Precyzyjna spektroskopia isotopów Be^+ i jądrowe promienie ładunkowe

Krzysztof Pachucki

Universytet Warszawski

14 styczeń 2009, IFD Uniwersytet Warszawski

wsparte przez *NIST Precision measurement Grant 60NANB7D6153*

Podstawy

- Rozwój zaawansowanych metod teoretycznych opartych na elektrodynamice kwantowej pozwala na precyzyjne wyznaczenie poziomów energetycznych
- atomy: H, He, Li i Be^+
- skończona masa jądra $\rightarrow$ przesunięcie izotopowe
- magnetyczny moment dipolowy i elektryczny kwadrupolowy $\rightarrow$ struktura nadsubtelna
- widoczny jest wpływ struktury jądra na widma atomowe: promień ładunkowy, polaryzowalność jądra, rozkład momentu magnetycznego wewnątrz jądra

Szkic

- Wpływ skończonych rozmiarów jądra na widma atomowe
- Poprawki relatywistyczne i QED
- Metody obliczeniowe dla atomów (jonów) 3-elektronowych
- Przesunięcie izotopowe w Be$^+$ i promienie ładunkowe

Średni kwadratowy promień ładunkowy jądra $r_{\rm ch}$

$$\langle r_{\rm ch}^2\rangle = \int d^3r\, r^2\, \rho(r)$$

$$\delta E = \frac{2\,\pi}{3}\, Z\,\alpha \left\langle \sum_a \delta^3(r_a)\right\rangle \langle r_{\rm ch}^2\rangle$$

$$= C\,\langle r_{\rm ch}^2\rangle$$

w przybliżeniu stanowi to 10^{-4} przesunięcia izotopowego

$$\nu_{\rm exp} - \nu_{\rm the} = C\,\delta\, r_{\rm ch}^2$$

mathematical formalism

$$E(\alpha) = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \cdots$$

$E^{(2)}$ is a nonrelativistic ground state energy E corresponding to Schrödinger H

$$H = \sum_a \frac{\vec{p}_a^{\,2}}{2\,m} - \frac{Z\,\alpha}{r_a} + \sum_{a>b} \frac{\alpha}{r_{ab}} + \frac{\vec{p}_N^{\,2}}{2\,m_N}$$

$E^{(4)}$ is the leading relativistic correction

$$E^{(4)} = \langle\phi|H^{(4)}|\phi\rangle$$

with $H^{(4)}$ being an effective Hamiltonian

Leading relativistic corrections

$$
\begin{aligned}
H^{(4)} \quad = \quad & \sum_a \left\{ -\frac{\vec{p}_a^{\,4}}{8\,m^3} + \frac{\pi\,Z\,\alpha}{2\,m^2}\,\delta^3(r_a) + \frac{Z\,\alpha}{4\,m^2}\,\vec{\sigma}_a \cdot \frac{\vec{r}_a}{r_a^3} \times \vec{p}_a \right\} \\
& + \sum_{a>b}\sum_b \left\{ -\frac{\pi\,\alpha}{m^2}\,\delta^3(r_{ab}) - \frac{\alpha}{2\,m^2}\,p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3} \right) p_b^j \right. \\
& - \frac{2\,\pi\,\alpha}{3\,m^2}\,\vec{\sigma}_a \cdot \vec{\sigma}_b\,\delta^3(r_{ab}) + \frac{\alpha}{4\,m^2}\,\frac{\sigma_a^i\,\sigma_b^j}{r_{ab}^3}\left(\delta^{ij} - 3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2} \right) + \frac{\alpha}{4\,m^2\,r_{ab}^3} \\
\times \quad & \left. \Big[2\,(\vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_a) + (\vec{\sigma}_b \cdot \vec{r}_{ab} \times \vec{p}_b - \vec{\sigma}_a \cdot \vec{r}_{ab} \times \vec{p}_a) \Big] \right\} \\
& + \sum_a \left\{ \frac{Z\,\alpha}{2\,m\,m_N}\,p_a^i \left(\frac{\delta^{ij}}{r_a} + \frac{r_a^i\,r_a^j}{r_a^3} \right) p_N^j - \frac{Z\,\alpha}{2\,r_a^3}\,\vec{\sigma}_a \cdot \vec{r}_a \times \vec{p}_N \right\}
\end{aligned}
$$

Leading QED corrections:

$$E^{(5)} = -\frac{4\,Z\,\alpha^2}{3}\left(\frac{1}{m}+\frac{Z}{M}\right)^2\left\langle\sum_a\delta^3(r_a)\right\rangle\ln k_0+\sum_a\langle H^{(5)}_{aN}\rangle+\sum_{a>b,\,b}\langle H^{(5)}_{ab}\rangle+E_{\rm pol}\,,$$

$$H^{(5)}_{aN} = \frac{Z\,\alpha^2}{2\,\pi\,m^2\,r_a^3}\left[\vec{s}_a\cdot\vec{r}_a\times\vec{p}_a-\frac{m}{M}\,\vec{s}_a\cdot\vec{r}_a\times\vec{p}_N\right]+\left[\frac{19}{30}+\ln(\alpha^{-2})\right]\frac{4\,\alpha^2\,Z}{3\,m^2}\,\delta^3(r_a)$$
$$+\left[\frac{62}{3}+\ln(\alpha^{-2})\right]\frac{(Z\,\alpha)^2}{3\,m\,M}\,\delta^3(r_a)-\frac{7}{6\,\pi}\,\frac{m^2}{M}\,(Z\,\alpha)^5\,P\left[\frac{1}{(m\,\alpha\,r_a)^3}\right]$$
$$+\frac{4}{3}\,\frac{Z^3\,\alpha^2}{M^2}\,\ln\left(\frac{M}{m\,\alpha^2}\right)\delta^3(r_a),$$

$$H^{(5)}_{ab} = \frac{\alpha^2}{\pi\,m^2}\left[\frac{s_a^i\,s_b^j}{r_{ab}^3}\left(\delta^{ij}-3\,\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^2}\right)-\frac{1}{2\,r_{ab}^3}\,(\vec{s}_a+\vec{s}_b)\cdot\vec{r}_{ab}\times(\vec{p}_a-\vec{p}_b)\right]$$
$$+\frac{\alpha^2}{m^2}\left[\frac{164}{15}+\frac{14}{3}\,\ln\alpha\right]\delta^3(r_{ab})-\frac{7}{6\,\pi}\,m\,\alpha^5\,P\left[\frac{1}{(m\,\alpha\,r_{ab})^3}\right],$$

Li: nonrelativistic wave function

- Hylleraas basis set:

$$\begin{aligned}\psi &= \mathcal{A}[\phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)\,\chi]\\ \phi(\vec{r}_1, \vec{r}_2, \vec{r}_3) &= \exp(-\alpha_1\, r_1 - \alpha_2\, r_2 - \alpha_3\, r_3)\, r_{23}^{n_1}\, r_{31}^{n_2}\, r_{12}^{n_3}\, r_1^{n_4}\, r_2^{n_5}\, r_3^{n_6}\\ \chi &= [\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2)]\,\alpha(3)\end{aligned}$$

- with many $\sim 10^4\ \phi's$
- correct analytic properties

Li: matrix elements

Matrix elements of the Hamiltonian

$$\begin{aligned}\langle\psi|H_0|\psi'\rangle &= \langle 2\,\phi(1,2,3)+2\,\phi(2,1,3)-\phi(3,1,2)-\phi(2,3,1)\\ &\quad -\phi(1,3,2)-\phi(3,2,1)|H_0\,|\phi'(1,2,3)\rangle/6\,.\end{aligned}$$

are expressed in terms of Hylleraas integral

$$\begin{aligned} f &= f(n_1,n_2,n_3,n_4,n_5,n_6)\\ &= \int\frac{d^3r_1}{4\,\pi}\int\frac{d^3r_2}{4\,\pi}\int\frac{d^3r_3}{4\,\pi}\,e^{-w_1\,r_1-w_2\,r_2-w_3\,r_3}\\ &\quad\times r_{23}^{n_1-1}\,r_{31}^{n_2-1}\,r_{12}^{n_3-1}\,r_1^{n_4-1}\,r_2^{n_5-1}\,r_3^{n_6-1}\end{aligned}$$

Li and Be^+: contributions to the isotope shift, MHz

correction	$^{11-7}$Li$(3S_{1/2} - 2S_{1/2})$	$^{11-9}$Be$(2P_{1/2} - 2S_{1/2})$
$\Delta\nu^{(2,1)}$	25 104.520 2(1)	31 568.577 3(8)
$\Delta\nu^{(2,2)}$	−2.967 9	0.765 7(2)
$\Delta\nu^{(4,1)}$	0.037 8(4)	−10.035 0(2)
$\Delta\nu^{(5,1)}$	−0.106 4(15)	0.877 7(36)
$\Delta\nu^{(6,1)}$	−0.020(5)	−0.092(23)
$\Delta\nu_{\mathrm{pol}}$	0.039(4)	0.208(21)
$\Delta\nu_{\mathrm{the}}$	25 101.502 8(64)(27)	31 560.302(31)(12)
$\Delta\nu_{\mathrm{the}}$[Drake]	25 101.470(5)	31 560.01(6)

^{11}Be: Nuclear polarizability

- ^{11}Be with the one halo neutron
- its size is close to ^{92}U
- nucleus polarized by the electric field of electrons what significantly shifts atomic energy levels

$$E_{\rm pol} = -m\,\alpha^4 \left\langle \sum_a \delta^3(r_a) \right\rangle (m^3\,\tilde{\alpha}_{\rm pol})$$

$$\tilde{\alpha}_{\rm pol} = \frac{8\,\pi\,\alpha}{9} \int_{E_T} \frac{dE}{E}\,\frac{1}{e^2}\,\frac{dB(E1)}{dE}\left[\frac{19}{6} + 5\,\ln\left(\frac{2\,E}{m}\right)\right]$$

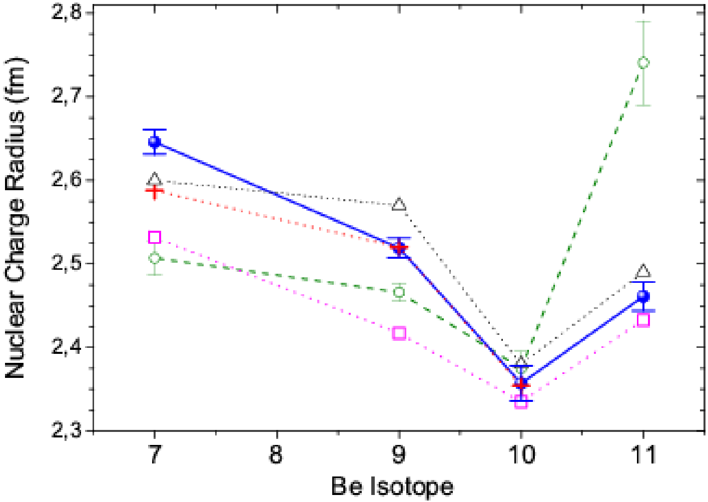
Be: charge radii

Measurement by Nörtershäuser *et al.* at ISOLDE in CERN (2008), $r_{\rm ch}(^9{\rm Be}) = 2.519(12)$ fm

isotope	$\nu_{\rm exp}$[MHz]	$\nu_{\rm the}$[MHz]	$r_{\rm ch}$[fm]
$^7{\rm Be}^+$	−49 236.81(88)	−49 225.736(35)(9)	2.645(14)
$^{10}{\rm Be}^+$	17 323.8(13)	17 310.437(13)(11)	2.358(16)
$^{11}{\rm Be}^+$	31 564.96(93)	31 560.302(31)(12)	2.464(16)

$$E_{\rm fs} = \frac{2\,\pi}{3}\,Z\,\alpha^4\,m^3\,r_{\rm ch}^2\langle\sum_a \delta^3(r_a)\rangle = \nu_{\rm exp} - \nu_{\rm the}$$

Plot of Be charge radii from Nörtershäuser *at al.*



Problems

- charge radii of reference nuclei are not very accurate
- precision of theoretical predictions is not sufficient for direct determination of charge radii
- development of computational methods for the 4-,5-electron systems
- finding the appropriate atomic transitions in B or B^+