

Relativistic calculations of isotope shifts in highly charged ions

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The isotope shifts of forbidden transitions in Be- and B-like argon ions are calculated. It is shown that only using the relativistic recoil operator can provide a proper evaluation of the mass isotope shift, which strongly dominates over the field isotope shift for the ions under consideration. Comparing the isotope shifts calculated with the current experimental uncertainties indicates very good perspectives for a first test of the relativistic theory of the recoil effect in middle- Z ions.

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I. INTRODUCTION

Recent high-precision measurements of forbidden transitions in highly charged argon ions [1] provide very good possibilities for tests of relativistic and quantum electrodynamic (QED) effects in middle- Z few-electron systems. In particular, in the case of Ar^{13+} the QED contribution to the $2s^2 2p^2 P_{1/2} - 2P_{3/2}$ transition energy is by four orders of magnitude larger than the corresponding experimental error. From the theoretical side, however, large efforts must be undertaken to achieve this accuracy [for the current theoretical results, see Ref. [1]]. The main goal of this paper is to calculate the isotope shifts of forbidden transitions in Be-like and B-like argon and to examine a possibility for their experimental determination.

The isotope shifts in the atomic transition energies arise from the finite nuclear mass (recoil effect) and from the finite nuclear size (field or volume shift). Generally, the field shift, caused by the penetration of the electron wave functions into the nuclear region, dominates for heavy atoms whereas the mass shift dominates for light atoms.

The relativistic units ($\hbar = c = 1$) are used in the paper.

II. MASS SHIFT

The nonrelativistic (nr) theory of the mass shift for many-electron atoms was first formulated by Hughes and Eckart [2]. This shift can be represented as the sum of two parts, the normal mass shift (NMS) and the specific mass shift (SMS). The normal-mass-shift operator is a one-particle operator. It is given by

$$H_{\text{NMS}}^{(\text{nr})} = \frac{1}{2M} \sum_i \mathbf{p}_i^2, \quad (1)$$

where \mathbf{p}_i is the momentum operator and M is the nuclear mass. The specific-mass-shift operator, which is a two-particle operator, can be written in the form

$$H_{\text{SMS}}^{(\text{nr})} = \frac{1}{2M} \sum_{i \neq j} \mathbf{p}_i \cdot \mathbf{p}_j. \quad (2)$$

The sum of expressions (1) and (2) defines the total recoil operator in the nonrelativistic theory.

The full relativistic theory of the nuclear recoil effect can be formulated only within quantum electrodynamics. Such a theory was first formulated in Ref. [3], where the complete αZ - dependence formulas for the recoil corrections to the atomic energy levels to first order in m/M were derived. Later, these formulas were rederived in simpler ways for the case of a hydrogenlike atom [4,5] as well as for a general case of a many-electron atom [6] (see also Ref. [7]). Full relativistic calculations of the recoil effect, based on these formulas, were performed for H- and Li-like ions [8–10]. In Ref. [5], they were employed to calculate the recoil corrections in H-like atoms to order $(\alpha Z)^6 m^2/M$, where α is the fine-structure constant. As follows from these formulas, within the lowest-order relativistic approximation ($\sim v^2/c^2$) and to first order in m/M , the recoil corrections can be derived by using the following recoil Hamiltonian:

$$H_M = \frac{1}{2M} \sum_{i,j} \left[\mathbf{p}_i \cdot \mathbf{p}_j - \frac{\alpha Z}{r_i} \left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right) \cdot \mathbf{p}_j \right], \quad (3)$$

where $\boldsymbol{\alpha}$ is a vector incorporating the Dirac matrices. The expectation value of H_M on the Dirac wave function yields the recoil correction to the atomic energy level to first order in m/M (here and in what follows, the Dirac wave functions are the eigenvectors of the Dirac-Coulomb-Breit Hamiltonian). An independent derivation of Hamiltonian (3) was presented in Ref. [11]. In Ref. [12], this Hamiltonian was employed to calculate the $(\alpha Z)^4 m^2/M$ corrections to the energy levels of He- and Li-like middle- Z ions.

According to expression (3), the lowest-order relativistic correction to the one-electron recoil operator is given by

$$H_{\text{NMS}}^{(\text{r})} = -\frac{1}{2M} \sum_i \frac{\alpha Z}{r_i} \left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right) \cdot \mathbf{p}_i, \quad (4)$$

The corresponding two-electron correction is

$$H_{\text{SMS}}^{(r)} = -\frac{1}{2M} \sum_{i \neq j} \frac{\alpha Z}{r_i} \left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right) \cdot \mathbf{p}_j. \quad (5)$$

To the lowest order in m/M , the mass isotope shift is determined as the difference of the expectation values of the recoil Hamiltonian for two different isotopes:

$$\delta E_{\text{MS}} = \langle \psi | (H_{M_1} - H_{M_2}) | \psi \rangle = -\frac{\delta M}{M_1 M_2} K, \quad (6)$$

where $\delta M = M_1 - M_2$ is the nuclear mass difference, $|\psi\rangle$ is the eigenvector of the Dirac-Coulomb-Breit Hamiltonian, and the constant K is defined by

$$K/M = \langle \psi | H_M | \psi \rangle. \quad (7)$$

It should be stressed here that our approach to the relativistic recoil effect differs from those in Refs. [13–16], where the nonrelativistic recoil Hamiltonian was evaluated with the Dirac wave functions. Averaging the nonrelativistic recoil operator with the Dirac wave functions strongly overestimates the relativistic correction to the recoil effect. It is caused by the fact (see Refs. [3,8]) that the relativistic contribution that results from averaging the nonrelativistic nuclear recoil operator with the Dirac wave functions is considerably canceled by the contribution of the relativistic correction operator defined by Eqs. (4) and (5). For this reason, the relativistic wave functions must be employed only in calculations with the relativistic recoil Hamiltonian (3).

III. FIELD SHIFT

The field isotope shift is caused by different nuclear charge distributions for different isotopes. For the nuclear charge distribution we used the Fermi model:

$$\rho(r, R) = \frac{N}{1 + \exp[(r - c)/a]}, \quad (8)$$

where the parameter a was chosen to be $a = 2.3/4 \ln 3$ and parameters N and c can be obtained from the known value of the root-mean-square (rms) nuclear charge radius $R = \langle r^2 \rangle^{1/2}$ and from the normalization condition for $\rho(r, R)$:

$$\int dr \rho(r, R) = 1. \quad (9)$$

With a high accuracy, N and c can be determined by the following analytical formulas (see, e.g., Ref. [17]):

$$N = \frac{3}{4\pi c^3} \left(1 + \frac{\pi^2 a^2}{c^2} \right)^{-1},$$

$$c = \sqrt{\frac{5}{3} \langle r^2 \rangle - \frac{7}{3} \pi^2 a^2}. \quad (10)$$

The potential of an extended nucleus is given by

$$V_N(r, R) = -4\pi\alpha Z \int_0^\infty dr' r'^2 \rho(r', R) \frac{1}{r_{>}},$$

$$r_{>} = \max(r, r'). \quad (11)$$

This potential was used in the Dirac-Coulomb-Breit Hamiltonian to obtain the relativistic wave functions. The field isotope shift can be determined by the formula

$$\delta E_{\text{FS}} = \left\langle \psi \left| \sum_i \delta V_N(r_i, R) \right| \psi \right\rangle, \quad (12)$$

where

$$\delta V_N(r) = V_N(r, R + \delta R) - V_N(r, R), \quad (13)$$

δR is the difference of the rms nuclear charge radii for two isotopes. Within the precision required, the direct evaluation of the field isotope shift by solving the Dirac-Coulomb-Breit equation for two different isotopes yields the same results.

Concluding this section, we note that in the case of a hydrogenlike atom the isotope shift can easily be calculated according to analytical formulas presented in Ref. [17].

IV. METHOD OF CALCULATION

In this work, the large-scale configuration-interaction (CI) Dirac-Fock (DF) method was used to solve the Dirac-Coulomb-Breit equation and to calculate the energies and the

TABLE I. The specific-mass-shift contribution to the isotope shift constant K (GHz amu) for the $3p_{1/2}-3s$ transition in Na-like ions. NSMS, nonrelativistic specific-mass shift; SMS, specific mass shift calculated with the Dirac wave function; RSMS, relativistic-operator correction to the specific mass shift; total, SMS + RSMS.

Ion	NSMS	SMS	SMS – NSMS	RSMS	Total	SMS [15]
Na	–100.1	–101.0	–0.9	2.5	–98.5	–97
Mg ¹⁺	–412.7	–416.1	–3.4	10.0	–406.1	–362
Al ²⁺	–926.3	–934.8	–8.5	24.0	–910.8	–837
Cl ⁶⁺	–5082.9	–5162.4	–79.5	183.2	–4979.3	–4846
Ar ⁷⁺	–6648.2	–6765.7	–117.5	261.6	–6504.1	–6363
Fe ¹⁵⁺	–26677	–27713	–1036	1995.3	–25718.6	–25662
Xe ⁴³⁺	–200802	–240996	–40194	69295	–171701	

TABLE II. Field-shift constant F (MHz/fm²) for the $3p_{1/2}$ - $3s$ transition in Na-like ions. $\langle r^2 \rangle^{1/2} = 0.836A^{1/3} + 0.570$ (A is the atomic mass number). NFS, nonrelativistic field-shift constant; FS, relativistic field-shift constant.

Ion	NFS	FS	FS [15]
Na	34.6	36.45	38.4
Mg ¹⁺	115.9	123.2	125.8
Al ²⁺	247.3	265.3	268.4
Cl ⁶⁺	1538.8	1726.2	1729.7
Ar ⁷⁺	2133.8	2423.4	2426.5
Fe ¹⁵⁺	14095.9	18107.9	18115
Xe ⁴³⁺	373760	965738	

isotope shifts of the forbidden transitions in Ar¹⁴⁺, Ar¹³⁺, and Kr²²⁺. The many-electron wave function $\Psi(\gamma J)$ with quantum numbers γ and J was expanded in terms of a large number of the configuration state functions (CSFs) with the same J ,

$$\Psi(\gamma J) = \sum_{\alpha} c_{\alpha} \Phi_{\alpha}(J). \quad (14)$$

For every relativistic atomic configuration the CSFs $\Phi_{\alpha}(J)$ are eigenfunctions of the square of total angular momentum J^2 and they can be obtained as the linear combinations of the Slater determinants corresponding to this configuration. The set of the CSFs in expansion (14) was generated including all single and double excitations and some part of triple excitations.

The Slater determinants are constructed from one-electron four-component Dirac spinors (orbitals). For the occupied shells these orbitals (φ_j) were obtained by the multiconfiguration DF method. The other vacant orbitals ($\tilde{\varphi}_j$) were obtained by solving the Dirac-Fock-Sturm equations

$$[h^{\text{DF}} - \varepsilon_{j_0}] \tilde{\varphi}_j = \lambda_j W(r) \tilde{\varphi}_j, \quad (15)$$

where h^{DF} is the Dirac-Fock operator, ε_{j_0} is the one-electron energy of the occupied DF orbital φ_{j_0} , and $W(r)$ is a constant sign weight function. The parameter λ_j in Eq. (15) can be considered as an eigenvalue of the Sturmian operator. If $W(r) \rightarrow 0$ at $r \rightarrow \infty$, all Sturmian functions φ_j have the same asymptotics at $r \rightarrow \infty$. It is clear that for $\lambda_j = 0$ the Sturmian

function coincides with the reference DF orbital φ_{j_0} . The widely known choice of the weight function is $W(r) = 1/r$, which leads to the well-known ‘‘charge quantization.’’ In the relativistic case this choice of the weight function is not very successful. In our calculations we used the following weight function:

$$W(r) = \frac{1 - \exp[-(ar)^2]}{(ar)^2}. \quad (16)$$

In contrast to $1/r$, this weight function is regular at origin. It is well known that the Sturmian operator is Hermitian and it does not contain continuum spectra in contrast to the Fock operator. Therefore, the set of the Sturmian eigenfunctions forms the discrete and complete basis set of one-electron wave functions.

V. RESULTS AND DISCUSSION

Before discussing our results for the isotope shifts in argon ions, we examine our calculations of the specific mass shift for the $3p_{1/2}$ - $3s$ transition in Na-like ions and compare them with the related results from Ref. [15]. In Table I we present our results for the SMS contribution to the isotope-shift constant K , defined by Eq. (7). The second column shows the nonrelativistic values of this contribution. These values were obtained within the same CIDF method and the same computer code, as described above, by the 1000-times increase of the velocity of light (in atomic units). We verified this nonrelativistic limit by comparing the total energies for the Dirac-Coulomb-Breit Hamiltonian with the total energies obtained by the fully nonrelativistic method based on the Schrödinger Hamiltonian and on the same calculation scheme. The total energies exactly coincide with each other for all the ions. In the third column we present the results obtained by averaging the nonrelativistic-recoil-operator (2) on the Dirac wave functions. The fourth column indicates the relativistic correction that results from using the Dirac wave functions in the calculation of the nonrelativistic-recoil-operator contribution. In the fifth column we give the relativistic correction obtained by averaging the relativistic correction operator (5). In the sixth column the total relativistic data are listed. The last column indicates the results of Ref. [15], based on averaging the nonrelativistic recoil operator

TABLE III. Individual contributions to the isotope shifts of the forbidden transition in ⁴⁰Ar: ³⁶Ar and ⁸⁶Kr: ⁸⁴Kr (cm⁻¹). The rms nuclear charge radii used in the calculation are $\langle r^2 \rangle^{1/2} = 3.390, 3.427, 4.188,$ and 4.184 fm for ³⁶Ar, ⁴⁰Ar, ⁸⁴Kr, and ⁸⁶Kr, respectively [20]. NMS, normal mass shift calculated with the Dirac wave function; SMS, specific mass shift calculated with the Dirac wave function; RNMS, relativistic-operator correction to the normal mass shift; RSMS, relativistic-operator correction to the specific mass shift; FS, field shift.

Ion	Transition	NMS	SMS	RNMS	RSMS	FS	Total
Ar ¹³⁺	$2s^2 2p^1 \ ^2P_{1/2} - \ ^2P_{3/2}$	0.1053	-0.0742	-0.0822	0.1151	-0.0005	0.0635
Ar ¹⁴⁺	$2s^1 2p^1 \ ^3P_1 - \ ^3P_2$	0.0797	-0.0698	-0.0627	0.0887	-0.0001	0.0358
Kr ²²⁺	$3s^2 3p^2 \ ^3P_1 - \ ^3P_2$	0.0053	0.0010	-0.0025	0.0000	0.0001	0.0039

TABLE IV. Energies of forbidden transitions for Ar and Kr ions and the isotope shifts in ^{40}Ar : ^{36}Ar and ^{86}Kr : ^{84}Kr .

Ion	Transition	Theory [22,23] λ (nm, air)	Theory [1], this work λ (nm, air)	Experiment [1] λ (nm, air)	Isotope shifts (nm)
Ar^{13+}	$2s^2 2p^1 \ ^2P_{1/2} - ^2P_{3/2}$	440.99	441.16(27)	441.2559(1)	0.00126
Ar^{14+}	$2s^1 2p^1 \ ^3P_1 - ^3P_2$	593.88	594.24(30)	594.3880(3)	0.00136
Kr^{22+}	$3s^2 3p^2 \ ^3P_1 - ^3P_2$		383.70(65)	384.1146(2)	0.00005

with the Dirac wave functions. Comparing the relativistic corrections, presented in the fourth and fifth columns, we observe that the absolute value of the second relativistic correction is larger than the absolute value of the first one and, as a result, the total relativistic correction and the correction that accounts only for the relativistic effects on the wave functions are of opposite sign. This means that using only the nonrelativistic part of the recoil operator in calculations based on employing the Dirac wave functions gives strongly incorrect results for the relativistic recoil effect.

For the $3p_{1/2} - 3s$ transition in neutral Na, the experimental value of the isotope shift amounts to $-758.5(0.7)$ MHz [18]. To derive the corresponding SMS we have to subtract the NMS and FS (field shift) from the experimental isotope shift. The nonrelativistic NMS has been evaluated as the $-m(1/M_1 - 1/M_2)$ fraction of the nonrelativistic transition energy, obtained as the difference between the experimental value of the transition energy (16956.2 cm^{-1}) and the related relativistic correction (45.4 cm^{-1}), calculated in this work. As a result, the nonrelativistic NMS was obtained to be -547.5 MHz. The sum of this value and the relativistic NMS correction (-9.7 MHz), calculated in this work, yields -557.2 MHz for the total NMS value. Subtracting this NMS value and our theoretical FS value (6.9 MHz) from the experimental isotope shift, we obtain the value -208.2 MHz for the SMS and -105.8 GHz amu for the SMS contribution to the constant K . This value differs from our theoretical result -98.5 GHz amu (Table I) by 7% and from the result of Ref. [15] by 9%. The disagreement between the theoretical and experimental values is mainly caused by the correlation effects, which are extremely large for neutral Na. It is very difficult to compute the isotope shift parameters for neutral Na with high accuracy. For systematic investigations of the nonrelativistic isotope shift by the multiconfiguration Hartree-Fock method we refer to Ref. [19], where an extremely large CI expansion was used. Although in our relativistic calculations the CI expansion is not so large, it is sufficient to show the role of the relativistic effects in the series of Na-like ions. Adding our relativistic correction to the nonrelativistic contribution from [19] yields $K = -103.9$ GHz amu that is in fair agreement with the experimental value presented above.

Table II shows the field-shift constant F , defined by $\delta E_{\text{FS}} = -F \delta \langle r^2 \rangle$, for the $3p_{1/2} - 3s$ transition in Na-like ions. The comparison of the nonrelativistic (second column) and relativistic (third column) data demonstrates the role of the relativistic effects in the field isotope shifts. Our relativistic field-shift constants are in a good agreement with the related

data from Ref. [15], presented in the fourth column of the table.

In Table III we present the results of our calculations for the isotope shifts in $^{40}\text{Ar}^{13+}$: $^{36}\text{Ar}^{13+}$, $^{40}\text{Ar}^{14+}$: $^{36}\text{Ar}^{14+}$, and $^{86}\text{Kr}^{22+}$: $^{84}\text{Kr}^{22+}$. To calculate the field isotope shift, we used the rms nuclear charge radii given in Ref. [20]. Since we consider transitions between levels which differ from each other only by the total angular momentum, the corresponding transition energies are completely determined by relativistic and QED effects. In particular, it means that all the mass- and field-shift contributions given in the table are of pure relativistic origin. Comparing the individual mass-shift contributions given in the Table III, we again observe a very significant cancellation of the contributions from the nonrelativistic part of the recoil operator ($H_{\text{NMS}}^{(\text{nr})} + H_{\text{SMS}}^{(\text{nr})}$) by the corresponding contributions from the relativistic part of the recoil operator ($H_{\text{NMS}}^{(\text{r})} + H_{\text{SMS}}^{(\text{r})}$). It can also be seen that the mass isotope shift strongly dominates over the field isotope shift for the ions under consideration.

In Table IV, we compare the isotope shifts calculated in this paper with the total theoretical and experimental values for the transition energies under consideration [1]. The non-QED parts of the theoretical values for the transition energies were obtained by the large-scale CIDF method described in the preceding section. The QED corrections were evaluated by using the one-electron Lamb shift data taken from Ref. [21] with an effective nuclear charge number Z_{eff} . For a given one-electron state, Z_{eff} was chosen to reproduce the related DF electron charged density at the Compton wavelength distance from the nucleus. For the argon ions, these results are also in a fair agreement with the corresponding results of Refs. [22,23] presented in the third column. In the sixth column of Table IV we present the total isotope shifts in $^{40}\text{Ar}^{13+}$: $^{36}\text{Ar}^{13+}$. These data were obtained with the Dirac multiconfiguration wave functions and their relative errors are determined by the relative errors in the wave functions. As one can see from the table, the isotope shift in $^{40}\text{Ar}^{13+}$: $^{36}\text{Ar}^{13+}$ is by an order of magnitude larger than the current experimental error. This provides very good perspectives for a first test of the relativistic theory for the recoil effect in middle- Z ions.

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