1 Distributed Magnetization

Let us assume that we have a nucleus with a distributed moment described by a magnetization vector $\boldsymbol{M}(r)$ and magnetic moment $\boldsymbol{\mu}$ related by

$$\boldsymbol{\mu} = \int d^3r \boldsymbol{M}(\boldsymbol{r})$$

The vector potential of a point dipole with magnetic moment $\boldsymbol{\mu}$:

$$\boldsymbol{A} = \frac{\mu_0}{4\pi} \frac{\boldsymbol{\mu} \times \boldsymbol{r}}{r^3} \,,$$

is then generalized to

$$\boldsymbol{A} = \frac{\mu_0}{4\pi} \int d^3s \, \frac{\boldsymbol{M}(\boldsymbol{s}) \times (\boldsymbol{r} - \boldsymbol{s})}{|\boldsymbol{r} - \boldsymbol{s}|^3} \,.$$

Let us suppose that $\boldsymbol{M}(\boldsymbol{r})$ points along the z-axis and that its magnitude depends only on r. Then, $\boldsymbol{\mu} = \mu \, \hat{z}$ with

$$\mu = 4\pi \int dr \, r^2 \, M(r) \,.$$

We may rewrite the vector potential as

$$\boldsymbol{A} = \frac{\mu_0}{4\pi} \, \hat{z} \times \int d^3s \; M(s) \, \frac{\boldsymbol{r} - \boldsymbol{s}}{|\boldsymbol{r} - \boldsymbol{s}|^3} \,. \tag{1}$$

This can be conveniently rewritten as

$$\boldsymbol{A} = -\frac{\mu_0}{4\pi} \, \hat{z} \times \boldsymbol{\nabla} \, \Phi_M(r) \,, \tag{2}$$

where the magnetic scalar potential is $\Phi_M(r)$ is defined by

$$\Phi_M(r) = \int d^3s \, \frac{M(s)}{|\boldsymbol{r} - \boldsymbol{s}|} = 4\pi \left[\frac{1}{r} \int_0^r ds \, s^2 \, M(s) + \int_r^\infty ds \, s \, M(s) \right] \,. \tag{3}$$

One easily shows that

$$-\boldsymbol{\nabla} \, \Phi_M(r) = \frac{\boldsymbol{r}}{r^3} \, 4\pi \int_0^r ds \, s^2 \, M(s) \,.$$

It follows that we may write the vector potential for distributed magnetization in the form

$$\boldsymbol{A} = \frac{\mu_0}{4\pi} \, \frac{\boldsymbol{\mu} \times \boldsymbol{r}}{r^3} \, f(r) \,, \tag{4}$$

where

$$f(r) = \frac{4\pi}{\mu} \int_0^r ds \, s^2 \, M(s) = \int_0^r ds \, s^2 \, M(s) \; \div \int_0^\infty ds \, s^2 \, M(s) \,.$$

1.1 Uniform Distribution

If $M(r)$ is constant inside a sphere of radius R and vanishes outside, then

$$f(r) = \begin{cases} r^3/R^3, & r \leq R \\ 1, & r > R \end{cases} \tag{5}$$

From this, it follows that

$$\boldsymbol{A} = \frac{\mu_0}{4\pi} \begin{cases} \dfrac{\boldsymbol{\mu} \times \boldsymbol{r}}{R^3}\,, & r \leq R \\ \dfrac{\boldsymbol{\mu} \times \boldsymbol{r}}{r^3}\,, & r > R\,. \end{cases} \tag{6}$$

A simple prescription to use in this case is to let

$$\frac{1}{r^2} \to \frac{r}{R^3}, \quad r < R$$

in the point dipole formula!

1.2 Fermi Distribution

Let $M(r)$ be described by a Fermi distribution:

$$M(r) = \frac{M_0}{1 + \exp[(r-c)/a]}. \tag{7}$$

The total magnetic moment is then given by

$$\mu = 4\pi \left[\frac{c^3}{3} + \sum_{n=1}^{\infty} (-1)^n \; e^{-nc/a} \int_0^c ds\, s^2 \; e^{ns/a} \right. \\ \left. - \sum_{n=1}^{\infty} (-1)^n \; e^{nc/a} \int_c^{\infty} ds\, s^2 \; e^{-ns/a} \right] \tag{8}$$

From Maple, we obtain

$$\int_0^c ds\, s^2 \; e^{ns/a} = e^{nc/a} \left(\frac{ac^2}{n} - 2\frac{a^2 c}{n^2} + 2\frac{a^3}{n^3} \right) - 2\frac{a^3}{n^3}\,, \tag{9}$$

so that the first sum becomes

$$\sum_{n=1}^{\infty} (-1)^n \; e^{-nc/a} \int_0^c ds\, s^2 \; e^{ns/a} = ac^2 \sum_1^{\infty} \frac{(-1)^n}{n} \\ -2a^2 c \sum_1^{\infty} \frac{(-1)^n}{n^2} + 2a^3 \sum_1^{\infty} \frac{(-1)^n}{n^2} - 2a^3 \sum_1^{\infty} \frac{(-1)^n}{n^3} e^{-nc/a}\,. \tag{10}$$

For the second integral, we obtain

$$\int_c^{\infty} ds\, s^2 \; e^{-ns/a} = e^{-nc/a} \left(\frac{ac^2}{n} + 2\frac{a^2 c}{n^2} + 2\frac{a^3}{n^3} \right) \tag{11}$$

so the second sum becomes

$$\sum_{n=1}^{\infty}(-1)^n \ e^{nc/a} \int_c^{\infty} ds\, s^2 \ e^{-ns/a} = ac^2 \sum_1^{\infty} \frac{(-1)^n}{n}$$
$$+2a^2 c \sum_1^{\infty} \frac{(-1)^n}{n^2} + 2a^3 \sum_1^{\infty} \frac{(-1)^n}{n^2} \,. \tag{12}$$

Combining, we find

$$\mu = 4\pi M_0 \left[\frac{c^3}{3} - 4a^2 c \sum_1^{\infty} \frac{(-1)^n}{n^2} - 2a^3 \sum_1^{\infty} \frac{(-1)^n}{n^3} e^{-nc/a} \right] \,. \tag{13}$$

Making use of the fact that

$$\sum_1^{\infty} \frac{(-1)^n}{n^2} = -\frac{\pi^2}{12} \,,$$

and defining

$$S_k(x) = \sum_1^{\infty} \frac{(-1)^{n-1}}{n^k} e^{-nx} \,,$$

we may rewrite the expression above as

$$\mu = \frac{4\pi}{3} c^3 M_0 \left[1 + \frac{a^2}{c^2}\pi^2 + 6 \ \frac{a^3}{c^3} \ S_3\left(\frac{c}{a}\right) \right] \,. \tag{14}$$

Now, we may evaluate the factor $f(r)$ in Eq. (5) using Maple

$$f(r, r<c) = \frac{4\pi M_0}{\mu} \left[\frac{r^3}{3} + \sum_{n=1}^{\infty} (-1)^n \ e^{-nc/a} \int_0^r ds\, s^2 \ e^{ns/a} \right]$$
$$= \frac{4\pi M_0}{\mu} \left[\frac{r^3}{3} - ar^2 S_1\left(\frac{c-r}{a}\right) + 2a^2 r S_2\left(\frac{c-r}{a}\right) \right.$$
$$\left. - 2a^3 S_3\left(\frac{c-r}{a}\right) + 2a^3 S_3\left(\frac{c}{a}\right) \right] \,. \tag{15}$$

Similarly, again using Maple, we find

$$f(r, r>c) = \frac{4\pi M_0}{\mu} \left[\frac{c^3}{3} + \frac{a^2 c}{3}\pi^2 + 2a^3 \ S_3\left(\frac{c}{a}\right) \right.$$
$$\left. -ar^2 \ S_1\left(\frac{r-c}{a}\right) - 2a^2 r \ S_2\left(\frac{r-c}{a}\right) - 2a^3 \ S_3\left(\frac{r-c}{a}\right) \right] \tag{16}$$

These expressions may be simplified somewhat to give

$$f(r, r<c) = \frac{1}{\mathcal{N}} \left[\frac{r^3}{c^3} - 3\, \frac{ar^2}{c^3}\, S_1\left(\frac{c-r}{a}\right) + 6\, \frac{a^2 r}{c^3}\, S_2\left(\frac{c-r}{a}\right) \right.$$
$$\left. - 6\, \frac{a^3}{c^3}\, S_3\left(\frac{c-r}{a}\right) + 6\, \frac{a^3}{c^3}\, S_3\left(\frac{c}{a}\right) \right] \,, \tag{17}$$

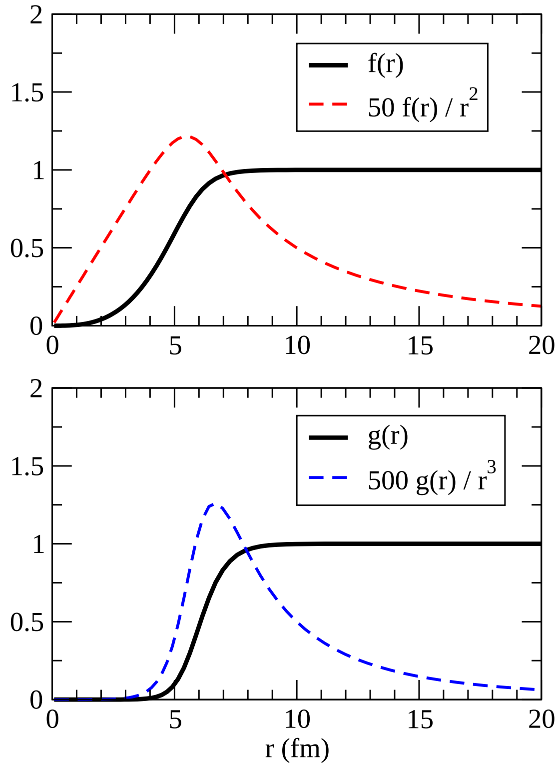

Figure 1: Upper panel: $f(r)$ and $50f(r)/r^2$ are shown for a Fermi distribution with $c = 5.748$ fm and $t = 2.3$ fm. Lower panel: $g(r)$ and $500g(r)/r^3$ are shown for a Fermi distribution with $c = 5.748$ fm and $t = 2.3$ fm.

and

$$f(r, r > c) = 1 - \frac{1}{\mathcal{N}}\left[3\,\frac{ar^2}{c^3}\,S_1\left(\frac{r-c}{a}\right) + 6\,\frac{a^2r}{c^3}\,S_2\left(\frac{r-c}{a}\right) + 6\frac{a^3}{c^3}\,S_3\left(\frac{r-c}{a}\right)\right], \quad (18)$$

where $\mathcal{N}$ is given by by

$$\mathcal{N} = \left[1 + \frac{a^2}{c^2}\pi^2 + 6\,\frac{a^3}{c^3}\;S_3\left(\frac{c}{a}\right)\right].$$

In the upper panel of Fig. 1, we plot the magnetic dipole scale factor $f(r)$ and the function $f(r)/r^2$ occurring in hyperfine integrals.

2 Distributed Quadrupole Moment

Now let us suppose that the nuclear quadrupole moment is distributed over the nucleus according to some radial distribution function $\rho(r)$. To analyze the resulting potential, we first consider a point quadrupole. The point quadrupole potential is given by

$$\Phi(\boldsymbol{r}) = \frac{1}{2}\sum_{ij} \frac{Q_{ij}}{4\pi\epsilon_0}\,\frac{x_i x_j}{r^5}.$$

Since the trace of Q_{ij} vanishes, we may replace

$$\frac{x_i x_j}{r^5} \rightarrow \frac{1}{3}\partial_j\partial_j\left(\frac{1}{r}\right)$$

in the expression for the potential. It follows that the potential of a quadrupole distributed symmetrically over the nucleus may be written

$$\Phi(\boldsymbol{r}) = \frac{1}{6}\sum_{ij} \frac{Q_{ij}}{4\pi\epsilon_0}\,\partial_j\partial_j \int \frac{4\pi x^2\rho(x)}{|\boldsymbol{r}-\boldsymbol{x}|}dx,$$

where $Q_{ij}\,\rho(r)$ is the distributed quadrupole moment density. The moment is normalized by requiring

$$\int_0^\infty 4\pi x^2\rho(x) = 1.$$

2.1 Uniform Distribution

Assuming that the distribution function $\rho(r) = \rho_0$ is constant over the nuclear volume, we have

$$\rho_0 = \frac{3}{4\pi R^3}$$

where R is the nuclear radius, and

$$\int \frac{4\pi x^2\rho(x)}{|\boldsymbol{r}-\boldsymbol{x}|}dx = \begin{cases} \frac{1}{R}\left(\frac{3}{2} - \frac{r^2}{2R^2}\right), & r < R \\ \frac{1}{r}, & r > R \end{cases}$$

Differentiating and dropping terms proportional to δ_{ij}, we find

$$\Phi = \frac{1}{2}\sum_{ij} \frac{Q_{ij}}{4\pi\epsilon_0}\,\frac{x_i x_j}{r^5}\,g(r),$$

where

$$g(r) = \begin{cases} 0, & r < R \\ 1, & r > R \end{cases}$$

2.2 Fermi Distribution

For a spherically symmetric distribution $\rho(x)$, we may write

$$\int \frac{4\pi x^2\rho(x)}{|\boldsymbol{r}-\boldsymbol{x}|}dx = 4\pi\left[\frac{1}{r}\int_0^r x^2\rho(x)dx + \int_r^\infty x^2\rho(x)dx\right].$$

Operating on this term with $\partial_j \partial_j$ leads to two terms, one proportional to $x_i x_j$ and one proportional to δ_{ij}. Only the former term is of interest here. We pick out the coefficient of $x_i x_j$ using

$$\partial_j \partial_j F(r) \rightarrow x_i x_j \times \frac{1}{r}\frac{d}{dr}\frac{1}{r}\frac{d}{dr}F(r).$$

It follows that

$$\frac{1}{3}\partial_i \partial_j \int \frac{4\pi x^2 \rho(x)}{|\boldsymbol{r}-\boldsymbol{x}|}dx \rightarrow \frac{4\pi x_i x_j}{r^5}\left[\int_0^r x^2 \rho(x)dx - \frac{r^3}{3}\rho(r)\right].$$

The potential for the distributed moment can therefore be written

$$\Phi(\boldsymbol{r}) = \frac{1}{2}\sum_{ij} \frac{Q_{ij}}{4\pi\epsilon_0}\frac{x_i x_j}{r^5}\, g(r).$$

with

$$g(r) = 4\pi \left[\int_0^r x^2 \rho(x)dx - \frac{r^3}{3}\rho(r)\right] \tag{19}$$

The two screening functions $f(r)$ and $g(r)$ are seen to be identical, except for the second term in Eq. (19)!

Now, let us determine $g(r)$ for a Fermi distribution

$$\rho(r) = \frac{\rho_0}{1+e^{(r-c)/a}}.$$

Carrying out the integrations in Eq. (19), we find

$$\begin{aligned} g(r, r<c) = \frac{1}{\mathcal{N}}\Bigg[&\frac{r^3}{c^3}\frac{1}{1+e^{(c-r)/a}} + 6\,\frac{a^3}{c^3}S_3\left(\frac{c}{a}\right) - 6\,\frac{a^3}{c^3}S_3\left(\frac{c-r}{a}\right) \\ &+6\,\frac{a^2 r}{c^3}S_2\left(\frac{c-r}{a}\right) - 3\,\frac{ar^2}{c^3}S_1\left(\frac{c-r}{a}\right)\Bigg], \end{aligned} \tag{20}$$

and

$$\begin{aligned} g(r, r>c) = 1 - \frac{1}{\mathcal{N}}\Bigg[&\frac{r^3}{c^3}\frac{1}{1+e^{(r-c)/a}} + 6\,\frac{a^3}{c^3}S_3\left(\frac{r-c}{a}\right) \\ &+6\,\frac{a^2 r}{c^3}S_2\left(\frac{r-c}{a}\right) + 3\,\frac{ar^2}{c^3}S_1\left(\frac{r-c}{a}\right)\Bigg]. \end{aligned} \tag{21}$$

In the above formulas, the normalization constant N is given by

$$\mathcal{N} = \left[1 + \frac{a^2}{c^2}\pi^2 + 6\frac{a^3}{c^3}S_3\left(\frac{c}{a}\right)\right] \tag{22}$$

The functions $S_n(x)$, as before, are defined by

$$S_n(x) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^n}\, e^{-kx} \equiv -\mathrm{Li}_n(-e^{-x}) \equiv -\mathrm{Polylog}(n, -e^{-x})$$

It might be noted that

$$S_1(x) = \log\left(1 + e^{-x}\right).$$

For small r, one finds

$$g(r) \to \frac{e^{c/a}\, r^4}{12\, a\, \mathcal{N}\left(1 + e^{c/a}\right)^2},$$

while for large r, $g(r) \to 1$. The function $g(r)$ is continuous at the point $r = c$. Indeed, the two forms are analytic continuations of a single function.

In the lower panel of Fig. 1, we plot the quadrupole scale factor $g(r)$ and the function $g(r)/r^3$ occurring in quadrupole integrals.

The functions $f(r)$ and $g(r)$ for a Fermi distribution are available numerically in the fortran subroutine nucfac.f.