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Nuclear structure effects in the isotope shift with halo nuclei

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Abstract Corrections to atomic energy levels due to nuclear structure effects are discussed. These are the finite nuclear size combined with relativistic and recoil corrections, and the nuclear polarizability. Good understanding of these effects is necessary for interpretation of high-precision measurements of the isotope shifts with neutron-rich nuclei ^{6,8}He, ^{11}Li and ^{11}Be. The summary of the results of the accurate atomic structure calculations is presented also.

Keywords isotope shift · nuclear structure · charge radius

1 Introduction

The size of light nuclei is about 10^{-5} times smaller than the typical atomic radius. In spite of this fact, precise measurements of atomic transition frequencies in light few-electron atoms made possible the determination of the root-mean-square (rms) charge radius of nuclei much more accurately than from the electron scattering measurements. Even for short-lived nuclei [1], one can obtain the rms radius with respect to the stable isotope from the atomic isotope shift measurement. The determination of the absolute value of the rms radius has not yet been possible, due to insufficient precision of theoretical predictions, with exception of hydrogenic systems. In the last few years precise measurements of the isotope shifts in light two- [2,3] and three-electron atomic systems [4,5] together with demanding accurate calculations of energy levels [6–10] brought the accurate values of the rms charge radii of neutron-rich isotopes: $^{6}\mathrm{He}(t_{1/2} = 807\mathrm{ms})$, $^{11}\mathrm{L}(t_{1/2} = 8\mathrm{ms})$, $^{8}\mathrm{He}(t_{1/2} = 119\mathrm{ms})$, and the very interesting $^{11}\mathrm{Be}(t_{1/2} = 14\mathrm{ms})$.

In order to determine rms charge radii difference the measurement of the isotope shift $\Delta\nu_{\rm exp}$ has to be collated with the theoretical predictions. The total isotope shift is split into the part independent on the size of the nuclei $\Delta\nu_{\rm the}$

$$\Delta\nu_{\rm exp} = \Delta\nu_{\rm the} + C_{AB}\,(r_A^2 - r_B^2). \tag{1}$$

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coming from different nuclei masses (the so called mass shift), and into the finite size contribution due to different nuclear charge radii (the so called volume shift). The mass shift for light atoms is about $\sim 10^4$ times larger in comparison to the volume shift, and thus has to be accurately calculated. It is in contrast to heavy atoms, where the volume shift is the dominating effect. The evaluation of $\Delta\nu_{\rm the}$ for light systems with few electrons is based on the expansion of energy levels in the fine structure constant α, thus giving series of coefficients associated to nonrelativistic, relativistic QED, and higher order QED corrections. Another expansion in the ratio of the reduced electron mass μ to the nuclear mass $\eta = -\mu/m_N$ is performed at the same time (see i.e. [10]). These finite nuclear mass effects are the most challenging in the isotope shift calculations due to their high complexity. Among others, theoretical calculations of the mass shift have reached a level of precision where tiny corrections due to nuclear structure and dynamics are necessary in order to interpret the results of high-precision measurements. In this paper we are focused on these effects in the isotope shift and its importance for the determination of the rms nuclear charge radii.

2 Finite nuclear size effects

The finite size contribution to the transition frequency is proportional to the square of the nuclear rms charge radius r_c

$$\nu_{\rm fs} = C\, r_c^2. \tag{2}$$

Effects coming form higher momenta of the charge distribution are negligible at the present accuracy level of spectroscopic mesurements in few electron atoms. In the above expression C as a function of α and η is expanded in the power series

$$C(\alpha,\eta) = \frac{R_\infty\, c\, \alpha^2}{\lambda\!\!\!^{-2}}\, (\mathcal{C}^{(4,0)} + \eta\, \mathcal{C}^{(4,1)} + \alpha^2\, \mathcal{C}^{(6,0)} + \ldots) \tag{3}$$

where $\mathcal{C}^{(n,m)}$ are dimensionless coefficients and λ is the electron Compton wavelength [12]. The leading-order term is proportional to the nonrelativistic wave function at the origin

$$\mathcal{C}^{(4,0)} = \frac{2\pi}{3} Z \left\langle \sum_a \delta^{(3)}(r_a) \right\rangle. \tag{4}$$

$C^{(6,0)}$ comes from the relativistic correction to the wave function at the origin [11]

$$\mathcal{C}^{(6,0)} \approx -Z^2\, \ln(Z\, \alpha\, m\, r)\, \mathcal{C}^{(4,0)}. \tag{5}$$

$C^{(4,1)}$ is a small finite mass correction consisting of two terms, the first is from the mass scaling and the second from the mass polarization.

$$\mathcal{C}^{(4,1)} = \frac{2\pi}{3} Z \left\langle \sum_a (3\, \delta^{(3)}(r_a) + [\delta^{(3)}(r_a)]_{\rm mp}) \right\rangle \tag{6}$$

where $[\delta^{(3)}(r_a)]_{\rm mp}$ is a second order operator

$$[\ldots]_{\rm mp} = 2\, [\ldots]\, \frac{1}{(H-E)'} \sum_{a>b} \mathbf{p}_a \cdot \mathbf{p}_b. \tag{7}$$

Table 1 Finite size corrections $C^{(n,k)} = \frac{R_\infty c}{\lambda^2}\,\alpha^{n-2}\,\eta^k\,\mathcal{C}^{(n,k)}$ to the constant C in MHz/fm^2 for the transitions in different isotopes of He(3^3P $\rightarrow$ 2^3S), Li(3^2S $\rightarrow$ 2^2S), Be(2^2P $\rightarrow$ 2^2S)

	^{4}He	^{6}He	^{8}He	^{7}Li	^{11}Li	^{9}Be$^+$	^{11}Be$^+$
$C^{(4,0)}$	−1.008496	−1.008496	−1.008496	−1.566501	−1.566501	−16.913491	−16.913491
$C^{(6,0)}$	−0.002077	−0.002032	−0.002046	−0.006687	−0.006675	−0.123447	−0.123788
$C^{(4,1)}$	0.000351	0.000233	0.000175	0.000363	0.000231	0.002006	0.001640
C	−1.010222	−1.010295	−1.010367	−1.572825	−1.572945	−17.034932	−17.035638

Table 2 Numerical results for the finite size constants C_{AB}. The overall uncertainty is estimated to be 25% of the relativistic correction

Isotope shift	C_{AB}(MHz/fm^2)
^{6}He-^{4}He(3^3P $\rightarrow$ 2^3S)	−1.0104(5)
^{8}He-^{4}He(3^3P $\rightarrow$ 2^3S)	−1.0108(5)
^{11}Li-^{7}Li(3^2S $\rightarrow$ 2^2S)	−1.5768(17)
^{11}Be-^{9}Be(2^2P $\rightarrow$ 2^2S)	−17.020(31)

Since these higher order $\mathcal{C}$ terms are small, we can express the constant C_{AB} in Eq. (1), for the isotope shift between atoms A and B, as the following combination

$$C_{AB} = \frac{r_{A0}^2\,C_A - r_{B0}^2\,C_B}{r_{A0}^2 - r_{B0}^2} \tag{8}$$

where r_{A0} and r_{B0} are initial approximate values of charge radii. In practice rms radius of one of the nuclei, let say B, is well known, and the mean square radius r_A^2 of A-nucleus is obtained with respect to r_B^2, according to Eq. (1).

Numerical results for C-coefficients of the transition frequencies for different isotopes of He, Li and Be$^+$ ion are presented in Table 1. The overall uncertainty of C is due to estimation of the relativistic correction to the wave function at origin on the basis of a known result for hydrogenic systems. As compared to the leading term $C^{(4,0)}$, the $C^{(4,1)}, C^{(6,0)}$ corrections are of the order $10^{-3} - 10^{-4}$. Thus, they are significant in the systematic studies of the isotope shift at the current level of theoretical uncertainties in $\nu_{\rm the}$. The obtained numerical results for constants C_{AB} for the relevant isotope shifts, using Eq. (8) are presented in Table 2.

3 Dipole electric polarizability of nuclei

Atomic transition frequencies are affected by the electric polarizability [8,13] of its nucleus, which reflects the possibility of nuclear excitations due to orbiting atomic electrons. To estimate this effect, let us employ the effective interaction Hamiltonian of a nucleus with the electromagnetic field

$$H_{\rm int} = q\,A^0 - \mathbf{d}\cdot\mathbf{E} - \boldsymbol{\mu}\cdot\mathbf{B} - \frac{q}{6}\,r_c^2\,\nabla\cdot\mathbf{E}, \tag{9}$$

which is valid as long as the characteristic momentum of the electromagnetic field is smaller than the inverse of the nuclear size. This is the main approximation of this approach, which may not always be valid. It was checked however that higher order polarizabilities are quite small (below 1 kHz) for deuterium [14,15], and this is similar for He, Li and Be isotopes. Within this low electromagnetic momentum approximation, the nuclear polarizability correction to the energy is given by the following formula [8]

$$\nu_{\rm pol} = -R_\infty\, c\, \alpha^2 \left\langle \sum_a \delta^3(r_a) \right\rangle (m^3\, \tilde{\alpha}_{\rm pol}), \tag{10}$$

where m is the electron mass and the expectation value of the Dirac δ is taken with the electron wave function in atomic units, (for hydrogenic systems it is equal to Z^3/π). In the equation above, $\tilde{\alpha}_{\rm pol}$ is a *weighted* electric polarizability of the nucleus given by the double integral [8]

$$\begin{aligned}\tilde{\alpha}_{\rm pol} = {} & \frac{16\,\alpha}{3} \int_{E_T}^{\infty} dE\, \frac{1}{e^2}\, |\langle \phi_N | \mathbf{d} | E \rangle|^2 \int_0^\infty \frac{dw}{w}\, \frac{E}{E^2 + w^2} \\ & \times \frac{1}{(\kappa + \kappa^\star)} \left[1 + \frac{1}{(\kappa+1)(\kappa^\star+1)} \left(\frac{1}{\kappa+1} + \frac{1}{\kappa^\star + 1} \right) \right]\end{aligned} \tag{11}$$

where $\kappa = \sqrt{1 + 2\, i\, m/w}$ and E_T is the excitation energy for the breakup threshold. This integral with respect to E includes implicitely nuclear excitations to discrete levels. The kets $|\phi_N\rangle$ and $|E\rangle$ denote the ground state of the nucleus and a dipole excited state with excitation energy E, respectively. The square of the dipole moment is related to the so called $B(E1)$ function by the relation

$$|\langle \phi_N | \mathbf{d} | E \rangle|^2 = \frac{4\,\pi}{3}\, \frac{dB(E1)}{dE} \tag{12}$$

in units e^2 fm^2 MeV^{-1}.

If E_T is much larger than the electron mass m, one can perform a small electron mass expansion and obtain a simplified formula [16]:

$$\tilde{\alpha}_{\rm pol} = \frac{19}{6}\, \alpha_{\rm E} + 5\, \alpha_{\rm Elog} \tag{13}$$

$$\begin{aligned}\alpha_{\rm E} &= \frac{2\,\alpha}{3}\, \frac{1}{e^2} \left\langle \phi_N \middle| \mathbf{d}\, \frac{1}{H_N - E_N}\, \mathbf{d} \middle| \phi_N \right\rangle \\ &= \frac{8\,\pi\,\alpha}{9} \int_{E_T} \frac{dE}{E}\, \frac{1}{e^2}\, \frac{dB(E1)}{dE}\end{aligned} \tag{14}$$

$$\begin{aligned}\alpha_{\rm Elog} &= \frac{2\,\alpha}{3}\, \frac{1}{e^2} \left\langle \phi_N \middle| \mathbf{d}\, \frac{1}{H_N - E_N}\, \ln\!\left(\frac{2(H_N - E_N)}{m} \right) \mathbf{d} \middle| \phi_N \right\rangle \\ &= \frac{8\,\pi\,\alpha}{9} \int_{E_T} \frac{dE}{E}\, \frac{1}{e^2}\, \frac{dB(E1)}{dE}\, \ln\!\left(\frac{2\,E}{m} \right),\end{aligned} \tag{15}$$

where $\alpha_{\rm E}$ is the static electric dipole polarizability and $\alpha_{\rm Elog}$ is the logarithmical modified polarizability. This approximation is valid for example for ^{3}He and ^{4}He isotopes, but not for ^{11}Li or ^{11}Be.

In the opposite situation, i.e. when m is much larger that E_T, that corresponds to the nonrelativistic limit, the polarizability correction adopts the form (with m being the reduced mass here):

$$E_{\rm pol} = -m\, \alpha^4 \left\langle \sum_a \delta^3(r_a) \right\rangle \frac{32\,\pi\,\alpha\, m^2}{9} \int_{E_T} dE\, \frac{1}{e^2}\, \frac{dB(E1)}{dE}\, \sqrt{\frac{m}{2\,E}}. \tag{16}$$

This approximation is justified for muonic helium atoms or ions, because the muon mass ($\sim$ 106 MeV) is much larger than the threshold energy E_T. This formula requires, however few significant corrections, namely Coulomb distortion and formfactor corrections. They were obtained by Friar [17] in the calculation of the polarizability correction in $\mu\,^4$He. This nonrelativistic approximation, however, is not valid for electronic atoms since the typical nuclear excitation energy in light nuclei is larger than the electron mass. This indicates possible limitation in the comparison of charge radii obtained from electronic and muonic atoms, as the nuclear structure effects are much different. Finally, the $B(E1)$ function is directly related to the photoabsorption cross section at photon energies E

$$\sigma(E) = \frac{16\,\pi^3}{9}\,\alpha E\left(\frac{1}{e^2}\,\frac{dB(E1)}{dE}\right) \tag{17}$$

which allows us to obtain the $B(E1)$ function from experimental data.

In Table 3 we collected data for nuclear polarizabilities of He, Li and Be isotopes. Most of the values for $\tilde{\alpha}_{\rm pol}$ are taken form the published results, some of them are new like for stable isotopes ^{7}Li, ^{9}Be. In all the cases, we recalculated the shift $\nu_{\rm pol}$ in the corresponding transition frequency. The polarizabilities for ^{4}He and ^{6}He were calculated in Ref. [13]. Here, we recalculated $\tilde{\alpha}_{\rm pol}$ for ^{8}He, using the measured electric dipole strength $B(E1)$ [18] for dissociation of ^{8}He into ^{6}He and 2 neutrons. Since it is not the complete possible way of excitation, we added the value of $\tilde{\alpha}_{\rm pol}$ for ^{4}He. Certainly this is not the best approach to obtain total nuclear polarizability, further improvements require more experimental data, therefore we associate rather large uncertainty of about 25% to $\tilde{\alpha}_{\rm pol}$ of ^{8}He. The related contribution to transition frequency $\nu_{\rm pol}$ is in agreement with the results obtained in [3]. The total $\tilde{\alpha}_{\rm pol}$ for ^{8}He is relatively small. This demonstrates the specific property of ^{8}He nucleus, which is more spherical and rigid as compared to the two-neutron halo ^{6}He nucleus. The effects of the nuclear polarizability to the isotope shift as a difference in $\tilde{\alpha}_{\rm pol}$ between nuclei is presented in the last column in Table 3. We observe, that the result is nonnegligible for ^{6}He, while it can be neglected for ^{8}He.

The $\tilde{\alpha}_{\rm pol}$ for ^{11}Li comes from Ref. [8] which based on the $B(E1)$ measurement in Ref. [19]. For the stable ^{7}Li nucleus, the polarizability $\tilde{\alpha}_{\rm pol}$ as calculated for the continuum above α and triton threshold [20], is 20 times smaller than $\tilde{\alpha}_{\rm pol}$ for ^{11}Li nucleus. Therefore its contribution to the isotope shift is very small, as we pointed this out in Ref. [8]. The opposite situation was found in the beryllium case. In Ref. [10] we used the experimental [21] and the theoretical line strength data [22] for ^{11}Be. Both data give consistent values for $\tilde{\alpha}_{\rm pol}$, what supports the significance of nuclear polarizability in ^{11}Be. However, not much smaller is the polarizability of ^{9}Be. The value of $\tilde{\alpha}_{\rm pol}$ in this case, was obtained using experimental data from Ref. [23]. There is a low lying, $E_{1/2+} = 1.684(7)$ MeV, 1/2+ excited state with the large transition dipole strength $B(E1)$ to the ground state, while the contribution from the other excited states can be neglected. The resulting nuclear polarizability $\tilde{\alpha}_{\rm pol}$ is only 2.5 times smaller than that of ^{11}Be, and can not be neglected.

4 Charge radii of halo nuclei from the atomic isotope shift

Results of our reevaluation of nuclear charge radii of halo nuclei are presented in Table 4. The experimental $\Delta\nu_{\rm exp}$ and theoretical $\Delta\nu_{\rm the}$ data for the helium isotope shift

Table 3 Nuclear polarizability data. The polarizability of ^{8}He is due to 2n dissociation and includes in addition the polarizability of ^{4}He

	$S \equiv E_T$ [MeV]	$\tilde{\alpha}_{\rm pol}\,[m^{-3}\,10^{-7}]$	Transition	$\nu_{\rm pol}$ [MHz]
^{4}He	$S_p = 19.8, S_n = 20.6$	0.36(4)	$3^3P_J \to 2^3S_1$	0.00129(13)
^{6}He	$S_{2n} = 0.975$	4.3(9)	$3^3P_J \to 2^3S_1$	0.0154(31)
^{8}He	$S_{2n} = 2.140$	0.64(16)	$3^3P_J \to 2^3S_1$	0.0023(6)
^{7}Li	$S_{\alpha+t} = 2.467$	0.47(5)	$3^2S_{1/2} \to 2^2S_{1/2}$	0.0017(2)
^{11}Li	$S_{2n} = 0.376(5)$	10.6(1.1)	$3^2S_{1/2} \to 2^2S_{1/2}$	0.039(4)
^{9}Be	$E_{1/2+} = 1.684(7)$	2.90(29)	$2^2P_{1/2} \to 2^2S_{1/2}$	0.083(8)
^{11}Be	$S_{2n} = 0.504$	6.90(69)	$2^2P_{1/2} \to 2^2S_{1/2}$	0.208(21)

Table 4 Summary of the isotope shift and the charge radii for halo isotopes of He, Li and Be. Reference radii: $r_{\rm c}(^4{\rm He}) = 1.676(8)$ fm [24], $r_{\rm c}(^7{\rm Li}) = 2.390(30)$ fm [25], $r_{\rm c}(^9{\rm Be}) = 2.519(12)$ fm [26], the first uncertainty of $\nu_{\rm the}$ for Li and Be comes from unknown higher order QED terms, second uncertainty is due to the atomic mass

	$\Delta\nu_{\rm exp}$[MHz]	$\Delta\nu_{\rm the}$[MHz]	$\delta r_{\rm c}^2$[fm^2]	$r_{\rm c}$[fm]
^{6}He-^{4}He (3^3P$_J \to 2^3$S$_1$)	43 194.660(10)^a	43 196.138(1)^a	1.463(36)	2.067(11)
^{8}He-^{4}He (3^3P$_J \to 2^3$S$_1$)	64 701.340(52)^a	64 702.257^a	0.908(95)	1.928(26)
^{11}Li-^{7}Li (3^2S$_{1/2} \to 2^2$S$_{1/2}$)	25 101.226(125)^b	25 101.501 1(64)(27)	0.174(79)	2.426(34)
^{11}Be-^{9}Be (2^2P$_{1/2} \to 2^2$S$_{1/2}$)	31 564.96(93)^c	31 560.156(31)(12)	−0.282(55)	2.462(33)

a - Ref. [3], b - Ref. [4], c - Ref. [5]

are the J-averaged values from Ref. [3]. In addition and in contrast to this Reference, we include $\nu_{\rm pol}$ within $\Delta\nu_{\rm the}$. In the determination of the rms charge radii of ^{6}He and ^{8}He we used improved constant C_{AB} as presented in Table 2, with including logarithmic relativistic correction to the wave function at the origin and with the leading finite mass correction. The effect of these corrections is rather small, our difference in square charge radii 1.463(36) fm^2 only slightly differs from that of Ref. ([3]) which is 1.466(36).

The experimental values $\Delta\nu_{\rm exp}$ have been obtained for lithium in [4] and for beryllium ion in [5]. Details of our calculations of $\Delta\nu_{\rm the}$ for lithium and beryllium ion are presented in Ref. [10]. Here, we additionally include electric polarizabilities of stable nuclei ^{7}Li and ^{9}Be, the last one is nonnegligible in the determination of ^{11}Be radius. There is also an additional correction for the $2^2P_{1/2}$ state in the beryllium ion coming from the hyperfine mixing of $2^2P_{1/2}$ and $2^2P_{3/2}$ states [27]. It contributes −57kHz to the IS in beryllium ion and is added to $\Delta\nu_{\rm the}$ value in Table 4. Apart from this theoretical isotope shifts $\Delta\nu_{\rm the}$ are in agreement with the former results [8–10].

5 Summary

The systematic analysis of the nuclear size and the nuclear structure effects in spectra of light atoms is presented. Improved theoretical predictions for the isotope shifts allowed us to refine the charge radii difference for exotic isotopes of ^{6,8}He, ^{11}Li and ^{11}Be. We find that the magnitude of the nuclear structure corrections to the atomic energy levels are comparable to the current experimental precision of isotope shift. Since for heavier elements, nuclear structure effects becomes more significant, they should be well understood before conclusions on nuclear charge radii are drawn.

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