overlap contribution
(magnetic hyperfine interaction)

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overlap in the charge-charge interaction

What did we have for the charge-charge interaction:

order	multipole moment / field	first order quasi moment / quasi field	second order quasi moment / quasi field	…
$\mathcal{O}(0)$	$M \propto r^0 Y_{00}$, $V \propto v(0)$ } MI [a]	$\tilde{M}^{(1)} \propto \{r^2 Y_{00}\}$, $\tilde{V}^{(1)} \propto \Delta v(0)$ } $MS^{(1)}$ [d]	$\tilde{M}^{(2)} \propto \{r^4 Y_{00}\}$, $\tilde{V}^{(2)} \propto \Delta^2 v(0)$ } $MS^{(2)}$	…
$\mathcal{O}(2)$	$Q \propto r^2 Y_{20}$, $V_{ij} \propto \partial_{ij} v(0)$ } QI [b]	$\tilde{Q}^{(1)} \propto \{r^4 Y_{20}\}$, $\tilde{V}^{(1)}_{ij} \propto \partial_{ij} \Delta v(0)$ } $QS^{(1)}$ [e]	$\tilde{Q}^{(2)} \propto \{r^6 Y_{20}\}$, $\tilde{V}^{(2)}_{ij} \propto \partial_{ij} \Delta^2 v(0)$ } $QS^{(2)}$	…
$\mathcal{O}(4)$	$H \propto r^4 Y_{40}$, $V_{ijkl} \propto \partial_{ijkl} v(0)$ } HDI [c]	$\tilde{H}^{(1)} \propto \{r^6 Y_{40}\}$, $\tilde{V}^{(1)}_{ijkl} \propto \partial_{ijkl} \Delta v(0)$ } $HDS^{(1)}$	$\tilde{H}^{(2)} \propto \{r^8 Y_{40}\}$, $\tilde{V}^{(2)}_{ijkl} \propto \partial_{ijkl} \Delta^2 v(0)$ } $HDS^{(2)}$	…
…	…	…	…	…

0th order contribution for a point nucleus

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overlap in the charge-charge interaction

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…	…	…	…	…

first order correction to 0th order for overlap (or 'extended nucleus')

$$-\frac{eZ}{6\epsilon_0}\,\rho_e(\mathbf{0})\,\langle r_n^2\rangle$$

➔ vanishes if the nucleus is a point...
➔ ...even if the charge density at r=0 is not zero
➔ correction is small w.r.t. regular monopole term.

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overlap in the current-current interaction

Translate this to the leading term of the current-current interaction

	dipole contribution	first order correction due to overlap
O(1)	$-\hat{\boldsymbol{\mu}}_I \cdot \hat{\boldsymbol{B}}(\mathbf{0})$	

- orbital
- spin

- Fermi contact contribution

$$-\frac{2\mu_B\mu_0}{3}\left(|\psi_{e,\uparrow}(\mathbf{0})|^2 - |\psi_{e,\downarrow}(\mathbf{0})|^2\right)$$

➔ does not vanish if nucleus becomes a point

- field related to Bohr-Weisskopf effect

overlap ⇔ extended nucleus !

'correction' is often dominant w.r.t. regular dipole term (see bcc-Fe)

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Bohr-Weisskopf effect

Two different isotopes of the same element have a different nuclear moment. The spatial distribution of this moment over the nuclear volume need not to be homogeneous:

$$E_{mag} = -\int_{nuc} \boldsymbol{B}_{hf} \cdot d\boldsymbol{\mu}_I$$

1) Bring the two naked nuclei in an externally applied B and measure the magnetic interaction energy. B is constant over the nuclear volume and goes out of the integral:

$$\frac{E_1}{E_2} = \frac{\boldsymbol{\mu}_{I1}}{\boldsymbol{\mu}_{I2}}$$

2) Bring both nuclei in the same hyperfine field. This varies over the nuclear volume and interacts with the (differently) distributed magnetic moments. B does not get out the integral, which leads to:

$$\frac{E_1}{E_2} = \frac{\boldsymbol{\mu}_{I1}}{\boldsymbol{\mu}_{I2}}\,(1+\Delta)$$

➔ Bohr-Weisskopf effect

Δ: hyperfine anomaly (up to 2%)

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