The isotope shift

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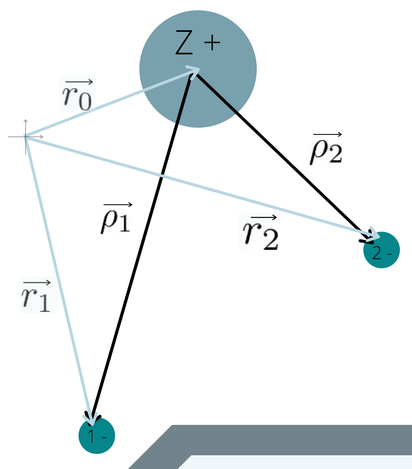
The isotope shift is the difference in the atomic state energies appearing for different isotopes of the same element. We present an inclusion of second-order perturbation theory for the specific mass (energy) shift. We also introduce an analysis of new *ab initio* calculations of isotope shifts in singly ionised calcium, by comparing them to recent empirical data, using King plot formalisms.

Atomic isotopes

Atomic Hamiltonian

Laboratory system

$$H(\vec{r}_0,\vec{r}_1,\vec{r}_2,\cdots,\vec{p}_0,\vec{p}_1,\vec{p}_2,\cdots) = \frac{p_0^2}{2M_A} + \sum_i \frac{p_i^2}{2m_e} + \sum_i V_{e-N}(\vec{r}_i-\vec{r}_0) + \frac{1}{2}\sum_{i\neq j} V_{e-e}(\vec{r}_i-\vec{r}_j)\,.$$



Center of mass system

$$H(\vec{\rho}_1,\vec{\rho}_2,\cdots,\vec{\pi}_1,\vec{\pi}_2,\cdots) = \sum_i \frac{\pi_i^2}{2\mu} + \sum_i V_{e-N}(\vec{\rho}_i) + \frac{1}{2}\sum_{i\neq j} V_{e-e}(\vec{\rho}_i-\vec{\rho}_j) + \frac{1}{M_A}\sum_{i\neq j}\vec{\pi}_i\cdot\vec{\pi}_j\,.$$

Different contributions to overall isotope shift

Mass shifts :

Normal mass shift

$$E_\mu = \frac{\mu}{m_e}E_\infty \qquad \mu = \frac{m_e M_n}{m_e + M_n}$$

Specific mass shift

$$H_{mpe} = -\frac{1}{M_n}\sum_{i=1}^{N}\sum_{j>i}^{N}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j}$$

$$E_{mpe} = -\frac{1}{M_n}\left\langle \psi^{(0)} \left| \sum_{i=1}^{N}\sum_{j>i}^{N}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j} \right| \psi^{(0)} \right\rangle$$

Field shift :

$$H_{vol}(r_i \le r_n) = \frac{Z}{2r_n}\left(\frac{2r_n}{r_i} + \frac{r_i^2}{r_n^2} - 3\right)$$

$$E_{vol} = \langle \psi_{n00}(\mathbf{r}_i) | H_{vol}(r_i) | \psi_{n00}(\mathbf{r}_i) \rangle$$

Second order theoretical specific mass shift results

First order

$$\delta E_{SMS} = \frac{M_A}{(M_A+m_e)^2}\left\langle \sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j \right\rangle$$

Second order

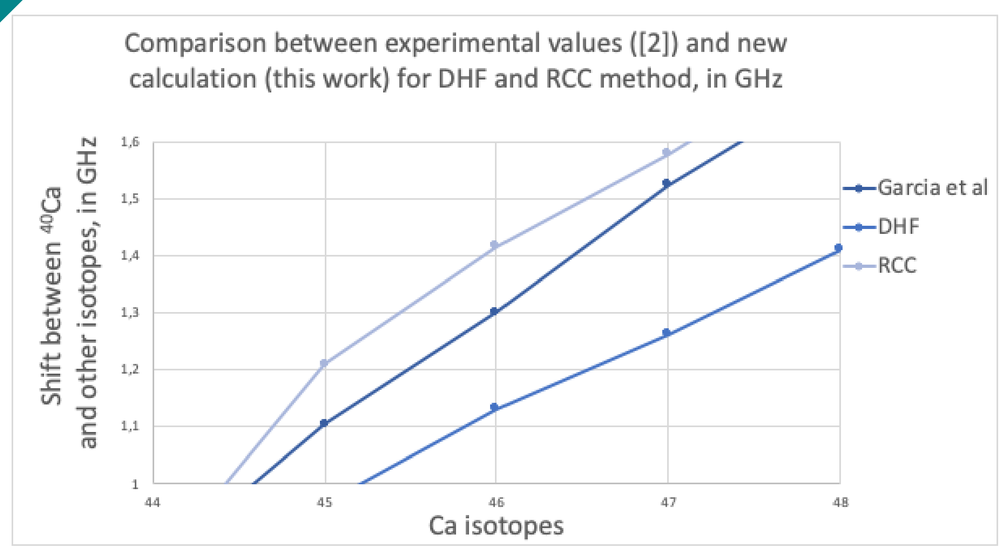
$$\delta E_{SMS} = \left| \frac{M_A}{(M_A+m_e)^2}\left\langle \sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j \right\rangle \right|^2$$

$$\vec{p}_i = \vec{\pi}_i + \frac{m_e}{M_T}\vec{P}$$

$$\vec{p}_0 = -\sum_i \vec{\pi}_i + \frac{M_A}{M_T}\vec{P}$$

Numerical shift calculations

First order



Etat	DHF method	RCC method
Field Shift constant (MHz/fm²)		
4s	-215,697	-261,921
4p 1/2	-0,417	20,238
4p 3/2	-0,0000104	20,627
Normal Mass Shift constant (GHz.amu)		
4s	2383,856	1556,449
4p 1/2	1619,66	1139,921
4p 3/2	1611,921	1138,666
Specific Mass Shift constant (GHz.amu)		
4s	-926,112	-152,95
4p 1/2	-501,109	-163,504
4p 3/2	-492,553	-158,492

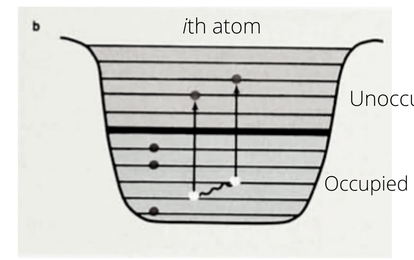
Isotope shift calculations done using DHF and RCC method

The coupled cluster numerical method

$$\hat{T}_2 = \sum_i \hat{t}_i$$

$$\Psi = \Phi_0 + \hat{T}_2\Phi_0 + \tfrac{1}{2!}\hat{T}_2{}^2\Phi_0 + \tfrac{1}{3!}\hat{T}_2{}^3\Phi_0 + \cdots = e^{\hat{T}_2}\Phi_0$$

$\hat{t}_i$



King plot approach

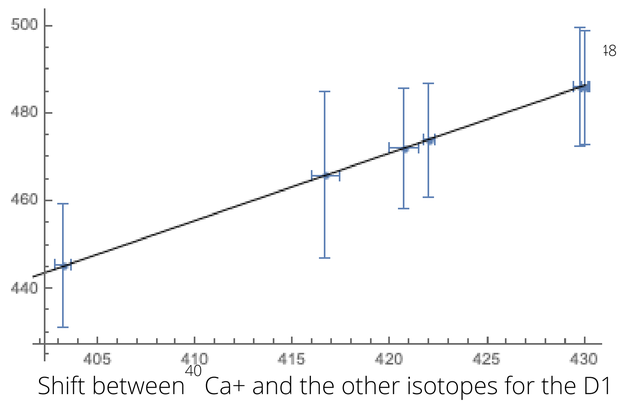
$$\mu_{(P,Q)}IS^a_{P,Q} = MS^a_{S,T} + \mu_{(P,Q)}FS^a_{P,Q}$$

$$\mu_{(P,Q)}IS^b_{P,Q} = MS^b_{S,T} + \mu_{(P,Q)}FS^b_{P,Q}$$

$$\mu_{(P,Q)} = \frac{(M_S - M_T)(M_P + m)(M_Q + m)}{(M_P - M_Q)(M_S + m)(M_T + m)}$$

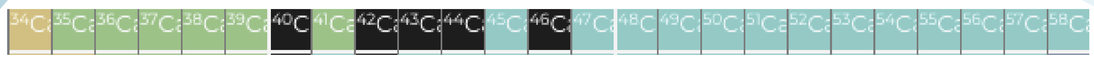
King plot analysis of empirical data for the D1 - D2 transitions in Ca+

Shift between ^{40}Ca+ and the other isotopes for the D2 transition, in MHz [2]

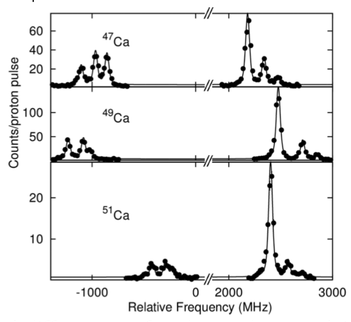


Shift between ^{40}Ca+ and the other isotopes for the D1 transition, in MHz [1]

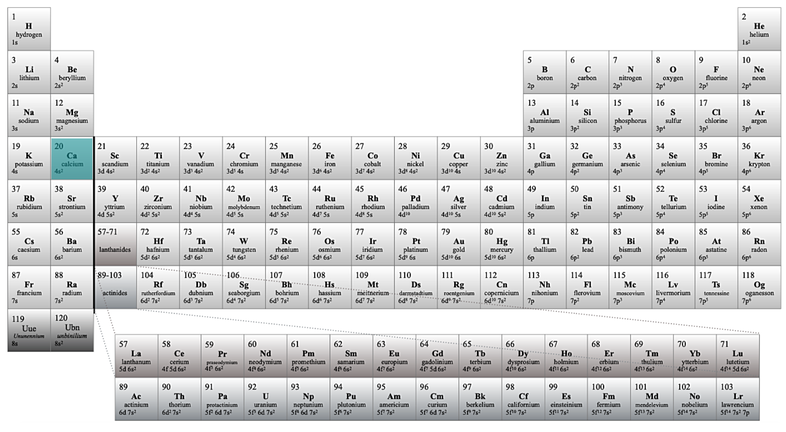
Calcium



Difference in hyperfine structure spectrums of ^{49}Ca, ^{47}Ca and ^{51}Ca



The spectral differences for these three calcium isotopes are subtle but clearly detectable with high-resolution spectroscopy. This is a manifestation of the isotope shift.



References

- [1] A. Andl et al., Phys. Rev. C (1982)
- WR Johnson, Many-Body Calculations of the Isotope Shift (2001)
- [2]Garcia Ruiz et al. Nature Phys 12, 594–598 (2016)

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