Prob 2 Li Isotope Shift

Specific Mass Shift: We use the formula $T = -\sum_a \langle v || C_1 || a \rangle^2 P(va)^2$, where $P(va)$ is the radial matrix elements of the momentum operator, to evaluate the 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.

\[
P_a(r) = 2 Z_a^{3/2} r e^{-Z_a r}
\]
\[
P_v(r) = \frac{1}{2\sqrt{6}} Z_v^{5/2} r^2 e^{-Z_v r/2}.
\]

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)

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