Multipole expansion of electric potential PhL 11.16.07

This is a horribly complicated subject when you dredge the outer limits, but I will try to summarize things here as best I can. I will show the logic flow, but won't actually derive any of the equations. We can do that some rainy day after the flow is well understood. The expansion of *vector* quantities does not appear here, see a separate older doc on that subject.

Contents:

1. Spherical Multipole Expansion of the Electric Potential
2. Taylor Expansion of the Electric Potential
3. Comments on the above two sections.
4. Multipole (Taylor) expansion of the potential energy in a charge distribution.
5. Can you write a multipole expansion for the charge density itself ??
6. Multipole Expansion using the angle γ.
7. Multipole expansion of the energy of two overlapping charge densities.
8. Angular Momentum Algebra
9. Derive formula (17.11) of Levitt.
10. Raab and De Lang Cartesian multipole expansions (from Google site)
(a) electric potential through octupole (1.3)
(b) electric field to same order (1.13)
(c) magnetic potential A through quadrupole order, definition of m_{jk}
(d) magnetic field through quadrupole order
(e) force and torque between a B field and the magnetic moments (1.59), (1.64)
(f) magnetic potential energy (interaction Hamiltonian) through quadrupole (1.67)

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1. Spherical Multiple Expansion of the Electric Potential

credits: http://en.wikipedia.org/wiki/Spherical_multipole_moments

First of all, we can write the potential of a point charge q at location **r'** viewed from position **r** as follows:

$$\Phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon}\frac{1}{R} = \frac{q}{4\pi\varepsilon}\frac{1}{\sqrt{r^2 + r'^2 - 2r'r\cos\gamma}}.$$

where R = | **r** - **r'**| and **r'** is the location of the charge in space, and we are here in SI units which have an extra $1/4\pi\varepsilon$ compared to Jackson equations like (1.48) on page 20. [I think Jackson may have changed to SI units in his later editions]. We know that γ is the angle between the two vectors **r** and **r'**. The above expression on the right is derived from simple geometry. The above is symmetric in r and r', it happens.

Imagine the inverse square root as a function of x= (r'/r) and cosγ. Expand it in a power series in x of the form $\sum_\ell x^\ell f_\ell(\cos\gamma)$, then integrate to determine the f_ℓ functions and you find they are P_ℓ's. Dealing with the inside and outside issues, you then end up with this single-sum expansion of the potential

$$\Phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^{l} P_l(\cos\gamma)$$

where now we have assumed that r = max(|**r**|, |**r'**|) and r' = min(|**r**|, |**r'**|). The next step is to expand the Legendre in a factorized summation form where now we have the polar angles of **r** and **r'** :

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)Y_{lm}^{*}(\theta',\phi')$$

// "addition theorem"

Inserting this then gives the result:

$$\Phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^{l}\left(\frac{4\pi}{2l+1}\right)\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)Y_{lm}^{*}(\theta',\phi')$$

with r and r' max and min as noted earlier. This appears in Jackson on page 679 as (3.70).

Now, suppose instead of having a single point charge q, we have a charge density ρ(**r'**) where we recall that **r'** is the location of the charge and **r** is the viewing point. We now assume that r > r' for all of ρ(**r'**) so we are viewing from outside a sphere containing the entire charge distribution. Suppose we then integrate the above formula over the **r'** angles. We could then define:

$$Q_{lm} \stackrel{\text{def}}{=} \int d\mathbf{r}'\rho(\mathbf{r}')\,(r')^{l}\sqrt{\frac{4\pi}{2l+1}}Y_{lm}^{*}(\theta',\phi')$$

and in terms of this $Q_{\ell m}$ thing we could write our potential expansion as follows:

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(\frac{Q_{lm}}{r^{l+1}}\right)\sqrt{\frac{4\pi}{2l+1}}Y_{lm}(\theta,\phi)$$

This then is the "multipole expansion of the electric potential of a charge distribution ρ as viewed from a point **r** which lies outside the entire charge distribution." The quantities $Q_{\ell m}$ care called the "electric multipole moments" of the charge distribution.

Notice that we don't see any "spatial derivatives of the potential" appearing in this formula.

2. Taylor Expansion of the Electric Potential

Imagine a unit point charge located at position **r**, and we view the potential from point **R**. We are going to do a Taylor expansion of the potential about the origin r = 0 (not about point R!). Thus, our expansion will be reasonable if the charge is somewhere "close to the origin" so **r** is "small". We get,
[Greek letters represent Cartesian x,y,z components, sum on repeats]

$$\phi(\mathbf{R};\mathbf{r}) = 1/|\mathbf{r}-\mathbf{R}| = \phi(r=0) + r_\alpha\partial_\alpha\phi + (1/2)\, r_\alpha r_\beta\partial_\alpha\partial_\beta\phi + (1/3!)\, r_\alpha r_\beta r_\gamma\partial_\alpha\partial_\beta\partial_\gamma\phi + \ldots$$

where all the derivatives shown are evaluated at $\mathbf{r} = 0$. Normally we would write just $\phi(\mathbf{R})$ for the potential at viewing point $\mathbf{R}$, but the potential is a function of both variables $\mathbf{R}$ and $\mathbf{r}$, and it happens that we are expanding in the variable $\mathbf{r}$. The factors in front are just overcount correctors. We have shown the dipole, quadrupole and octupole terms here, and higher terms have the same pattern. Now we can go off and compute these derivatives. Consider: [∂_α means diff with respect to r_α]

$$f = 1/|\mathbf{r}-\mathbf{R}| \qquad \partial_\alpha f = -(1/2)\,[\,1/|\mathbf{r}-\mathbf{R}|^3\,]\,2\,(r_\alpha - R_\alpha) \qquad \Rightarrow \partial_\alpha f|^{r=0} = +R_\alpha/R^3$$

Using the $\partial_\alpha f$ shown right above here, we can apply ∂_β to get

$$\partial_\beta(\partial_\alpha f) = -\delta_{\alpha\beta}/|\mathbf{r}-\mathbf{R}|^3 + 3\,(r_\alpha - R_\alpha)(r_\beta - R_\beta)/|\mathbf{r}-\mathbf{R}|^5$$

$$\Rightarrow \partial_\beta(\partial_\alpha f)^{|r=0} = -\delta_{\alpha\beta}/R^3 + 3R_\alpha R_\beta/R^5 = (1/R^5)\,[\,3R_\alpha R_\beta - \delta_{\alpha\beta}R^2]$$

As a side comment, notice that trace($\partial_\alpha\partial_\beta\phi$) = 0. But this says $\partial_\alpha\partial_\alpha\phi = 0$ which is Laplace's equation, so this serves to confirm the correctness (somewhat) of our last calculation.

Next, let's throw out the octupole term for the moment, and rewrite the quadrupole term as follows: [we now just show the "viewing point argument R" inside $\phi(\mathbf{R})$.]

$$\phi(\mathbf{R}) = 1/|\mathbf{r}-\mathbf{R}| = \phi(0) + r_\alpha\partial_\alpha\phi + (1/6)\,[\,3r_\alpha r_\beta - \delta_{\alpha\beta}r^2\,]\,\partial_\alpha\partial_\beta\phi + \text{octupole and higher terms}$$

In the [...] bracket, the first term replicates the term we had in the first place, and the second term is really zero because $\partial_\alpha\partial_\alpha\phi = 0$. The advantage of this last step is that the bracket is now traceless and looks very much like our second derivative. Now let's install our derivatives to get:

$$\phi(\mathbf{R}) = 1/|\mathbf{r}-\mathbf{R}| = 1/R + (r_\alpha R_\alpha)/R^3 + (1/6)\,[\,3r_\alpha r_\beta - \delta_{\alpha\beta}r^2\,]\,[\,3R_\alpha R_\beta - \delta_{\alpha\beta}R^2]/R^5 + \ldots$$

and we can marvel at the extreme symmetry of the result. Now, if $\mathbf{R}$ is located close to the charge, so $\mathbf{R}$ and $\mathbf{r}$ are the same order of magnitude, then all the terms are order 1/R and our expansion is not converging! That is, each term is the same general size. We want the terms to be getting smaller. That requires that R be large compared to r. Then the terms are 1/R, $1/R^2$, $1/R^3$ and so on.

Now imagine a set of charges q_i placed at locations $\mathbf{r_i}$. We assume each charge is close to the origin, so we are justified in doing the expansion separately for each charge! That is to say, for the charge at $\mathbf{r_i}$, we are expanding around $\mathbf{r_i} = 0$. We then generalize our result above as follows by adding the contribution of each term in the potential, each having its own expansion:

$$\phi(\mathbf{R}) = \Sigma_i\, q_i/|\mathbf{r_i}-\mathbf{R}|$$

$$= \{\Sigma_i\, q_i\}/R + R_\alpha\{\Sigma_i\, q_i\, r_{i\alpha}\}/R^3 + (1/6)\,[\,3R_\alpha R_\beta - \delta_{\alpha\beta}R^2\,]\,\{\,\Sigma_i\, q_i\,[\,3r_{i\alpha}r_{i\beta} - \delta_{\alpha\beta}r_i^2]\,\}/R^5 + \ldots$$

At this point, we isolate the {} bracketed quantities as follows:

$Q = \Sigma_i \; q_i$ = "monopole moment" = the total charge

$P_\alpha = \{\Sigma_i \; q_i \; r_{i\alpha} \}$ = "the dipole moment"

$Q_{\alpha\beta} = \{\Sigma_i \; q_i \; [\; 3r_{i\alpha}r_{i\beta} - \delta_{\alpha\beta}r_i^2] \}$ = "the quadrupole moment"

For continuous distributions of charge, we would write these as:

$$Q = \int d^3\mathbf{r} \; \rho(\mathbf{r})$$

$$\mathbf{P} \;\; = \int d^3\mathbf{r} \; \rho(\mathbf{r}) \; \mathbf{r}$$

$$Q_{\alpha\beta} = \int d^3\mathbf{r} \; \rho(\mathbf{r}) \;\; (3r_\alpha r_\beta - \delta_{\alpha\beta}r^2)$$

This Q thing is the "Cartesian quadrupole moment" as opposed to the $Q_{\ell m}$ thing appearing above in our spherical harmonic expansion.

In terms of these moments, we can then write

$$\phi(\mathbf{R}) = Q/R + \mathbf{R}\bullet\mathbf{P}/R^3 + (1/6) \; [\; 3R_\alpha R_\beta \; - \delta_{\alpha\beta}R^2 \;] \; Q_{\alpha\beta}/R^5 \qquad + ...$$

In order to get reasonable convergence of this expansion, we must have R >> a where a is the diameter of a sphere bounding all the charges.

One normally expresses this final result by rewriting in terms of a lower-case **r**, so now we change our viewing point from **R** to **r** and write:

$$\phi(\mathbf{r}) = Q/r + \mathbf{r}\bullet\mathbf{P}/r^3 + (1/6) \; [\; 3r_\alpha r_\beta \; - \delta_{\alpha\beta}r^2 \;] \; Q_{\alpha\beta}/r^5 \qquad + ...$$

Notice the symmetry here. Both **r** and **P** are vectors. Both $[\; 3r_\alpha r_\beta \; - \delta_{\alpha\beta}r^2 \;]$ and $Q_{\alpha\beta}$ are traceless tensors. I wonder what the octupole term looks like.

3. Comments on the above two sections.

In Section 1, we write a formula expressing a potential $\phi(r)$ in terms of the moments of a charge distribution using the angular momentum basis functions. But we don't do any Taylor expansion in this section. In Section 2 we do the Taylor expansion in order to find the Cartesian moment expansion of the same $\phi(r)$ potential. The first expansion is easy to write to all orders, but the second we only write through quadrupole order.

4. Taylor expansion of the potential energy in a charge distribution.

Start with Jackson's formula (1.53) on page 21 which says

$$W = (1/2) \int d^3\mathbf{r}\ \rho(\mathbf{r})\phi(\mathbf{r})$$

Now treat the potential $\phi(\mathbf{r})$ as a function of $\mathbf{r}$ and Taylor expand it about the origin $\mathbf{r} = 0$:

$$\phi(\mathbf{r}) = \{ \phi(0) + r_\alpha \partial_\alpha \phi + (1/6) [3r_\alpha r_\beta - \delta_{\alpha\beta} r^2] \partial_\alpha \partial_\beta \phi \} + \text{octupole and higher terms}$$

where derivatives are now evaluated at $\mathbf{r} = 0$. This time we don't know the potential ϕ, so we just leave these derivatives in place. The derivatives are just constants since evaluated at r=0, so insert to get

$$W = (1/2) \int d^3\mathbf{r}\ \rho(\mathbf{r}) \{ \phi(0) + r_\alpha \partial_\alpha \phi + (1/6) [3r_\alpha r_\beta - \delta_{\alpha\beta} r^2] \partial_\alpha \partial_\beta \phi \}$$

$$= (1/2)[\phi(0) \int d^3\mathbf{r}\ \rho(\mathbf{r}) + (\partial_\alpha \phi) \int d^3\mathbf{r}\ \rho(\mathbf{r})\ r_\alpha + (1/6) (\partial_\alpha \partial_\beta \phi) \int d^3\mathbf{r}\ \rho(\mathbf{r})\ [3r_\alpha r_\beta - \delta_{\alpha\beta} r^2] + ...$$

We now of course recognize the moments defined above,

$$Q = \int d^3\mathbf{r}\ \rho(\mathbf{r}) \qquad \mathbf{P} = \int d^3\mathbf{r}\ \rho(\mathbf{r})\ \mathbf{r} \qquad Q_{\alpha\beta} = \int d^3\mathbf{r}\ \rho(\mathbf{r})\ (3r_\alpha r_\beta - \delta_{\alpha\beta} r^2)$$

so we end up with

$$W = (1/2)\phi(0)Q + (\partial_\alpha \phi) P_\alpha + (1/6)(\partial_\alpha \partial_\beta \phi) Q_{\alpha\beta} + \text{octupole and higher}$$

Comment: this is the expansion Levitt refers to on page 172.

5. Can you write a multipole expansion for the charge density itself ??

AKA : How to expand any scalar function $\rho(\mathbf{r})$ using spherical harmonics.

Following the previous section, we would write:

$$\rho(\mathbf{r}) = \{ \rho(0) + r_\alpha \partial_\alpha \rho + (1/6) [3r_\alpha r_\beta - \delta_{\alpha\beta} r^2] \partial_\alpha \partial_\beta \rho \} + \text{octupole and higher terms}$$

This is not a very useful concept I suspect. For example, if you try to integrate this term by term over all space, each term blows up.

But suppose we try to expand $\rho(\mathbf{r})$ in the following manner: [for each value of r, $\rho(r,\theta,\phi)$ is some function $g(\theta,\phi)$ and you can expand any reasonable $g(\theta,\phi)$ on the spherical harmonics, that is my argument at least.]

$$\rho(\mathbf{r}) = \Sigma_{\ell m}\ f_{\ell m}(r)\ Y_{\ell m}(\theta,\phi)$$

Multiply both sides by $Y_{\ell' m'}(\theta,\phi)$ and integrate over $d\Omega$, then you get

$$\int d\Omega\ \rho(\mathbf{r}) Y_{\ell m}(\theta,\phi) = f_{\ell m}(r)$$

so you could compute the part of $\rho(r)$ that belongs to each multipole. Namely:

$$\rho_{\ell m}(\mathbf{r}) = f_{\ell m}(r)\ Y_{\ell m}(\theta,\phi)$$

Then you could express your total charge density as the Levitt like sum:

$$\rho(\mathbf{r}) = \Sigma_{\ell m}\ \rho_{\ell m}(\mathbf{r})$$

So, I guess you really can expand a charge density in this way, and this is what Levitt means by his equation (7.3). You can expand any reasonable scalar function in this way. The only problem using this with ρ is that ρ doesn't solve something simple like the Laplace equation, so we don't know what the $f_{\ell m}(r)$ are until someone hands you a $\rho(r)$ and then you can compute $f_{\ell m}(r)$. But these functions must exist for any ρ because we how to compute them.

6. Multipole Expansion using the angle γ.

Back in section 1 we had we took $\phi = (1/4\pi\varepsilon_0)\ 1/\ |\mathbf{r} - \mathbf{r'}|$ and expanded in this way

$$\Phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^{l} P_l(\cos\gamma)$$

where γ is the angle between r and r' and $r = \max(|\mathbf{r}|, |\mathbf{r'}|)$ and $r' = \min(|\mathbf{r}|, |\mathbf{r'}|)$. The charge q is located at position r'. Let's do our same trick of having a set of charges q_i at positions $\mathbf{r_i'}$ and make sure that $\mathbf{r}$ is outside all these charges. Then we have: [I will ignore the $4\pi\varepsilon_0$ from now on]

$$\phi(r) = \Sigma_i\ q_i\ (1/r)^{\ell+1}\ \Sigma_\ell\ (r'_i)^\ell\ P_\ell(\cos\gamma_i) = \Sigma_\ell\ (1/r)^{\ell+1}\ [\ \Sigma_i\ q_i\ (r'_i)^\ell\ P_\ell(\cos\gamma_i)\ ]$$

Now you could write $q_i = q_i(\gamma_i, r_i)$ meaning that the two variables γ_i and r_i determine where this charge is. And we could then write that as a continuous charge density $\rho(\gamma,r)$. Then the bracketed quantity in the above becomes $\int d^3r\ \rho(\gamma,r)\ (r\ )^\ell\ P_\ell(\cos\gamma)$. Write $d_3r = 2\pi\ r^2\ dr\ d(\cos\gamma)$ where we pre-integrate over the azimuthal coordinate. Ie, we are using spherical coordinates where θ is γ. So we have

$$[\ \Sigma_i\ q_i\ (r'_i)^\ell\ P_\ell(\cos\gamma_i)\ ] = 2\pi \int r^2 dr \int d(\cos\gamma)\ \rho(\gamma,r)\ (r\ )^\ell\ P_\ell(\cos\gamma) = \int dV\ \rho(r)\ (r\ )^\ell\ P_\ell(\cos\gamma)$$

At this point we can replace γ with the more usual name θ and have

$$M_\ell = 2\pi \int r^{2+\ell}\ dr \int d(\cos\theta)\ \rho(\mathbf{r})\ P_\ell(\cos\theta)$$

Since $P_0 = 1$ and $P_1 = x$ and $P_2 = (3x^2 - 1)/2$ [see MM page 98] we have:

$M_0 = \int dV\, \rho(\mathbf{r}) =$ total charge

$M_1 = \int dV\, \rho(\mathbf{r})\, r \cos\theta = \int dV\, \rho(\mathbf{r})\, z$

$M_2 = 1/2 \int dV\, \rho(\mathbf{r})\, r^2 (3\cos^2(\theta) - 1) = 1/2 \int dV\, \rho(\mathbf{r})\, (3z^2 - r^2) = 1/2\, Q_0$

Convention seems to define Q_0 without the factor of 1.2, so [this is really Q_{20}]

$Q_0 = \int dV\, \rho(\mathbf{r})\, (3z^2 - r^2)$ $\qquad$ $M_2 = Q_0/2$

This thing Q_0 is also called a quadrupole moment, but is different from the two things we found earlier which we also called by the same name: $Q_{\ell m}$ and $Q_{\alpha\beta}$. Notice that if $\rho(r)$ is radially symmetric, you get the integral $\int dx\, (3x^2-1)$ on [-1,1] which is exactly 3*2/3 - 2 = 0, so no quadrupole moment. A nucleus with a quad moment has a flattened charge shape of some sort.

7. Multipole expansion of the energy of two overlapping charge densities.

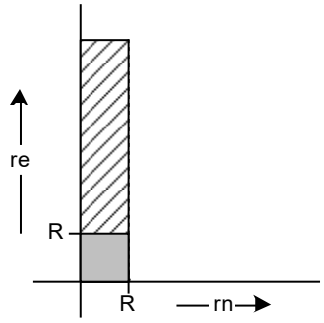
This is taken from a PDF I now have (and printed), written by Jerschow, chemistry NYU late 2004. The energy of interest is this: [this appears in Jackson on page 21 as equation (1.52), but Jackson has an extra 1/2 out front to correct for overcounting. That is because he is computing the self-energy of a single charge distribution. Since we are dealing with two separate distributions, there is no factor 1/2 since there is no overcounting.]

$$E = \frac{1}{4\pi\epsilon_0} \iint dr_e dr_n \frac{\rho_e(r_e)\rho_n(r_n)}{|\mathbf{r}_e - \mathbf{r}_n|}$$

where we are thinking explicitly that e = electron charge density and n = nuclear charge density.
We expand the denominator in the usual manner,

$$\frac{1}{|\mathbf{r}_e - \mathbf{r}_n|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-1}^{l} \frac{1}{2l+1} \frac{r_{\text{small}}^l}{r_{\text{large}}^{l+1}} Y_l^{m*}(\theta_n, \phi_n) Y_l^m(\theta_e, \phi_e)$$

Even though it is not true inside the nucleus itself, we still just assume that $r_{small} = r_n$ and $r_{large} = r_e$. That is, we assume this at all points in space, even though not true inside the tiny nucleus. If we think about the volume of the double integration in terms of the radial magnitudes we can draw this picture:



Most of the integral contribution comes from a thin vertical strip as shown, because we think the charge density of the nucleus stops abruptly at some radius R, due to the nuclear force. By making the assumption just stated, we are going to make an error in the grey square area, but this is so tiny compared to the infinitely high cross hatched region, that we think this error will be negligible.

Once we insert the 1/R expansion as shown (which really now has r_n^{ℓ} / $r_e^{\ell+1}$ inside), because each term in the sum factorizes between the two coordinate systems, we can move say the dr_e integral all the way to the right where only the factors $1/ r_e^{\ell+1}$ and $Y_{\ell m}(\theta_e,\phi_e)$ lie to its right. Then the dr_n integral picks up the other factors. We choose where to put our overall constants and then get this result:

$$E = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} A_l^m B_l^{m*}$$

where

$$A_l^m = \sqrt{\frac{4\pi}{2l+1}} \int \mathrm{d}r_\mathrm{n} \rho_\mathrm{n}(r_\mathrm{n}) r_\mathrm{n}^l Y_l^m(\theta_\mathrm{n}, \phi_\mathrm{n})$$

and

$$B_l^m = \frac{1}{4\pi\epsilon_0} \sqrt{\frac{4\pi}{2l+1}} \int \mathrm{d}r_\mathrm{e} \rho_\mathrm{e}(r_\mathrm{e}) r_\mathrm{e}^{-l-1} Y_l^m(\theta_\mathrm{e}, \phi_\mathrm{e})$$

So this then is a multipole expansion of the electrostatic energy stored in two overlapping charge distributions where the n one is very small. the numbers $A_{\ell m}$ exactly our $Q_{\ell m}$ shown in Section 1 above, which we would call the spherical moments of the nuclear charge distribution. The $B_{\ell m}$ are something else, not clear what you would call it, some kind of moments of the electron charge distribution.

The objects $Y_{\ell m}(\theta,\phi)$ are simply functions, and the $A_{\ell m}$ and $B_{\ell m}$ are complex numbers.

8. Angular Momentum Algebra

Right now I don't have a perfect source with all this stuff, so I will piece things together from the web

$$\left[J_i, J_j\right] = i\hbar\varepsilon_{ijk}J_k \qquad J_\pm = J_x \pm iJ_y \qquad \left[J_z, J_\pm\right] = \pm\hbar J_\pm$$

$$J_{\mp}J_{\pm} = \left(J_x \mp iJ_y\right)\left(J_x \pm iJ_y\right) = J_x^2 + J_y^2 \pm i\left[J_x, J_y\right]$$
$$= J^2 - J_z^2 \mp \hbar J_z$$

$$\vec{J}^2\left|j,m\right\rangle = j(j+1)\hbar^2\left|j,m\right\rangle$$
$$J_z\left|j,m\right\rangle = m\hbar\left|j,m\right\rangle$$
$$\left\langle j,m\middle|j,m\right\rangle = 1$$

$$J_+\left|j,m\right\rangle = \sqrt{j(j+1)-m(m+1)}\hbar\left|j,m+1\right\rangle$$
$$J_-\left|j,m\right\rangle = \sqrt{j(j+1)-m(m-1)}\hbar\left|j,m-1\right\rangle.$$

$$\langle\theta,\phi|l,m\rangle = Y_{l,m}(\theta,\phi)$$ spherical harmonics

$$[L^2, L_\pm] = 0$$

$$L_x = \frac{1}{2}(L_+ + L_-)$$
$$L_y = \frac{1}{2i}(L_+ - L_-)$$

Now the $|\ell m\rangle$ span a Hilbert space whose states diagonalize L^2 and L_z . When we close with $\langle\theta\phi|$ we obtain these vectors expressed in a coordinate representation, and those are the spherical harmonic functions. We can find representations of the various angular momentum operators in this space, such as

$$L^2 = -\frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{\hbar^2}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$L_x = -\mathrm{i}\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right), \tag{530}$$

$$L_y = -\mathrm{i}\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right), \tag{531}$$

$$L_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi}, \tag{532}$$

$$L_\pm = \hbar\,\mathrm{e}^{\pm\mathrm{i}\phi}\left(\pm\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}\right).$$

Consider these results from above:

$L^+ | \ell m\rangle = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ |\ell\ m+1\rangle$
$L^- | \ell m\rangle = [\ \ell(\ell+1) - m(m-1)\ ]^{1/2}\ |\ell\ m-1\rangle$

If we close on the left with $|\theta\phi\rangle$ we get

$\langle\theta\phi | L^+ | \ell m\rangle = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ \langle\theta\phi\ |\ell\ m+1\rangle$
$\langle\theta\phi | L^- | \ell m\rangle = [\ \ell(\ell+1) - m(m-1)\ ]^{1/2}\ \langle\theta\phi\ |\ell\ m-1\rangle$

For the top line we can do this: note that $\langle\theta\phi\ |\ell m\rangle\ L^+_{op}\ (1) = 0$

$<\theta\phi \mid L^{+} \mid \ell m> = L^{+}_{op} <\theta\phi \mid \ell m> = [\ L^{+}_{op},\ <\theta\phi \mid \ell m>]$

This equation exists in the space of complex numbers, not differential operators or abstract operators. In this space we can therefore write [here "op" means the angle differential operators shown above]

$[\ L^{+}_{op},\ <\theta\phi \mid \ell m>\ ] = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ <\theta\phi \mid \ell\ m+1>$
$[\ L\text{-}^{+}_{op},\ <\theta\phi \mid \ell m>\ ] = [\ \ell(\ell+1) - m(m-1)\ ]^{1/2}\ <\theta\phi \mid \ell\ m-1>$
$[\ L_3{}^{op},\ <\theta\phi \mid \ell m>\ ] = m\ <\theta\phi \mid \ell m>$

But this tells us that:

$[\ L^{+}_{op},\ Y_{\ell m}(\theta,\phi)\ ] = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ Y_{\ell m+1}(\theta,\phi)$
$[\ L^{-}_{op},\ Y_{\ell m}(\theta,\phi)\ ] = [\ \ell(\ell+1) - m(m-1)\ ]^{1/2}\ Y_{\ell m-1}(\theta,\phi)$
$[\ L^{3}_{op},\ Y_{\ell m}(\theta,\phi)\ ] = m\ Y_{\ell m}(\theta,\phi)$

Now we make a definition: Suppose you have a set of *operators* $A_{\ell m}$ that obey the above equations written in operator space:

$[\ L^{+},\ A_{\ell m}\ ] = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ A_{\ell m+1}$
$[\ L^{-},\ A_{\ell m}\ ] = [\ \ell(\ell+1) - m(m-1)\ ]^{1/2}\ A_{\ell m-1}$
$[\ L^{3},\ A_{\ell m}\ ] = m\ A_{\ell m}$

Any operator in the abstract Hilbert space spanned by the $\mid \ell m>$ that obeys there rules is defined to be a **spherical tensor operator**.

Here is a little extra I would like to add to this section. Consider two vectors a and b. We define the + and - components of these vectors as we did for L/J above

$$L_x = \frac{1}{2}(L_+ + L_-)$$
$$L_y = \frac{1}{2i}(L_+ - L_-)$$

and $$J_{\pm} = J_x \pm iJ_y$$

and you then find that

$a \bullet b = a_z b_z + (1/2)\ [\ a_- b_+ + a_+ b_-]$

9. Derive formula (17.11) of Levitt.

We start with our result of Section 7 above,

$$E = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} A_l^m B_l^{m*}$$

where

$$A_l^m = \sqrt{\frac{4\pi}{2l+1}} \int \mathrm{d}r_\mathrm{n} \rho_\mathrm{n}(r_\mathrm{n}) r_\mathrm{n}^l Y_l^m(\theta_\mathrm{n}, \phi_\mathrm{n})$$

and

$$B_l^m = \frac{1}{4\pi\epsilon_0} \sqrt{\frac{4\pi}{2l+1}} \int \mathrm{d}r_\mathrm{e} \rho_\mathrm{e}(r_\mathrm{e}) r_\mathrm{e}^{-l-1} Y_l^m(\theta_\mathrm{e}, \phi_\mathrm{e})$$

As an aside, notice that $Y_{\ell m}(\theta,\phi)^* = (-1)^m Y_{\ell m}(\theta,\phi)$ so that: $B_{\ell m}{}^* = (-1)^m B_{\ell,-m}$

where E is the electrostatic energy stored in the nuclear + electronic charge densities. The above is a classical result only, the A and B are just numbers.

Now comes the "transition from classical to quantum mechanics". We want to take the above energy formula and interpret it as a Hamiltonian operator in the Hilbert space spanned by the nuclear spin vectors we write as | I,M>. These are good quantum numbers for the nucleus, they do form a Hilbert space, and it seems a reasonable assumption that we have a correct Hamiltonian by so doing. We can interpret the charge distribution scalar function as this expectation value: $\langle\psi \mid \rho(\mathbf{r}) \mid \psi\rangle$ = where **r** is now an operator in our Hilbert space and $|\psi\rangle = |\psi_{IM}\rangle$ is our nuclear state (probably our ground state). The angles in the spherical harmonic functions can also be imagined as operators, and the integration is a summation of operators, and the sums $A_{\ell m}$ and $B_{\ell m}$ are themselves now operators. We replace the * with † on the B operator in our new Hamiltonian which is now this:

$$H = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{l,m} B_{l,m}^\dagger$$

I suppose you could show that this H is in fact a Hermitian operator, but I don't want to get sidetracked on that right now. Because $Y_{\ell m}(\theta,\phi)$ satisfies the usual commutation relations which define a spherical tensor operator (see previous section), we know that the summations which form $A_{\ell m}$ and $B_{\ell m}$ are also spherical tensor operators!

Now let's look specifically at the quadrupole operator A_{2m} . First, we go look up this fact:

$$Y_2^{-2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\, e^{-2i\varphi}$$
$$Y_2^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\theta\,\cos\theta\, e^{-i\varphi}$$
$$Y_2^{0}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\,(3\cos^2\theta - 1)$$
$$Y_2^{1}(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\theta\,\cos\theta\, e^{i\varphi}$$

$$Y_2^2(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\, e^{2i\varphi}$$

and we keep in mind these facts

x = r sinθ cosϕ
y = r sinθ sinϕ
z = r cosθ

We then have:

$A_{\ell m}$ = sqrt(4π/5) * $\int$ dr ρ(r) r^2 $Y_{2,m}(\theta,\phi)$

Notice that we then have $r^2 \sin^2\theta\, e^{2i\phi}$ = (r sinθ [cosϕ + isinϕ])^2 = (x + iy)^2 . Putting this in, and replacing the integral (for some reason) by a discrete charge sum, we find that

$$A_{2,0} = \frac{1}{2}\sum_i e_i(3z_i^2 - r_i^2)$$

$$A_{2,\pm1} = \mp\sqrt{\frac{3}{2}}\sum_i e_i z_i(x_i \pm \mathrm{i}y_i)$$

$$A_{2,\pm2} = \sqrt{\frac{3}{8}}\sum_i e_i(x_i \pm \mathrm{i}y_i)^2$$

Again, the coordinates like x_i for the i^{th} nucleon are operators in our Hilbert space. We have just written out explicitly the 5 ℓ=2 spherical operator components.

The authors of our PDF paper now make this definition:

eQ = 2 < I,M=I | A_{20} | I, M=I > = <II | Σ$_i$ e_i (3 z_i^2 - r_i^2) | II>

We are now thinking $|\ell,m> \rightarrow |$ I,M> where I is the nuclear spin.

Now comes the Wigner-Eckart part of the derivation. We know from the WE theorem that ALL the matrix elements of a tensor operator can be obtained if you know ANY ONE of the matrix elements. The WE theorem says this: [see http://electron6.phys.utk.edu/qm2/modules/m4/wigner.htm]

$$<\alpha',j',m'|T^k_q|\alpha,j,m> = <j,k;m,q|j,k,j',m'>\frac{<\alpha',j'\|T^k\|\alpha,j>}{\sqrt{2j'+1}} = C^{j'}_{mq}\frac{<\alpha',j'\|T^k\|\alpha,j>}{\sqrt{2j'+1}}$$

$$= (-1)^{j+k-m'}\begin{pmatrix} j & k & j' \\ m & q & -m' \end{pmatrix} <\alpha',j'\|T^k\|\alpha,j> = (-1)^{j'-m'}\begin{pmatrix} j' & k & j \\ -m & q & m \end{pmatrix} <\alpha',j'\|T^k\|\alpha,j> .$$

where it is too bad the paste looks bad, but we can read it I think. The theorem is interested in the matrix element of a tensor operator T, $<\alpha',j',m' | T_{kq} | \alpha,j,m>$, where we previously have written $T_{\ell m}$. Here, the α indicates quantum numbers *other than* angular momentum. The object $<\alpha',j' || T_k || \alpha,j>$ is called the reduced matrix element, and it is just some function of α', j', k, α, j. The point is that all (2j+1)*(2k+1)*(2j'+1) matrix elements specified by $<\alpha',j',m' | T_{kq} | \alpha,j,m>$ are all Clebsch-Gordon coefficients times this reduced matrix element number, whatever it is. Our author has written the RHS of the WE theorem in 4 different ways because he is writing the C-G coefficients in 4 different ways -- the reduced matrix element is the same in all cases. The second way with $C^{j'}_{mq}$ looks wrong to me because there are not enough labels on the C symbol, but that is just the way this symbol is define. Consider:

$$|j_1,j_2;j,m>=\sum_{m_1}\sum_{m_2} C^{j}_{m_1m_2}|j_1,j_2;m_1,m_2>.$$

$$|j_1,j_2;m_1,m_2>=\sum_{j} C^{j}_{m_1m_2}|j_1,j_2;j,m>$$

.

The first line tells you a j-j coupling state as a sum over L-S states, so to speak. This is the details of what we mean by saying $j = j_1 \otimes j_2$. The second line shows the reverse direction where $m = m_1 + m_2$. Here are some properties of the CG coefficients written as Wigner 3-j symbols:

Properties of the Wigner 3-j symbols:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \quad \text{unless} \quad m_1 + m_2 + m_3 = 0.$$

We can permute the columns of the 3-j symbol. An even permutation does not alter its value. An odd permutation multiplies the initial value by $(-1)^{j_1+j_2+j_3}$. Moreover,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}.$$

This implies

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}$$

or

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = 0 \quad \text{unless} \quad j_1 + j_2 + j_3 = even.$$

I could probably find a better website than http://electron6.phys.utk.edu/qm2/modules/m4/wigner.htm and get cleaner copies of these things, but it is at least readable.

Now we are going to apply this theorem to our situation (these pastes are stolen from

http://books.google.com/books?id=0BSOg0oHhZ0C&pg=PA78&lpg=PA78&dq=quadrupole+moment+quantum&source=web&ots=VRbCjb5ZRn&sig=oxAyXWcB_gFxc3EAbUe6IXFJNDk#PPA78,M1

$$Q = (j\ j|Q_0^{(2)}|j\ j) = (j||\mathbf{Q}^{(2)}||j)\begin{pmatrix} j & j & 2 \\ -j & j & 0 \end{pmatrix}$$

Let's see if we agree with this. The quoted theorem has k = 2 in the middle, but we want to permute the columns by one column to get the above. That picks up a phase factor $(-1)^{j+j+2} = (-1)^{2j}$ and remember that j can be half-integral. The phase appearing in our theorem above is $(-1)^{-j+2-j} = (-1)^{2j}$ and this cancels away with our permuting factor, so the above is exactly correct.

So we have embodied our reduced matrix element into the number "Q". But now, we say this:

$$\begin{aligned}(j\ m|Q_0^{(2)}|j\ m) &= (j||\mathbf{Q}^{(2)}||j)\begin{pmatrix} j & j & 2 \\ -m & m & 0 \end{pmatrix} \\ &= (-1)^{j-m}Q\begin{pmatrix} j & j & 2 \\ -m & m & 0 \end{pmatrix}\Big/\begin{pmatrix} j & j & 2 \\ -j & j & 0 \end{pmatrix} \\ &= Q\cdot\frac{3m^2 - j(j+1)}{j(2j-1)}\end{aligned}$$

I have not verified these steps, but I know that the resulting CG coefficient is some function of m and j, so the result seems quite reasonable:

Now comes the very tricky step. Suppose we make this operator *replacement*:

$$Q^{(2)}_0 \ \rightarrow\ [Q/j(2j-1)]\ [\ 3\ J_3^2 - J^2\ ]$$

where J_3 and J^2 are our usual spin operators. If we took the above matrix element of either the original operator *or* its replacement, we get the same expectation value!! That is,

$$< j\ m\ |\ Q^{(2)}_0\ |\ jm\ > \ =\ [Q/j(2j-1)] < j\ m\ |\ [\ 3\ J_3^2 - J^2\ ]\ |\ jm >$$

Thus, if all we are going to do is evaluate these diagonal matrix elements, then the two operators are equally useful. We are not saying this:

$$Q^{(2)}_0 \ =\ [Q/j(2j-1)]\ [\ 3\ J_3^2 - J^2\ ] \qquad \text{// not true}$$

There is no way in the world that some coordinate-based operator $Q^{(2)}_0$ which knows nothing about nuclear spins is going to be *equal to* the spin operator shown. It is just that we may make the replacement if all we want to do is evaluate diagonal matrix elements! That is the point to understand here. The replacement is a convenient way to track those CG coefficients, that is all it really is.

So, with this meaning in mind, we make this replacement:

$$< I,M\ |\ A_{20}\ |\ I,\ M >\ \ =\ \ [Q/I(2I-1)] < I,M\ |\ [\ 3\ I_3^2 - I^2\ ]\ |\ I,\ M >$$

But our PDF authors used Q_{pdf} where $Q = eQ_{pdf}/2$, so we make this change to get back into alignment with the notation of the PDF paper:

$$< I,M \mid \mathbf{A_{20}} \mid I, M > \;=\; [eQ/2I(2I-1)] < I,M \mid [\, 3\,\mathbf{I_3}^2 - \mathbf{I}^2\,] \mid I, M >$$

If we now define a new Q tensor object as follows:

$$\mathbf{Q_{2,0}} \;=\; [eQ/2I(2I-1)]\,[\;[\,3\,\mathbf{I_3}^2 - \mathbf{I}^{\,2}\,]$$

Then we have shown that

$$< I,M \mid \mathbf{A_{20}} \mid I, M > \;= < I,M \mid \mathbf{Q_{2,0}} \mid I, M >$$

I think the PDF author has made a few errors. First, the use I(I+1) instead of I^2, and secondly they have a wrong factor of α two lines above their line (23).

Now, we know that $\mathbf{Q_{2,0}}$ is the 2,0 element of a 5-element set of tensor operators, and we should be able to compute the other elements using raising or lowering operators. So let's start with one of our results in the angular momentum section above:

$$[\; L^+,\; A_{\ell m}\,] \;= [\,\ell(\ell+1) - m(m+1)\,]^{\,1/2}\;\; A_{\ell m+1}$$

which we now modify to our current needs,

$$[\; I^+,\; \mathbf{Q_{2,0}}\,] \;= [\,2(2+1) - 0(0+1)\,]^{\,1/2}\;\; \mathbf{Q_{2,1}} \;=\; [\,6\,]^{\,1/2}\,\mathbf{Q_{2,1}}$$

But we now get

$$[\; I^+,\; \mathbf{Q_{2,0}}\,] \;= \{\, eQ/2I(2I-1)\,\}\;\; [\; I^+,\, 3\,\mathbf{I_3}^2 - \mathbf{I}^{\,2}\,] \;= \{\, eQ/4*3\}\,[\; I^+,\, 3\mathbf{I_3}^2\,] \;= \{\, eQ/4*3\}\; 3\,[\; I^+,\, \mathbf{I_3}^2\,]$$

We do know from our ang mom section above that $[\, I_3,\, I^+\,] = \hbar\, I_+$ so $[\; I^+,\, \mathbf{I_3}\,] = -I^+$ if we ignore the $\hbar$ units, setting it to 1. We know that $[a,b^2] = [a,b]\,b + b\,[a,b]$ so we get

$$[\; I^+,\, \mathbf{I_3}^2\,] \;= [\; I^+,\, \mathbf{I_3}\,]\; I_3 + I_3\;\; [\; I^+,\, \mathbf{I_3}\,] \;=\;\; -I^+\;\; I_3 + I_3\,(\,-I^+\,) \;= -\,[\; I^+ I_3 + I_3\, I^+\,]$$

So we end up with:

$$\mathbf{Q_{2,1}} = [\,6\,]^{\,-\,1/2}\;\; [\;\, I^+,\;\, \mathbf{Q_{2,0}}\,] \;=\; [\,6\,]^{\,-\,1/2}\;\; \{\, eQ/4*3\}\; 3\,(-1)\,[\; I^+ I_3 + I_3\, I^+\,]$$

$$= \;-\,[\,1/6\,]^{\,1/2}\;(\alpha/2)\;3\;\;[\; I^+ I_3 + I_3\, I^+\,] \;= -\,[1/6*4\,]^{\,-\,1/2}\;\; 3\,\alpha\;\; [\; I^+ I_3 + I_3\, I^+\,]$$

$$= -\,[\,9/6*4\,]^{\,1/2}\alpha\;\; [\; I^+ I_3 + I_3\, I^+\,] \;=\; -\,\alpha\,[3/8]^{1/2}\;\; [\; I^+ I_3 + I_3\, I^+\,]$$

and this agrees with our PDF equation (20), exactly. If we were to repeat the calculation with the - sign, the square root 6 does not change, but we have $[\; I^-,\, \mathbf{I_3}\,] = I^-$ so we get an overall sign change and this gives us the second of equation (20).

Now let's do one more:

$[\ L^+,\ A_{\ell m}\ ] = [\ \ell(\ell+1) - m(m+1)\ ]^{1/2}\ A_{\ell m+1}$

$[\ I^+,\ \mathbf{Q_{2,1}}\ ] = [\ 2(2+1) - 1(1+1)\ ]^{1/2}\ \mathbf{Q_{2,1}} = [\ 4\ ]^{1/2}\ \mathbf{Q_{2,2}} = 2\ \mathbf{Q_{2,2}}$

Then we have to compute // remember that

$[\ I^+,\ \mathbf{Q_{2,1}}\ ] = -\alpha\ [3/8]^{1/2}\ [\ I^+,\ I^+ I_3 + I_3 I^+\ ]$

and we remember that

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

So $[\ I^+,\ I^+ I_3] = I^+\ [\ I^+, I_3] = -I^{+\,2}$. And also $[\ I^+,\ I_3 I^+] = [\ I^+,\ I_3]\ I^+ = -I^{+\,2}$. So we get

$[\ I^+,\ \mathbf{Q_{2,1}}\ ] = -\alpha\ [3/8]^{1/2}\ [\ I^+,\ I^+ I_3 + I_3 I^+\ ] = -\alpha\ [3/8]^{1/2}\ (-1)\ 2\ I^{+\,2}$

and then

$\mathbf{Q_{2,2}} = 1/2\ [\ I^+,\ \mathbf{Q_{2,1}}\ ] = \alpha\ [3/8]^{1/2}\ I^{+\,2}$

which then agrees with our PDF paper equation (21).

The net result is that we know all 5 members of our tensor operator $Q_{2,m}$ as follows:

$$Q_{2,0} = \alpha\frac{1}{2}(3I_z^2 - I(I+1)) \qquad (19)$$

$$Q_{2,\pm 1} = \mp\alpha\sqrt{\frac{3}{8}}(I_z I_\pm + I_\pm I_z) \qquad (20)$$

$$Q_{2,\pm 2} = \alpha\sqrt{\frac{3}{8}}I_\pm^2, \qquad (21)$$

where we have to replace I(I+1) in (19) with I^2 (they just have an error there). So this was a good exercise of computing all members of a tensor operator if you are just given one member, using the raising and lowering operators in the commutator relations which define a spherical tensor operator in the first place.

We are pondering right now the quadrupole term of our Hamiltonian

$$H = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{l,m}B_{l,m}^{\dagger}$$

so we are interested in:

$H_{quadrupole} = \Sigma_m\ A_{2m}\ B^{\dagger}_{2m}\ \sim\ \Sigma_m\ Q_{2m}\ B^{\dagger}_{2m} = \Sigma_m\ Q_{2m}\ (-1)^m\ B_{\ell,-m}$ // see note in Sec 6

where we have done the replacement of the A operator with the Q operator as outlined above. What are we going to do with our B operators?

$$B_l^m = \frac{1}{4\pi\epsilon_0}\sqrt{\frac{4\pi}{2l+1}}\int \mathrm{d}r_\mathrm{e}\rho_\mathrm{e}(r_\mathrm{e})r_\mathrm{e}^{-l-1}Y_l^m(\theta_\mathrm{e},\phi_\mathrm{e})$$

Let's look at B_{20} which we can write out as

$B_{20} = (1/4\pi\varepsilon_0)\ \mathrm{sqrt}(4\pi/5)\ \int d^3r\ \rho(r)/r^3\ Y_{20}(\theta,\phi)$

$= (1/4\pi\varepsilon_0)\ \mathrm{sqrt}(4\pi/5)\ \int d^3r\ \rho(r)/r^3\ (1/4)\ \mathrm{sqrt}(5/\pi)[\ 3\cos^2\theta - 1]$

$= (1/4\pi\varepsilon_0)\ 2/4\ \int d^3r\ \rho(r)/r^3\ [\ 3\cos^2\theta - 1]$

$= (1/4\pi\varepsilon_0)\ (1/2)\ \int d^3r\ \rho(r)/r^5\ [\ 3z^2 - r^2] = (1/4\pi\varepsilon_0)\ (1/2)\ \Sigma_i\ (-e)/r_i^5\ [\ 3z_i^2 - r_i^2\ ]$

where at the end we sum over all electrons that make up the electron $\rho(r)$, and each has the same charge of -e. Thus we have arrived at PDF equation (25).

At this point, let's go back and look at our Taylor series expansion for the energy of a charge distribution sitting in a potential, specifically [again, no factor of 1/2 because this is not a self-energy]

$W = \int d^3\mathbf{r}\ \rho_e(\mathbf{r})\phi_n(\mathbf{r})$

$\phi(\mathbf{r}) = \{\ \phi(0) + r_\alpha\partial_\alpha\phi + (1/6)\ [\ 3r_\alpha r_\beta - \delta_{\alpha\beta}r^2\ ]\ \partial_\alpha\partial_\beta\phi\ \}$ + octupole and higher terms

$W = [\ \phi(0)\ \int d^3\mathbf{r}\ \rho(\mathbf{r}) + (\partial_\alpha\phi)\ \int d^3\mathbf{r}\ \rho(\mathbf{r})\ r_\alpha + (1/6)\ (\partial_\alpha\partial_\beta\phi)\ \int d^3\mathbf{r}\ \rho(\mathbf{r})\ [\ 3r_\alpha r_\beta - \delta_{\alpha\beta}r^2\ ] + ...$

And recall our PDF paper's first equation

$$E = \frac{1}{4\pi\epsilon_0}\iint \mathrm{d}r_\mathrm{e}\mathrm{d}r_\mathrm{n}\frac{\rho_\mathrm{e}(r_\mathrm{e})\rho_\mathrm{n}(r_\mathrm{n})}{|\mathbf{r}_\mathrm{e}-\mathbf{r}_\mathrm{n}|} = \sum_{l=0}^{\infty}\sum_{m=-1}^{l}A_l^m B_l^{m*}$$

$$E = \frac{1}{4\pi\epsilon_0}\iint \mathrm{d}r_\mathrm{e}\mathrm{d}r_\mathrm{n}\frac{\rho_\mathrm{e}(r_\mathrm{e})\rho_\mathrm{n}(r_\mathrm{n})}{|\mathbf{r}_\mathrm{e}-\mathbf{r}_\mathrm{n}|}$$

So if we ignore the $(1/4\pi\varepsilon_0)$, we can think of E and W as being the same thing, where the r in the first integral is r_e and ρ is for the electrons ρ_e (r_e) and then $\phi(r_e) = \rho_n(r_n)/R$ = the potential that the electron sees at position r_e due to the nuclear charge distribution. In our Taylor expansion, we have a quadrupole term which is in Cartesian coordinates. I did not know how to do a Taylor expansion in spherical coordinates!

But let's look at just one of the terms in the "quadrupole" part of W shown above -- the term where $\alpha = \beta = 3$. That term is

$$W_{\text{quadrupole piece}} = (1/6)\,(\partial_z\partial_z\phi) \int d^3\mathbf{r}\,\rho(\mathbf{r})\,[\,3z^2 - r^2\,] =$$

We are tempted to associate this one term with the following term in our Hamiltonian sum:

$H_{\text{quadrupole}} = \Sigma_m\ A_{2m}\,B^{\dagger}_{2m}$ but only consider the $A_{20}B^{\dagger}_{20}$ term

Recall from the PDF paper also the fact that

$$A_{2,0} = \frac{1}{2}\sum_i e_i(3z_i^2 - r_i^2) \qquad (15)$$

Thus we can write

$$W_{\text{quadrupole piece}} = (1/6)\,(\partial_z\partial_z\phi)\ 2 * \{\,(1/2) \int d^3\mathbf{r}\,\rho(\mathbf{r})\,[\,3z^2 - r^2\,]\,\} = (1/3)\,(\partial_z\partial_z\phi)\ A_{20}$$

We would be tempted now to make this identification

$B^{\dagger}_{20} = (1/3)\,(\partial_z\partial_z\phi)$ // but something is wrong here ....

and this is equation (26) except they have 1/2 and I have 1/3 ! I suspect by rotational symmetry you should triple the result since the ∂_{xx} and ∂_{yy} terms must be the same. So then I am missing 1/2.

Let's now go after this same type of result in a **different way that is more direct**. Recall that

$$B_{20} = (1/4\pi\varepsilon_0)\,(1/2)\,\Sigma_i\,(-e)/r_i^5\ [\,3z_i^2 - r_i^2\,]$$

We could write the electric potential due all these electrons (marked i) as follows:

$\phi(r) = (1/4\pi\varepsilon_0)(-e)\,\Sigma_i\,(1/|r-r_i|)$ // where r is the viewing point

As calculated in Section 2 above, we know that

$$\partial_\beta\,(\partial_\alpha\phi)^{|r=0} = (1/4\pi\varepsilon_0)(-e)\,\Sigma_i(1/R^5)\ [\ 3R_\alpha R_\beta - \delta_{\alpha\beta}R^2]$$ // imagine each R as r_i

In particular, this says

$\partial_z(\partial_z\phi)^{|r=0} = (1/4\pi\varepsilon_0)(-e)\,\Sigma_i(1/r_i^5)\,[\,3\,z_i^2 - r_i^2\,] = 2\,B_{20}$

from which we conclude that

$B_{20} = (1/2)\,\partial_{zz}V(\mathbf{r})^{|r=0}$ // now this agrees with (26)

Let's now try to produce the $B_{2,1}$ object:

$$B_{l,m} = -e\,\frac{1}{4\pi\epsilon_0}\sqrt{\frac{4\pi}{2l+1}}\sum_{i=1}^{N} r_i^{-l-1}Y_l^m(\theta_i,\phi_i) \qquad Y_2^1(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\theta\,\cos\theta\,e^{i\varphi}$$

So we get

$B_{2,1} = (-e)\,(1/4\pi\varepsilon_o)\,\mathrm{sqrt}(4\pi/5)\,\Sigma_i\,(1/r_i)^3\,(-1/2)\,\mathrm{sqrt}(15/2\pi)\,\sin\theta_i\cos\theta_i\,[\,\cos\phi_i + i\sin\phi_i]$

Now make this replacement

$(1/r_i)^3\sin\theta_i\cos\theta_i\,[\,\cos\phi_i + i\sin\phi_i] = (1/r_i)^5\,z_i\,[\,x_i + i\,y_i]$

So then have

$B_{2,1} = (-e)\,(-1/2)\,(1/4\pi\varepsilon_o)\,\mathrm{sqrt}(6)\,\Sigma_i\,1/r_i)^5\,z_i\,[\,x_i + i\,y_i]$

Now recall from above that

$\partial_\beta(\partial_\alpha\phi)^{|r=0} = (1/4\pi\varepsilon_0)(-e)\,\Sigma_i(1/R^5)\,[\,3R_\alpha R_\beta - \delta_{\alpha\beta}R^2]$ // imagine each R as r_i

In particular, consider

$(\partial_x\partial_z\phi)^{|r=0} = (1/4\pi\varepsilon_0)(-e)\,\Sigma_i(1/R^5)\,[\,3x_iz_i\,] = \partial_{xz}\phi$

Then of course $\partial_{yz}\phi$ = same thing with $[\,3y_iz_i\,]$ so we can then say

$B_{2,1} = (-1/2)\,\mathrm{sqrt}(6)\,\Sigma_i\,(1/r_i)^5\,z_i\,[\,x_i + i\,y_i] = (-1/2)\,\mathrm{sqrt}(6)\,[\,\partial_{xz}\phi/3 + i\,\partial_{yz}\phi/3\,]$

$= -\,\mathrm{sqrt}(1/6)\,[\,[\,\partial_{xz}\phi + i\,\partial_{yz}\phi\,]$

and this does in fact agree with (27). I will just accept (28) as being true, I could show it without much trouble.

Now let's see if we have finally arrived at Levitt's (17.11). Here is our quadrupole Hamiltonian valid if we take an expectation value:

$H_{quadrupole} = \Sigma_m\,(-1)^mQ_{2,m}\,B_{2,-m}$ = where (19) below should be I^2 not I(I+1)

$$Q_{2,0} = \alpha \frac{1}{2}(3I_z^2 - I(I+1)) \qquad (19)$$

$$Q_{2,\pm 1} = \mp \alpha \sqrt{\frac{3}{8}}(I_z I_\pm + I_\pm I_z) \qquad (20)$$

$$Q_{2,\pm 2} = \alpha \sqrt{\frac{3}{8}} I_\pm^2, \qquad (21)$$

$$B_{2,0} = \frac{1}{2}\left(\frac{\partial^2 V}{\partial z^2}\right)_{r=0} = \frac{1}{2} V_{zz}.$$

$$B_{2,\pm 1} = \mp \frac{1}{\sqrt{6}}(V_{xz} \pm i V_{yz})$$

$$B_{2,\pm 2} = \frac{1}{2\sqrt{6}}(V_{xx} - V_{yy} \pm 2i V_{xy}).$$

where $\alpha = eQ/I(2I-1)$. So I will now assemble all these terms as follows:

$H_{quadrupole} = eQ/I(2I-1) * \{ (1/2)(3I_z^2 - I^2)(1/2)V_{zz}$ 2,0 for Q

$+ \text{ sqrt}(3/8)(I_zI_+ + I_+I_z)\ 1/\text{sqrt}(6)\ (V_{xz} - i\,V_{yz})$ 2,1

$+ \text{ sqrt}(3/8)(I_zI_- + I_-I_z)\ 1/\text{sqrt}(6)\ (V_{xz} + i\,V_{yz})$ 2,-1

$+ \text{sqrt}(3/8)\ I_+^2\ (1/2\ \text{sqrt}(6))\ (V_{xx} - V_{yy} - 2iV_{xy})$ 2,2

$+ \text{sqrt}(3/8)\ I_-^2\ (1/2\ \text{sqrt}(6))\ (V_{xx} - V_{yy} + 2iV_{xy})\ \}$ 2,2

Let's now divide outside by 4, multiple inside by 4. We then get

$\text{sqrt}(3/8) * 1/\text{sqrt}(6) * 4 = \text{sqrt}(16*3/8*6) = \text{sqrt}(48/48) = 1$

I then get this result

$H_{quadrupole} = eQ/4I(2I-1) * \{ (3I_z^2 - I^2)\ V_{zz}$ 2,0

$+ (I_zI_+ + I_+I_z)\ (V_{xz} - i\,V_{yz})$ 2,1

$+ (I_zI_- + I_-I_z)\ (V_{xz} + i\,V_{yz})$ 2,-1

$+ I_+^2\ (V_{xx} - V_{yy} - 2iV_{xy})/2$ 2,2

$$+ \; I_-^2 \; (V_{xx} - V_{yy} + 2iV_{xy})/2 \qquad \} \qquad 2,2$$

and I also have this definition of eQ:

$$eQ \; = 2 < I,M=I \; | \; A_{20} \, | \, I, M=I > \; = \; <II \, | \, \Sigma_i \, e_i \, (\, 3 \, z_i^2 - r_i^2) \, | \, II>$$

What are the **dimensions** of things here? We seem to have dim(H) = charge X^2 potential/X^2 which is then charge * potential V which is correct. When I think of I_+ in one of the above equations, I am thinking of having done everything with $\hbar = 1$. But the real operators I_j have $\hbar$ dimensions, so if you mean the real operators, you should divide the overall result by $\hbar^2$.

This agrees exactly with Levitt page 577 equation (17.11) *except* he has an extra overall factor of 3 which I do not have. Of course he has not said exactly how he has defined is "Q". Perhaps he defines his Q as follows:

$$Q_{Levitt} = 3Q \; = \; 3 \; <II \, | \, \Sigma_i \, e_i \, (\, 3 \, z_i^2 - r_i^2) \, | \, II>$$

If so, then we would be in agreement exactly. Recall our Cartesian moment definition

$$Q_{\alpha\beta} = \; \{\Sigma_i \; q_i \; \; [\, 3 r_{i\alpha} r_{i\beta} - \delta_{\alpha\beta} r_i^2] \, \} \qquad\qquad = \text{"the quadrupole moment"}$$

We can identify our Q with Q_{zz} . Wolfram page shows that $Q_{xx} + Q_{yy} + Q_{zz} = 0$.

To clean up this confusion, I would have to go consult the Electric Multipole chapter of this book: Slichter, *Principles of MR*, 1989. Amazon shows some of this chapter, and he does get to the point of saying $1/6 \; V_{\alpha\beta} Q_{\alpha\beta}$ which agrees in scale with me (Cartesiaon). But then the excerpt stops!

I have done enough on this little problem I think. At least I now understand *why* the nuclear spins appear in a Hamiltonian which purports to be related to an electric field interaction, which you would think would have nothing whatsoever to do with nuclear spin state | I,M> .

AHA!!!!! I just looked at Levitt's **errata** and he says:

"Page 577-578. There are several errors concerning the definitions of the quadrupolar interaction. In Eq.17.11, **the right-hand side should be divided by (3*hbar)**. In the first equation on page 578, the right-hand side should be divided by (3*hbar). See also pages 201-202."

I think he is right about dividing by 3, but I think he should divide by $\hbar^2$ not by $\hbar$. I will make a note of this in case I send him some email. ******

10. Multiple Expansions of the E and B fields.

Jackson does some of this stuff, and I could do this with the tensor harmonics and all that, but here is some nice stuff from Raab and De Lang's book, a piece of which I can see on the Google book search. First, here is the expansion of an electric potential:

From (1.1) and (1.2) we obtain the multipole expansion for the electrostatic potential at P relative to the origin O

$$\Phi(\mathbf{R}) = \frac{1}{4\pi\epsilon_0}\left[\frac{q}{R} + \frac{R_i}{R^3}p_i + \frac{3R_iR_j - R^2\delta_{ij}}{2R^5}q_{ij} + \frac{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})}{2R^7}q_{ijk} + \cdots\right]. \tag{1.3}$$

Here δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ if $i \neq j$) and q, p_i, q_{ij}, $q_{ijk}, \cdots$ are electric multipole moments, relative to the origin O, defined as follows:

$$q = \int_V \rho(\mathbf{r})\, dv \tag{1.4}$$

is the zeroth moment, or electric monopole moment,

$$p_i = \int_V r_i\, \rho(\mathbf{r})\, dv \tag{1.5}$$

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is the first moment, or electric dipole moment,

$$q_{ij} = \int_V r_i r_j\, \rho(\mathbf{r})\, dv \tag{1.6}$$

is the second moment, or electric quadrupole moment,

$$q_{ijk} = \int_V r_i r_j r_k \rho(\mathbf{r})\, dv \tag{1.7}$$

This is just straightforward Cartesian Taylor expansion and it is taken through the octupole term which is always nice. The q_{ij} are not here made traceless.

Now, if you take the gradient of the potential expansion shown above, you get an expansion for the electric field which is this:

The electric field $\mathbf{E} = -\boldsymbol{\nabla}\Phi$ can be found from (1.3). Writing $E_i = -\partial\Phi/\partial R_i$ we obtain

$$E_i(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{R_i}{R^3}q + \frac{3R_iR_j - R^2\delta_{ij}}{R^5}p_j + \frac{3}{2R^7}\left\{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})\right\}q_{jk} + \cdots\right]. \quad (1.13)$$

The expansions (1.3) and (1.13) show that:

(i) Each multipole contributes separately to the potential and field at an external point.

(ii) Each multipole behaves as if it were located at the origin. This is because its contribution to the potential and field contains, apart from the moment itself, only $\mathbf{R}$, the displacement of the field point P from the origin O.

(iii) The potential and field due to each multipole depend not only on its moment and on its distance R from the field point, but in general also on its orientation relative to $\mathbf{R}$. For example, the dipole contribution in (1.3) and (1.13) contains $R_ip_i = Rp\cos\theta$, where θ is the angle between $\mathbf{R}$ and $\mathbf{p}$.

(iv) The R-dependences of the potential and field, respectively, are charge: R^{-1} and R^{-2}; dipole: R^{-2} and R^{-3}; quadrupole: R^{-3} and R^{-4}, etc.

(v) At sufficiently large distances (distance $\gg$ dimensions of charge distribution), the potential and field are dominated by the leading non-vanishing term in $1/R$, all higher-order terms being negligible. Associated with the leading non-vanishing term is a unique multipole moment independent of choice of origin (see Section 1.2). Thus, at a distant point the $SO_4^{=}$ ion behaves like a charge, HCl like a dipole, CO_2 like a quadrupole, CH_4 like an octopole, etc., even though each has higher moments. If the distance to the field point is not sufficiently large, then higher-order moments contribute as well.

(vi) The potential and field external to a neutral spherically symmetric charge distribution are zero.

We will refer to (1.4)–(1.7) and (1.9)–(1.12) as primitive moments to distinguish them from traceless moments which can be constructed for all terms beyond the electric dipole. For example, a commonly used definition of a traceless electric quadrupole moment is [1,2]

$$\Theta_{ij} = \frac{1}{2}(3q_{ij} - q_{kk}\delta_{ij}). \quad (1.14)$$

Since $\delta_{ii} = 3$ we see that $\Theta_{ii} = 0$ as desired. According to (1.14), the quadrupole contribution to the potential (1.3) can be written as

$$\frac{1}{4\pi\varepsilon_0}\frac{3R_iR_j - R^2\delta_{ij}}{2R^5}\frac{1}{3}(2\Theta_{ij} + q_{kk}\delta_{ij}) = \frac{1}{4\pi\varepsilon_0}\frac{3R_iR_j - R^2\delta_{ij}}{3R^5}\Theta_{ij}.$$

Thus the term involving the trace q_{kk} in (1.14) does not contribute to the potential, and one can use either the primitive moment q_{ij} or the traceless moment Θ_{ij}

Here I have included the comments about the traceless form quadrupole moment. This is a little different from the traceless form of the factor we had in a previous section which required the Laplace equation. Here, the extra δ term contributes nothing just because that is what equation 1.3 says!

So let's look a bit at this electric field expansion:

$$E_i(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{R_i}{R^3}q + \frac{3R_iR_j - R^2\delta_{ij}}{R^5}p_j + \frac{3}{2R^7}\left\{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})\right\}q_{jk} + \cdots\right]. \quad (1.13)$$

You see the first point charge term has **E** = q**R**/R^3 as we expect. The quadrupole term has a complicated direction! I think it says **E** = [3**R**(**R**•**p**) - R^2 **p**]/R^5 and the next term is there as well. [Jackson p 101 !]

Now, of course we want to know next about the magnetic field situation! The Google thing skips some pages here, but we are allowed to see the results as follows:

With regard to the other terms in (1.40), it is not convenient to define the magnetic multipoles in terms of the integrals in this expansion. These are first transformed in a manner that facilitates comparison with electrostatics and with quantum-mechanical expressions (Chapter 2): it is shown in Appendix A that for magnetostatics (i)

$$R_j \int_V J_i r_j \, dv = (\mathbf{m} \times \mathbf{R})_i, \tag{1.43}$$

where

$$\mathbf{m} = \frac{1}{2} \int_V \mathbf{r} \times \mathbf{J} \, dv \tag{1.44}$$

and (ii)

$$(3R_j R_k - R^2 \delta_{jk}) \int_V J_i r_j r_k \, dv = \varepsilon_{ijl} (3R_k R_l - R^2 \delta_{kl}) m_{jk}, \tag{1.45}$$

where

$$m_{ij} = \frac{2}{3} \int_V (\mathbf{r} \times \mathbf{J})_i r_j \, dv. \tag{1.46}$$

Using (1.42), (1.43), and (1.45) in (1.40) we have the desired expression

$$A_i(\mathbf{R}) = \frac{\mu_0}{4\pi} \left[\frac{1}{R^3} (\mathbf{m} \times \mathbf{R})_i + \frac{1}{2R^5} \varepsilon_{ijl} (3R_k R_l - R^2 \delta_{kl}) m_{jk} + \cdots \right]. \tag{1.47}$$

Here $\mathbf{m}$ given by (1.44) is the magnetic dipole moment of the steady current distribution, and m_{ij} given in (1.46) is the magnetic quadrupole moment. The magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ of the steady currents can be obtained from (1.47). The calculation is outlined in Appendix B and it yields

$$B_i(\mathbf{R}) = \frac{\mu_0}{4\pi} \left[\frac{3R_i R_j - R^2 \delta_{ij}}{R^5} m_j + \frac{3}{2R^7} \left\{ 5R_i R_j R_k - R^2 (R_i \delta_{jk} + R_j \delta_{ki} + R_k \delta_{ij}) \right\} m_{jk} + \cdots \right]. \tag{1.48}$$

It is interesting to compare the dipole and quadrupole orders of the electrostatic scalar potential (1.3) with the corresponding orders for the magnetostatic vector potential (1.47). These result in similar expressions for the dipole contributions, and for the quadrupole contributions, to the electrostatic field (1.13) and the magnetostatic field (1.48) in terms of the respective multipole moments.

Here we first get the vector potential A expanded through the magnetic quadrupole order where you see that the Cartesian *magnetic quadrupole moments* m_{ij} are the integrals shown of the current density J. I don't think I have ever seen this nice result before. The dipole moment is also shown above. Then he does the messy ∇ x A calculation in an appendix and we get the B field as shown! Now let's compare:

$$E_i(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{R_i}{R^3}q + \frac{3R_iR_j - R^2\delta_{ij}}{R^5}p_j + \frac{3}{2R^7}\left\{5R_iR_jR_k - R^2(R_i\delta_{jk} + R_j\delta_{ki} + R_k\delta_{ij})\right\}q_{jk} + \cdots\right]. \quad (1.13)$$

The field expansions at least to this order are exactly the same, with the appropriate moments! And the potentials ϕ and A have similar expansions. This information came from:

http://books.google.com/books?id=axnYh8mx0UAC&pg=PA12&lpg=PA12&dq=%22magnetic+quadrupole+moment%22&source=web&ots=9VVsoWJGLM&sig=a2cjm_v2Z9S6-rpjABd4XbR0-pM#PPA11,M1

Multipole Theory In Electromagnetism: Classical, Quantum, And Symmetry Aspects, With Applications
(International Series of Monographs on Physics) (Hardcover)
by R. E. Raab (Author), O. L. de Lange (Author)
Hardcover: 248 pages
Publisher: Oxford University Press, USA (December 10, 2004) $40 used, $140 new!

I don't think this book does the ℓm type multipole expansions, by the way, just Cartesian.

First, force and torque due to magnetic field and current density:

1.8 Force and torque in an external magnetostatic field

Consider a finite distribution of steady currents in a static magnetic field $\mathbf{B}(\mathbf{r})$. The force on an element of charge dq moving with velocity $\mathbf{u}$ is

$$\begin{aligned} d\mathbf{F} &= dq\,\mathbf{u} \times \mathbf{B} \\ &= \mathbf{J} \times \mathbf{B}\,dv. \end{aligned} \tag{1.55}$$

The total force on the distribution is therefore

$$F_i = \varepsilon_{ijk} \int_V J_j\, B_k\, dv. \tag{1.56}$$

We assume a slowly varying field and make a series expansion about the origin O

$$B_k(\mathbf{r}) = B_k + (\nabla_l B_k) r_l + \frac{1}{2}(\nabla_m \nabla_l B_k) r_l r_m + \cdots. \tag{1.57}$$

Using (1.57) and (1.42) in (1.56) we have

$$F_i = \varepsilon_{ijk} \left[(\nabla_l B_k) \int_V J_j\, r_l\, dv + \frac{1}{2}(\nabla_m \nabla_l B_k) \int_V J_j\, r_l r_m\, dv + \cdots \right]. \tag{1.58}$$

In Appendix C it is shown how to express (1.58) in terms of the magnetic multipole moments (1.44) and (1.46). The result is

$$F_i = m_j \nabla_j B_i + \frac{1}{2} m_{jk} \nabla_k \nabla_j B_i + \cdots. \tag{1.59}$$

This result is similar to the corresponding electrostatic formula (1.30).

For the total torque on the distribution

$$\mathbf{N} = \int \mathbf{r} \times d\mathbf{F} \tag{1.60}$$

we first use (1.55) to express this as

$$\mathbf{N} = \int_V \mathbf{r} \times (\mathbf{J} \times \mathbf{B})\, dv. \tag{1.61}$$

Thus

$$N_i = \varepsilon_{ijk}\, \varepsilon_{klm} \int_V r_j J_l B_m\, dv. \tag{1.62}$$

In (1.62) we use the expansion (1.57). Then

$$N_i = \varepsilon_{ijk}\,\varepsilon_{klm} \int r_j J_l \,[B_m + (\nabla_n B_m) r_n + \cdots]\, dv. \tag{1.63}$$

In Appendix D it is shown how to express (1.63) in terms of the magnetic dipole and quadrupole moments. The result is

$$N_i = \varepsilon_{ijk} \left[m_j B_k + \frac{1}{2}(m_{jl} + m_{lj}) \nabla_l B_k + \cdots \right]. \tag{1.64}$$

This may be compared with the corresponding result (1.31) for the torque on a charge distribution in an electrostatic field. We see that the dipole terms are analogues of each other, as are the quadrupole terms. (In comparing the latter, recall that q_{jl} in (1.31) is symmetric and therefore equal to $\frac{1}{2}(q_{jl} + q_{lj})$.)

1.9 Potential energy of a current distribution in a magnetostatic field

The calculation is similar to that in Section 1.5 for a charge distribution in an electrostatic field. We assume that the external magnetic field varies slowly in the current distribution. The potential energy is given by (1.33) and (1.59). We also have $\boldsymbol{\nabla} \times \mathbf{B} = 0$ because the sources of the external field are outside the distribution and the currents are steady. Thus $\nabla_j B_i = \nabla_i B_j$ in (1.59), and (1.33) yields

$$\begin{aligned} W &= -\int_i^f \left[m_j \frac{\partial B_j}{\partial r_i} + \frac{1}{2} m_{jk} \frac{\partial}{\partial r_i} \nabla_k B_j + \cdots \right] dr_i \\ &= -\int_i^f \left[m_i\, dB_i + \frac{1}{2} m_{ij}\, d(\nabla_j B_i) + \cdots \right]. \end{aligned} \tag{1.65}$$

Here the field and its derivatives are evaluated at the origin, and the multipole moments are the total moments. From (1.65)

$$m_i = -\frac{\partial W}{\partial B_i}, \qquad m_{ij} = -2\,\frac{\partial W}{\partial (\nabla_j B_i)}, \qquad \text{etc.} \tag{1.66}$$

For a rigid (non-polarizable) distribution the multipole moments in (1.65) are constants, equal to the permanent moments $m_i^{(0)}$, $m_{ij}^{(0)}$, ... Then (1.65) yields

$$W = -m_i^{(0)} B_i - \frac{1}{2} m_{ij}^{(0)} \nabla_j B_i + \cdots. \tag{1.67}$$

This is the magnetostatic counterpart of (1.37).

This last result is what I am really after. It tells you the Hamiltonian describing the magnetic quadrupole interaction with a magnetic field! This is something not mentioned in Levitt, but there it is, big as day. I am not surprised at the form of the result. I have done this myself above for the electric stuff which is this:

$$W = (1/2)\phi(0)Q \;+\; (\partial_\alpha\phi)\, P_\alpha \;+\; (1/6)(\partial_\alpha\partial_\beta\phi)\, Q_{\alpha\beta} \;+ \text{octupole and higher}$$

But now replace $\partial_\alpha\phi = -E_\alpha$ to get

$$W = (1/2)\phi(0)Q \;- p_i E_i \;-\; (1/6)\, Q_{\alpha\beta}\, (\partial_\alpha E_\beta) \;+ \text{octupole and higher}$$

where I have used $Q_{\alpha\beta} = \int d^3\mathbf{r}\ \rho(\mathbf{r})\ (3r_\alpha r_\beta - \delta_{\alpha\beta}r^2)$. If one uses the simpler $q_{\alpha\beta} = \int d^3\mathbf{r}\ \rho(\mathbf{r})3r_\alpha r_\beta$, then my result becomes

$$W = (1/2)\phi(0)Q \;- p_i E_i \;-\; (1/2)\, q_{ij}\nabla_i E_j \;+ \text{octupole and higher}$$

and this makes the electric and magnetic dipole and quadrupole terms look exactly the same. [We don't get to see the book's result because Google does not have equation (1.37).]