Spherical average

Given a center, we evaluate the integral

$$f_{\text{avg}}(r) = \frac{\int_0^{2\pi}\int_0^{\pi} f(r,\theta,\phi) r^2 \sin\theta \, d\theta d\phi}{\int_0^{2\pi}\int_0^{\pi} r^2 \sin\theta \, d\theta d\phi}$$
$$= \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} f(r,\theta,\phi) r^2 \sin\theta \, d\theta d\phi$$

Because we have implemented radial splines defined as:

$$f_l^m(r) = \int_0^{2\pi}\int_0^{\pi} f(r,\theta,\phi) Y_l^m(\theta,\phi) \sin\theta \, d\theta d\phi$$

So if $f(r,\theta,\phi)$ is the function you wish to spherically average and it's around an atomic center (where we have the functionality), the spline associated with $Y_{l=0}^{m=0}$ is proportional to the spherical average,

$$f_{\text{avg}}(r) = \frac{1}{\sqrt{4\pi}} f_0^0(r)$$

I think I have computed the right prefactor but perhaps I'm off. It's easy to verify because $4\pi r^2 f_{\text{avg}}(r)$ will integrate to the number of electrons)

My notes on AtomDB should basically explain the procedure.

Once you have an atomic grid, you want to interpolate (using spherical harmonics). But you only want the spline for the l=0 spherical harmonic.
https://github.com/theochem/grid/blob/211ab55634bb4d8b6843904791809acc350a5623/src/grid/interpolate.py#L111
This gives values for r (you can also use splines for r directly) for each spherical harmonic, Y_l^m. Then choose the l=m=0 points. A test example is
https://github.com/theochem/grid/blob/211ab55634bb4d8b6843904791809acc350a5623/src/grid/tests/test_interpolate.py#L139