monopole shift

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overview for the charge-charge case

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]	$\tilde{M}^{(1)} \propto \{r^2 Y_{00}\}$ $\tilde{V}^{(1)} \propto \Delta v(0)$	$\mathrm{MS}^{(1)}$ [d]	$\tilde{M}^{(2)} \propto \{r^4 Y_{00}\}$ $\tilde{V}^{(2)} \propto \Delta^2 v(0)$	$\mathrm{MS}^{(2)}$	…
$\mathcal{O}(2)$	$Q \propto r^2 Y_{20}$ $V_{ij} \propto \partial_{ij} v(0)$	QI [b]	$\tilde{Q}^{(1)} \propto \{r^4 Y_{20}\}$ $\tilde{V}^{(1)}_{ij} \propto \partial_{ij} \Delta v(0)$	$\mathrm{QS}^{(1)}$ [e]	$\tilde{Q}^{(2)} \propto \{r^6 Y_{20}\}$ $\tilde{V}^{(2)}_{ij} \propto \partial_{ij} \Delta^2 v(0)$	$\mathrm{QS}^{(2)}$	…
$\mathcal{O}(4)$	$H \propto r^4 Y_{40}$ $V_{ijkl} \propto \partial_{ijkl} v(0)$	HDI [c]	$\tilde{H}^{(1)} \propto \{r^6 Y_{40}\}$ $\tilde{V}^{(1)}_{ijkl} \propto \partial_{ijkl} \Delta v(0)$	$\mathrm{HDS}^{(1)}$	$\tilde{H}^{(2)} \propto \{r^8 Y_{40}\}$ $\tilde{V}^{(2)}_{ijkl} \propto \partial_{ijkl} \Delta^2 v(0)$	$\mathrm{HDS}^{(2)}$	…
…	…		…		…		…

Table 1. Systematic overview of nuclear multipole and quasi multipole moments and electronic multipole and quasi multipole fields that appear in the multipole expansion of for two interacting (and overlapping) classical charge distributions. The first column gives the regular multipole expansion for point nuclei: the monopole interaction (labeled by [a]) which provides the unperturbed hamiltonian in a quantum frame-work. This is perturbed by [b] the quadrupole and [c] the hexadecapole interaction. The next columns give the quasi multipole moments/fields for every multipole interaction, denoted by a tilde. They provide first order corrections (shifts) to the multipole interactions of the first column, due to the extendedness of the nucleus. The box labeled [d] gives rise to the isomer/isotope shift, while the box labeled by [e] is the main topic of the present paper. Colored (gray) text is by extrapolation only, and is not systematically derived in this paper. The objects in each line are spherical tensors of a given rank (rank 0 for line 1, rank 2 for line 2, rank 4 for line 3, …).

- multipole interaction
- first order multipole shift
- second order multipole shift
- …

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overview for the charge-charge case

order	multipole moment / field		first order quasi moment / quasi field		second order quasi moment / quasi field		…
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…	…		…		…		…

This is what one usually does.

Example for a single atom (if Z=1 : hydrogen) :

$$
\begin{aligned}
Q_{00} &= \frac{\sqrt{4\pi}}{\sqrt{4\pi}} \int \rho_n(\vec{r})\, d\vec{r} \\
&= eZ \\
V_{00} &= \frac{1}{4\pi\epsilon_0} \frac{\sqrt{4\pi}}{\sqrt{4\pi}} \int \frac{\rho_e(\vec{r})}{r}\, d\vec{r} \\
&= \frac{-e}{4\pi\epsilon_0} \langle \Psi_e | \frac{1}{r} | \Psi_e \rangle
\end{aligned}
$$

$$
\begin{aligned}
E_0^{(0)} &= Q_{00} V_{00} \\
&= \frac{-e^2 Z}{4\pi\epsilon_0} \langle \Psi_e | \frac{1}{r} | \Psi_e \rangle
\end{aligned}
$$

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overview for the charge-charge case

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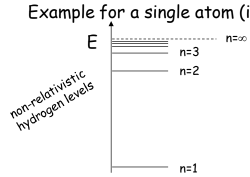
…	…		…		…		…

This is what one usually does.

Example for a single atom (if Z=1 : hydrogen) :



$$
\begin{aligned}
E_0^{(0)} &= Q_{00} V_{00} \\
&= \frac{-e^2 Z}{4\pi\epsilon_0} \langle \Psi_e | \frac{1}{r} | \Psi_e \rangle
\end{aligned}
$$

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overview for the charge-charge case

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…	…		…		…		…

Corrections due to the shape of the nucleus (quadrupole moment, hexadecapole moment,....) in the case without overlap

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overview for the charge-charge case

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…	…		…		…		…

The influence of overlap:

- first order monopole shift (well-known)
- first order quadrupole shift (recent advancement)
- first order hexadecapole shift (extremely small)

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overview for the charge-charge case

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...	...	...	...	...

The influence of overlap:

- second order monopole shift (known but exotic)
- (the rest is too small)

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first-order monopole shift

monopole term, no overlap :

$$E^{qq\,(0)}_{sh} = E_I + \left\langle \psi_e^{(0)} \otimes I \middle| \hat{T}_e + \hat{U}_{ee} - \frac{e^2 N Z}{4\pi\epsilon_0\, r_e} \middle| I \otimes \psi_e^{(0)} \right\rangle$$

$$= \underbrace{E_I + E_e + E_{ee}}_{E_\alpha} - \frac{e^2 N Z}{4\pi\epsilon_0} \langle I | I \rangle \underbrace{\left\langle \psi_e^{(0)} \middle| \frac{1}{r_e} \middle| \psi_e^{(0)} \right\rangle}_{\langle \frac{1}{r_e} \rangle}$$

$$= E_\alpha - \frac{e^2 N Z}{4\pi\epsilon_0} \left\langle \frac{1}{r_e} \right\rangle$$

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first-order monopole shift

monopole term, with overlap :

Look back at the gravitational result :

monopole shift : $\frac{1}{6}\, {}_cQ^{(0)}_{sz} \cdot {}_cV^{(0)}_{sz} = \frac{1}{6} \Delta V_2(\mathbf{0}) \langle r_1^2 \rangle$

$= \frac{4\pi G}{6} \rho_2(\mathbf{0}) \int \rho_1(r_1)\, r_1^2\, dr_1$

only if m_2 extends up to the origin !

Translate this to operators/expectation values for the quantum case:

monopole shift $\propto \langle \Psi_e \otimes I |\, \hat{\delta}(\vec{r}) \otimes \hat{r}^{\,2}\, | \Psi_e \otimes I \rangle$

small perturbation operator

unperturbed wave function

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first-order monopole shift

Final result :

$$E^{(0)}_{qq} = E_\alpha - \frac{e^2 N Z}{4\pi\epsilon_0} \left\langle \frac{1}{r_e} \right\rangle - \frac{eZ}{6\epsilon_0} \rho_e(\mathbf{0}) \langle r_n^2 \rangle$$

or

$$E^{(0)}_{qq} = E_\alpha + \tilde{\mathrm{Q}} \left\{ - \frac{eN}{4\pi\epsilon_0} \left\langle \frac{1}{r_e} \right\rangle \right\} + \tilde{\mathrm{Q}} \left\{ - \frac{1}{6\epsilon_0} \rho_e(\mathbf{0}) \langle r_n^2 \rangle \right\}$$

monopole moment = eZ

monopole field = potential at the nucleus, depends on integral property of electrons.

Extra potential at the nucleus, depends on point property of electrons and integral property of nucleus.

Vanishes if :
- the nucleus is a point, or
- the electrons do not enter the nucleus

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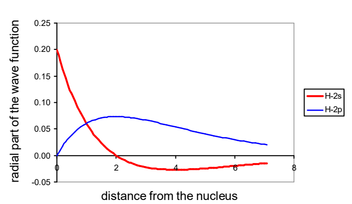
do electrons enter the nucleus ?

Go back to the H-atoms and check the equations on http://winter.group.shef.ac.uk/orbitron/
(take any orbital at the left, then choose the tab 'equations' on top).



Estimate the order of magnitude of the monopole shift energy (use the non-relativistic equation for H-atom s wave functions, and the nuclear radius trend seen in the first lecture.

- non-relativistic s-electrons do have a non-zero wave-function at r=0.
- the same holds for relativistic $p_{1/2}$ electrons

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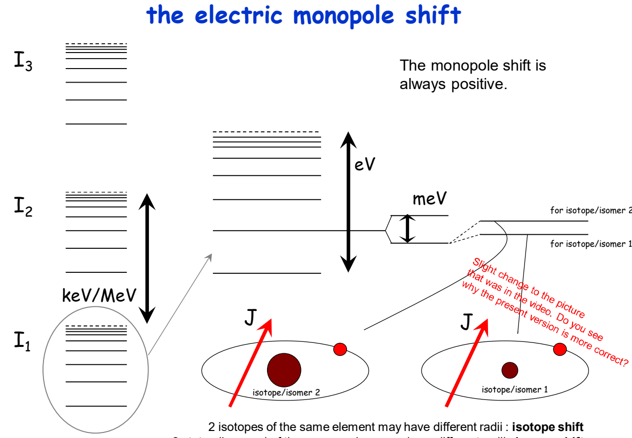
the electric monopole shift

The monopole shift is always positive.



2 isotopes of the same element may have different radii : **isotope shift**
2 states (isomers) of the same nucleus may have different radii : **isomer shift**

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experimental consequence: isotope shift

What:
levels in the atomic spectra of different isotopes of the same element are shifted (by the monopole shift).

We will later encounter the *isomer shift* :
for the same isotope, levels do depend on the nuclear state ("isomer").

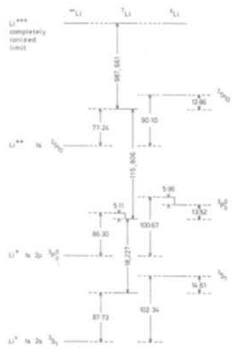

Fig. 4.1. *Calculated mass shifts in free Li ions. All energies are relative to the completely ionized limit. Energies are expressed in cm^{-1} (multiply by 0.5809 to get values in μeV). For instance, the $^3S_1$ configuration (1s^1 2s^1 with the two spins parallel) in infinitely heavy Li$^+$ has an energy which is 87.73 cm^{-1} (50.96 μeV) lower than the same configuration in ^{7}Li$^+$, and 102.34 cm^{-1} (59.44 μeV) lower than in ^{6}Li$^+$. Comparisons with an infinitely heavy ion cannot be checked experimentally, but the difference of 14.61 cm^{-1} (8.48 μeV) between the $^3S_1$ configurations of ^{7}Li$^+$ and ^{6}Li$^+$ is present in experiments. Similar interpretations can be made for the $^2S_{1/2}$ configuration, while the $^3P_1$ configuration contains complications not discussed in this text. (Picture taken from Isotope Shifts in Atomic Spectra, W. H. King, Plenum Press, 1984.)*

(shifts in this picture are due to the mass of the isotope -- see lecture 2 – as well as to the isotope shift)

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...	...	...	...	...

The influence of overlap:

• second order monopole shift (known but exotic)

➔ much smaller (4th power of the nuclear radius)
➔ nevertheless relevant for exotic cases: muonic atoms
(atoms where one of the electrons is replaced by a much heavier muon ➔ closer to the nucleus, more overlap)

http://en.wikipedia.org/wiki/Exotic_atom#Muonic_atoms

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