1 NMR Shielding

Shielding Tensor:

$$\sigma_{\beta\alpha}^{K} = \frac{\mathrm{d}^2 E}{\mathrm{d}B_\alpha\,\mathrm{d}m_{K_\beta}}\Big|_{\mathbf{B},\mathbf{m}_K=\mathbf{0}} \tag{1}$$

How do I parameterize energy E with $\mathbf{B}$ and $\mathbf{m}_K$?
The one-electronic Hamiltonian in magnetic field:

$$h(\mathbf{r},\mathbf{B},\mathbf{m}) = \frac{1}{2}\boldsymbol{\pi}^2 - \phi(\mathbf{r}) \tag{2}$$

in which:

$$\boldsymbol{\pi} = -i\boldsymbol{\nabla} + \mathbf{A} \tag{3}$$

is the kinetic momentum operator.

Vector potential:

$$\mathbf{A}_i = \mathbf{A}_0(\mathbf{r}_i) + \sum_K \mathbf{A}_K(\mathbf{r}_i) \tag{4}$$

with:

$$\mathbf{A}_0(\mathbf{r}_i) = \frac{1}{2}\mathbf{B}\times\mathbf{r}_0 \qquad \mathbf{B} = \nabla\times\mathbf{A}(\mathbf{r}) \tag{5}$$

$$\mathbf{A}_K(\mathbf{r}_i) = \alpha^2\frac{\mathbf{M}_K\times\mathbf{r}_K}{r_K^3} \qquad \mathbf{B}_K(\mathbf{r}) = \nabla\times\mathbf{A}_K(\mathbf{r}) \tag{6}$$

The first part is contribution from the external magnetic field, the second part from the nuclear magnetic moments.
Now parameterize with MO coefficients / densities?

2 SCF Level

$$E^{\mathrm{SCF}} = \sum_i^N h_{ii} + \frac{1}{2}\sum_{ij}^N \langle ij||ij\rangle \tag{7}$$

At SCF level, the NMR shielding tensor is given as:

$$\begin{aligned}\sigma_{\beta\alpha}^{\mathrm{SCF},K} &= \frac{\mathrm{d}^2 E^{\mathrm{SCF}}}{\mathrm{d}B_\alpha\,\mathrm{d}m_{K_\beta}}\Big|_{\mathbf{B},\mathbf{m}_K=0} \\ &= \end{aligned} \tag{8}$$