ProblemSet7

Prob 2 Li Isotope Shift

Specific Mass Shift: We use the formula $T = -\sum_a [v]^{-1} \langle v \| C_1 \| a \rangle^2 P(va)^2$, where $P(va)$ is the radial matrix elements of the momentum operator, to evaluate the the SMS. Since Li has only one core shell $(1s)^2$, the sum reduces to a single term. Moreover, since the reduced matrix element $\langle v \| C_1 \| a \rangle$ vanishes between two s states, the SMS vanishes for the 2s state. (This statement is true only in the independent particle approximation and is modified when correlation corrections are considered.) Introduce the Coulomb wave function $P_a(r)$ for the $1s$ core orbital and $P_v(r)$ for the $2p$ valence orbital.

$$\begin{aligned} P_a(r) = &\; 2Za(3/2re^{(-Z_a r)} \\ P_v(r) = &\; \frac{1}{2\sqrt{6}} {Z_v}^{5/2} r^2 e^{(-Z_v r/2)}. \end{aligned}$$

The valence-core radial matrix element $P(va)$ becomes

$$P(va) = -\frac{16\sqrt{6}(Z_a Z_v)^{(5/2}}{(2Z_a + Z_v)^4}$$

Substitute numerical values $Z_a = 3 - 5/16$ and $Z_v = 1 + 1/8$ to obtain $P(va) = -0.348975$

The reduced matrix element

$$\langle v \| C_1 \| a \rangle = 1$$

Put the above together to obtain the SMS (up to a factor 1/Ma)

$$T = -\frac{1}{3} |\langle v \| C_1 \| a \rangle|^2 P(va)^2 = -0.0405946$$