + 2(l - m)] C^L_{l-m} \} P_L^1 \mathbf{\hat{\phi}} 
\]

\[
- \sum_{L=1,3,\ldots} \frac{1}{(L+1)(2L+3)} C^{L+1}_m \{ (l - m)[L + 1 + 2(l + m + 1)] C^L_{l+m} - (l + m + 1)[L + 1 + 2(l - m)] C^L_{l-m} \} P_L^1 \mathbf{\hat{\phi}} + (l + m + 1) [L + 1 + 2(l - m)] C^{L+1}_m \} P_L^1 \mathbf{\hat{\phi}} \}
\]

(63)
With similar manipulations, we get from eq.(61)

\[ j_{j=l+\frac{1}{2},m_j} = \mu_B \frac{(-1)^m}{4\pi} \left[ \frac{\partial R_{nl}^2}{\partial r} - 2l R_{nl}^2 \right] \left[ \sum_{L=1,3,...}^{2l+1} \frac{1}{L(2L-1)} C_{l010}^{L-1 \cdot 0} \{ (l + m + 1)[L + (l + m + 1)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \} \right. \\
- 2(l + m + 1)]C_{l m l - m}^{L-1 \cdot 0} + (l + m + 1)[L - 2(l - m)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \left. \} C_{l m l}^{L+1 \cdot 0} \{ (l + m + 1)[L + 1 - 2(l + m + 1)]C_{l m l - m}^{L+1 \cdot 0} \} \right] \right] \phi. \]

Equations (63) and (64) can be further reduced to:

\[ j_{j=l+\frac{1}{2},m_j} = \mu_B \frac{(-1)^m}{4\pi} \left[ \frac{\partial R_{nl}^2}{\partial r} - 2l R_{nl}^2 \right] \left[ \sum_{L=1,3,...}^{2l+1} \frac{1}{L(2L-1)} C_{l010}^{L-1 \cdot 0} \{ (l - m)[L + (l - m)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \} \right. \\
- 2(l + m + 1)]C_{l m l - m}^{L-1 \cdot 0} + (l + m + 1)[L - 2(l - m)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \left. \} C_{l m l}^{L+1 \cdot 0} \{ (l + m + 1)[L + 1 - 2(l - m)]C_{l m l - m}^{L+1 \cdot 0} \} \right] \phi. \]

(64)

\[ j_{j=l+\frac{1}{2},m_j} = \mu_B \frac{(-1)^m}{4\pi} \left[ \frac{\partial R_{nl}^2}{\partial r} - 2l R_{nl}^2 \right] \left[ \sum_{L=1,3,...}^{2l+1} \left( \frac{1}{L(2L-1)} C_{l010}^{L-1 \cdot 0} \{ (l + m + 1)[L + (l + m + 1)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \} \right. \\
- 2(l - m)]C_{l m l - m}^{L-1 \cdot 0} + (l - m)[L + 2(l + m + 1)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \left. \} C_{l m l}^{L+1 \cdot 0} \{ (l + m + 1)[L + 1 - 2(l - m)]C_{l m l - m}^{L+1 \cdot 0} \} \right] \phi \]

(65)

\[ j_{j=l+\frac{1}{2},m_j} = \mu_B \frac{(-1)^m}{4\pi} \left[ \frac{\partial R_{nl}^2}{\partial r} - 2l R_{nl}^2 \right] \left[ \sum_{L=1,3,...}^{2l+1} \left( \frac{1}{L(2L-1)} C_{l010}^{L-1 \cdot 0} \{ (l + m + 1)[L + (l + m + 1)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \} \right. \\
- 2(l - m)]C_{l m l - m}^{L-1 \cdot 0} + (l - m)[L + 2(l + m + 1)]C_{l m l - (m + 1)}^{L-1 \cdot 0} \left. \} C_{l m l}^{L+1 \cdot 0} \{ (l + m + 1)[L + 1 - 2(l - m)]C_{l m l - m}^{L+1 \cdot 0} \} \right] \phi \]

(66)

where we have make use of the identity [4] \((l + m + 1)C_{l m l - (m + 1)}^{2 \cdot 0} = (l - m)C_{l m l - m}^{2 \cdot 0} \), which follows from the general expression for \( C_{a \beta b \beta}^{a + b} \), to eliminate and reduce the highest-order term sum in eqs.(63) and (64). These two equations may look discouraging but eminently suitable for numerical
calculation of particular cases, as will be demonstrated in section V. Also, the coefficients of the multipole expansion are universal in the sense the ones given in table 1 were found to be.

Table 2 The coefficients $\alpha_{j}^{m_j}$ in the multipole expansion of the total current density, see equation (2.54).

| $L$ | $j = l + \frac{1}{2}$ | $m_j$ | 1   | 3   | 5   | 7   |
|-----|----------------------|-------|-----|-----|-----|-----|
| $\frac{7}{2}$ | $\frac{7}{2}$ | $\frac{4}{3}$ | $-\frac{14}{33}$ | $\frac{4}{39}$ | $-\frac{5}{429}$ |
| $\frac{5}{2}$ | $\frac{5}{2}$ | $\frac{20}{21}$ | $\frac{10}{33}$ | $-\frac{92}{273}$ | $\frac{35}{429}$ |
| $\frac{3}{2}$ | $\frac{3}{2}$ | $\frac{4}{7}$ | $\frac{14}{33}$ | $\frac{68}{273}$ | $-\frac{35}{143}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{4}{21}$ | $\frac{2}{11}$ | $\frac{20}{91}$ | $\frac{175}{429}$ |
| $\frac{5}{2}$ | $\frac{5}{2}$ | $\frac{9}{7}$ | $-\frac{1}{3}$ | $\frac{1}{21}$ |
| $\frac{3}{2}$ | $\frac{3}{2}$ | $\frac{27}{35}$ | $\frac{7}{15}$ | $-\frac{5}{21}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{9}{35}$ | $\frac{4}{15}$ | $\frac{10}{21}$ |
| $\frac{3}{2}$ | $\frac{3}{2}$ | $\frac{6}{5}$ | $-\frac{1}{5}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{2}{5}$ | $\frac{3}{5}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | 1 |
Table 2 lists such coefficients according to the definition
\[
j_{j=m_j} = \pm \frac{\mu_B}{4\pi} \left\{ \frac{\partial R_{nl}^2}{\partial r} + [2 \mp (2j + 1)] \frac{R_{nl}^2}{r} \right\} \sum_{L=1,3,5...}^{2j} \alpha_{L}^{jm_j} P_{L}^1
\]  

(67)

The notation in this expression implies what is not immediately obvious from eqs. (65) and (66): the expansion coefficients are independent of \(l\). In other words: for instances, no matter whether a \(j = 5/2\) sextet involves a \(d\) or \(f\) electron, each of the three allowed multipole components of the current density will have the same relative strength for different \(m_j\) values in both cases. Again, this is a consequence of the Wigner-Eckart theorem, which is applicable, because the total current density has the same property as the orbital one: its multipole component of order \(L\) is an irreducible tensor operator of rank \(L\).

V Examples

V.I The magnetic field generated by the orbital current in the state \(|n = 3, l = 2, m_l = 1\rangle\)

Since the radial part of the wave function of the state \(|3, 2, 1\rangle\) is
\[
R_{32}(r) = \frac{2\sqrt{30}}{1215\sqrt{a_0}} e^{-\frac{r}{a_0}} r^2,
\]
(68)

after substitution of \(R_{32}^2\) and \(f_{21}(\theta)\) from table 1 into eq.(20) we get,
\[
j_\phi = \frac{-16\mu_B}{5(3^9)(a_0^6)} e^{-\frac{2r}{a_0}} P_1^1 + \frac{2}{8\pi} P_3^1
\]
(69)

Comparing the above equation with eq.(9) gives,
\[
j_1(r) = \frac{-2}{5(3^9)(a_0^6)\pi} e^{-\frac{2r}{a_0}} r^3\text{ and } j_3(r) = \frac{-4}{5(3^9)(a_0^6)\pi} e^{-\frac{2r}{a_0}} r^3.
\]

Substitution these js into eq.(17) and integrating using the identity [1],
\[
\int r^n e^{-r/a} dr = -ae^{-r/a} \left\{ r^n + nar^{n-1} + n(n-1)a^2r^{n-2} + ... + n!a^n \right\}
\]
(70)

we have,
\[
A_1 = \frac{\mu_0\mu_B\sin\theta}{4\pi a_0^2} \left\{ e^{-\frac{2r}{a_0}} \left( \frac{2}{(5)(3^6)} a_0^2 + \frac{8}{(5)(3^5)} a_0^2 \right) \right\} + \frac{19}{(5)(3^4)} a_0^2 + \frac{2}{9} a_0^2 \right\}
\]
(71)
IV.II The magnetic field generated by the state $|n = 3, l = 2, j = 3/2, m_j = 3/2 >$

Substitution of the radial wave function $R_{32}$ of the previous example and the coefficients $a_{Lm_j}$ of table 2 into eq.(67) gives
Following the same procedure of the above example, the expressions for the vector potential and for the magnetic field are,

\[
A_1 = \frac{3\mu_0\mu_B \sin \theta}{10\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{2}{9} \left\{ \frac{2}{a_0} \right\}
\]

\[
A_3 = -\frac{27\mu_0\mu_B (4 \cos^2 \theta \sin \theta - \sin^3 \theta)}{20\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{2}{3} \left\{ \frac{2}{a_0} \right\}
\]

\[
B_{r_1} = \frac{3\mu_0\mu_B \cos \theta}{10\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{2}{3} \left\{ \frac{2}{a_0} \right\}
\]

\[
B_{r_3} = -\frac{27\mu_0\mu_B (5 \cos^3 \theta - 3 \cos \theta)}{5\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{2}{3} \left\{ \frac{2}{a_0} \right\}
\]

\[
B_{\theta_1} = \frac{3\mu_0\mu_B \sin \theta}{10\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{8}{3} \left\{ \frac{2}{a_0} \right\}
\]

\[
B_{\theta_3} = -\frac{81\mu_0\mu_B (4 \cos^2 \theta \sin \theta - \sin^3 \theta)}{20\pi a_0^3} \left\{ \frac{2}{(5)(3^8)} a_0^3 \right\} + \frac{2}{(5)(3^4)} a_0^2 \left\{ \frac{2}{r} \right\} + \frac{2}{(5)(3^2)} a_0 \left\{ \frac{2}{r^2} \right\} + \frac{2}{3} \left\{ \frac{2}{a_0} \right\}
\]

\[
\frac{\partial}{\partial z} = \frac{4\mu_B r^3 e^{2\eta_0}}{\pi 5(3^4) a_0^3} (15a_0 - r) \left\{ \frac{-6}{5} P_1 + \frac{7}{35} P_3 \right\}
\]

(77)
Figure 2 is a graphical representation of the magnetic field in this case. The pattern is much simpler than the previous one; it is reminiscent of the field of a simple current loop. The same holds for the case $j = \frac{5}{2}, m_j = \frac{5}{2},$ as seen in fig. 3. This becomes understandable if one notices, using the coefficients of table 2, that $j(r, \theta)$ is proportional to $\sin^3 \theta$ for $j = m_j = \frac{3}{2}$ and to $\sin^5 \theta$ for $j = m_j = \frac{5}{2}$. Thus, with increasing $j$, the current tends to be confined in the ‘equatorial’ plane. Comparing figs. 3 and 4, one realizes the limits of the ‘universality’ of the relations summarized in table 2. Although in these two cases the $\theta$-dependence of $j$ is identical, the different r-dependences influence the resulting pattern of field lines in a qualitative way.

References

[1] Gough W 1996 Eur.J.Phys. 17 208 -215
[2] Trammell G T 1953 Phys. Rev. 92 1387-1393
[3] Hirst L L 1997 Rev. Mod. Phys. 69 607-626
[4] de Châtel P F and Ayuel K A 1999, to be published
[5] Arfken G 1985 Mathematical Methods for Physicists 3rd edn (Orlando, Fl: Academic ) p 639 and 640
Figure 1
