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Theoretical isotope shifts in neutral barium

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The present work deals with a set of problems in isotope shifts of neutral barium spectral lines. Some well-known transitions ($6s^2\,{}^1S_0$–$6s6p\,{}^{1,3}P_1^o$ and $6s^2\,{}^1S_0$–$6p^2\,{}^3P_0$) are investigated. Values of the changes in the nuclear mean-square charge radius are deduced from the available experimental isotope shifts using our *ab initio* electronic factors. The three sets $\{\delta\langle r^2\rangle^{A,A'}\}$ obtained from these lines are consistent with each other. The combination of the available nuclear mean-square radii with our electronic factors for the $6s5d\,{}^3D_{1,2}$–$6s6p\,{}^1P_1^o$ transitions produces isotope shift values in conflict with the laser spectroscopy measurements of U. Dammalapati *et al.* [Eur. Phys. J. D **53**, 1 (2009)].

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I. INTRODUCTION

The first isotope shift (IS) measurements on barium were done by Arroe [1], who studied the resonance transition $6s^2\,{}^1S_0$–$6s6p\,{}^1P_1^o$ of neutral barium located at a wavelength of $\lambda_1 = 553.7$ nm. One of the first attempts to obtain the differences in nuclear mean-square charge radii of the radioactive barium nuclides ${}^{140-134}$Ba was done by Fischer *et al.* [2], who investigated experimentally and theoretically the IS in the Ba II resonance line $6s\,{}^2S_{1/2}$–$6p\,{}^2P_{1/2}^o$ at $\lambda = 493.4$ nm. Their results are often used by other authors. Later, the Doppler-free spectroscopy was explored by Nowicki *et al.* [3,4], who studied the neutron-deficient isotopes ^{131}Ba and ^{128}Ba. Using the same procedure Bekk *et al.* [5] pursued the work of Nowicki *et al.* with other unstable isotopes. Concurrently but independently, Baird *et al.* [6] proposed a similar experiment. Years later, thanks to high-resolution laser spectroscopy, Grundevik *et al.* [7] explored the far-red transitions between the $6s5d$ and the $6p5d$ configurations and, in continuity, investigated the spin-forbidden transition $6s^2\,{}^1S_0$–$6s6p\,{}^3P_1^o$ at $\lambda_2 = 791.3$ nm [8]. In a work by Mueller *et al.* [9], collinear laser spectroscopy has been connected to the mass separator ISOLDE-II at CERN. One of the aims of this experiment was to extend the knowledge on fundamental nuclear properties into regions far from stability. In that context, ISs of barium isotopes in the mass range 122–146 have been measured for the λ_1 atomic transition. Finally, Wijngaarden and Li [10] (re)measured the IS of the same transition using a ring dye laser and obtained the most recent and precise IS values of this line. Many other measurements were also reported on highly excited states of Ba I [11,12].

Theoretical barium studies are far less advanced. In 1974, Trefftz *et al.* [13] performed calculations on various states of barium using MCHF wave functions generated with the code of Froese Fischer [14] but did not study IS. King and Wilson [15] used a modified version of the latter program that includes the mass velocity and Darwin terms in order to calculate electron densities at the nucleus. In addition, Fricke *et al.* [16] and Olsson *et al.* [17] used multiconfiguration Dirac-Hartree-Fock wave functions to compute electronic F factors. Finally, in an unpublished work, Kozlov and Korol [18] calculated the FS and MS of Ba I and Ba II using second-order many-body perturbation theory to take core-valence and valence correlations into account.

Our interest was stimulated by the paper of Dammalapati *et al.* [19], who reported the first laser spectroscopy measurements of the $6s5d\,{}^3D_{1,2}$–$6s6p\,{}^1P_1^o$ transitions for several isotopes. Observing that the resulting ISs strongly deviate from their expected behavior for odd isotopes in an analysis based on King plots, the authors pointed out that there were no theoretical calculations available for comparison.

II. ISOTOPE SHIFT THEORY

The main ideas of the IS theory are outlined here. The interested reader should look at the pioneer works by Shabaev [20–24] and Palmer [25], who expressed the theory of the relativistic MS as used in the present work. The tensorial form of the relativistic recoil operator was derived by Gaidamauskas *et al.* [26]. Based on those developments a module, called RIS3 (relativistic isotope shift), was designed [27] for the revised version of the GRASP2K package [28].

A. Mass shift

The finite mass of the nucleus gives rise to a recoil effect, called the mass shift (MS). The nuclear recoil corrections within the $(\alpha Z)^4 m^2/M$ approximation are obtained by evaluating the expectation values of the operator,

$$H_{\rm MS} = \frac{1}{2M}\sum_{i,j}^{N}\left(\mathbf{p}_i\cdot\mathbf{p}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\mathbf{r}_i)\,\mathbf{r}_i}{r_i^2}\right)\cdot\mathbf{p}_j\right). \tag{1}$$

Separating the one-body ($i = j$) and two-body ($i \neq j$) terms that, respectively, constitute the normal mass shift (NMS) and specific mass shift (SMS) contributions, Hamiltonian (1) becomes

$$H_{\rm MS} = H_{\rm NMS} + H_{\rm SMS}. \tag{2}$$

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The (mass-independent) NMS, $K_{\rm NMS}$, and SMS, $K_{\rm SMS}$, parameters are defined by the following expressions:

$$K_{\rm NMS} \equiv M\langle\Psi|H_{\rm NMS}|\Psi\rangle, \tag{3}$$

and

$$K_{\rm SMS} \equiv M\langle\Psi|H_{\rm SMS}|\Psi\rangle. \tag{4}$$

When discussing a transition IS, one needs to consider the variation of the mass parameter from one level to another. The corresponding line frequency isotope MS is written as the sum of the NMS and SMS contributions,

$$\delta\nu_{k,\rm MS}^{A,A'} = \delta\nu_{k,\rm NMS}^{A,A'} + \delta\nu_{k,\rm SMS}^{A,A'}, \tag{5}$$

with

$$\delta\nu_{k,\rm MS}^{A,A'} = \left(\frac{M'-M}{MM'}\right)\frac{\Delta K_{\rm MS}}{h} = \left(\frac{M'-M}{MM'}\right)\Delta\widetilde{K}_{\rm MS}, \tag{6}$$

where $\Delta K_{\rm MS} = (K_{u,\rm MS} - K_{\ell,\rm MS})$ is the difference of the $K_{\rm MS}$ $(= K_{\rm NMS} + K_{\rm SMS})$ parameters of the levels involved in the transition k. For $\widetilde{K}$, the unit (GHz u) is often used in the literature. As far as the conversion factors are concerned, we use $\Delta K_{\rm MS}[m_e E_{\rm h}] = 3609.4824\Delta\widetilde{K}_{\rm MS}[\rm GHzu]$.

B. Field shift

The energy shift arising from the difference in nuclear charge distributions between two isotopes, A and A', for levels $i = (\ell,u)$ involved in transition k, the frequency field shift (FS) of the spectral line k can be written as [29–31]

$$\delta\nu_{k,\rm FS}^{A,A'} = \frac{\delta E_{u,\rm FS}^{A,A'} - \delta E_{\ell,\rm FS}^{A,A'}}{h} \approx F_k\delta\langle r^2\rangle^{A,A'}. \tag{7}$$

F_k is the line electronic factor

$$F_k = \frac{2\pi}{3h}Z\left(\frac{e^2}{4\pi\epsilon_0}\right)\Delta|\Psi(0)|^2_k, \tag{8}$$

proportional to the change of the total probability density at the origin associated with the electronic transition between level ℓ and level u. In this approximation, the first-order frequency FS becomes

$$\begin{aligned}\delta\nu_{k,\rm FS}^{A,A'} &= F_k\;\delta\langle r^2\rangle^{A,A'}\\ &= \frac{Z}{3\hbar}\left(\frac{e^2}{4\pi\epsilon_0}\right)\;\Delta|\Psi(0)|^2_k\;\delta\langle r^2\rangle^{A,A'}. \end{aligned} \tag{9}$$

C. The total isotope shift

It is easy to estimate the total line frequency shift by merely adding the MS, (5), and FS, (7) or (9), contributions:

$$\delta\nu_k^{A,A'} = \overbrace{\delta\nu_{k,\rm NMS}^{A,A'} + \delta\nu_{k,\rm SMS}^{A,A'}}^{\delta\nu_{k,\rm MS}^{A,A'}} + \delta\nu_{k,\rm FS}^{A,A'} \tag{10}$$

$$= \left(\frac{M'-M}{MM'}\right)\Delta\widetilde{K}_{\rm MS} + F_k\delta\langle r^2\rangle^{A,A'}. \tag{11}$$

III. COMPUTATIONAL PROCEDURE

The multiconfiguration Dirac-Hartree-Fock method [32], as implemented in the GRASP2K program package [28,33], is employed to obtain approximate wave functions that we refer to as atomic state wave functions. An atomic state wave function is represented by a linear combination of configuration state functions (CSFs) with the same parity P, total angular momentum J, and component M_J along the z direction,

$$\Psi(\gamma\;PJM_J) = \sum_{j=1}^{\rm NCSFs} c_j\;\Phi(\gamma_j PJM_J), \tag{12}$$

where $\{c_j\}$ are the mixing coefficients and $\{\gamma_j\}$ the sets of quantum numbers needed for specifying unambiguously CSFs. The latter are built from single-electron orbital wave functions. Applying the variational principle, the mixing coefficients and single-electron orbital wave functions are optimized simultaneously in the relativistic self-consistent field method. The energy functional is estimated from the expectation value of the Dirac-Coulomb (DC) Hamiltonian [34],

$$H_{\rm DC} = \sum_{i=1}^{N}[c\boldsymbol{\alpha}_i\cdot\mathbf{p}_i + (\beta_i - 1)c^2 + V(r_i)] + \sum_{i<j}^{N}\frac{1}{r_{ij}}, \tag{13}$$

where $V(r_i)$ is the monopole part of the electron-nucleus interaction, $\boldsymbol{\alpha}$ and β are the (4×4) Dirac matrices, and c is the speed of light [$c = 1/\alpha$ in atomic units (a.u.), where α is the fine-structure constant].

To effectively capture major electron correlation, CSFs of a particular parity and symmetry are generated through substitutions within an active set of orbitals occupied in the reference configuration. As regards the hardware and software limitations, it is obviously impossible to use complete active-space wave functions that would include all CSFs with the right symmetry for a given orbital active set. The CSF expansions have to be constrained so that the major correlation excitations are taken into account. In our calculations an approach based on single (S) and restricted double (rD) substitutions was applied [38]. rD substitutions limit the excitations to maximum one hole in the core. In the case of barium ([Xe] $6s^2$, [Xe] $6s6p$, [Xe] $6p^2$, [Xe] $6s5d$), double excitations are applied to the valence shells but with the restriction that, at most, one electron is substituted from $1s2sp3spd4spd5sp$ [Xe] shells, the other(s) involving the $6s$, $5d$, or $6p$ valence shells of the considered reference configuration. All occupied orbitals in the reference configuration are treated as spectroscopic and are obtained in the Dirac-Hartree-Fock (DHF) single-configuration approximation. These orbitals are frozen in all subsequent calculations. The J levels belonging to a given term were optimized simultaneously with standard weights through the Extended Optimal Level (EOL) scheme and the set of virtual orbitals is increased layer by layer. Starting from the $n = 9$ correlation layer, the core is fully opened but the new CSFs are generated by single excitations from the reference. The effect of adding the Breit interaction to the DC Hamiltonian, (13), is estimated to be much smaller than the uncertainty in the transition IS parameters with respect to the correlation model. This interaction has therefore been neglected.

TABLE I. Sample from several sources of the nuclear rms radii and difference in the nuclear mean-square charge radii relative to that of ^{138}Ba (in fm and fm^2, respectively).

	Semiempirical formula (14)		From Angeli [35]		From Angeli and Marinova [36]	
	$\langle r^2\rangle^{1/2}$	$\delta\langle r^2\rangle^{138,A}$	$\langle r^2\rangle^{1/2}$	$\delta\langle r^2\rangle^{138,A}$	$\langle r^2\rangle^{1/2}$	$\delta\langle r^2\rangle^{138,A}$
^{138}Ba	4.8901	0.0	4.8385(48)	0.0	4.8378(46)	0.0
^{137}Ba	4.8798	0.1006	4.8326(48)	0.0571	4.8314(47)	0.0609(2)
^{136}Ba	4.8692	0.2040	4.8327(48)	0.0561	4.8334(46)	0.0422(2)
^{135}Ba	4.8586	0.3071	4.8273(48)	0.1082	4.8294(47)	0.0812(3)
			$\delta\langle r^2\rangle^{138,A}$ value from			
	Ref. [4]	Ref. [5]	Ref. [6]	Ref. [37]	Ref. [7]	Ref. [10]
^{138}Ba	0.0	0.0	0.0	0.0	0.0	0.0
^{137}Ba	0.049(2)	0.059(4)	0.067	0.072(6)	0.059(6)	0.049
^{136}Ba	0.034(3)	0.041(8)	0.061	0.044(4)	0.042(7)	0.034
^{135}Ba	0.066(5)	0.079(12)	0.108	0.088(7)	0.080(10)	0.065
^{134}Ba	0.044(7)	0.053(16)	0.095	0.051(7)	0.056(10)	/

IV. ISOTOPE SHIFTS OF NEUTRAL BARIUM

A. A large "choice" of nuclear radii

The reliability of the FS values obtained with the *ab initio* electronic F factor, (8), is a function of the accuracy of the calculations, but also of the level of confidence on the nuclear data $\delta\langle r^2\rangle^{A,A'}$. Table I lists nuclear root-mean-square (rms) charge radii and mean-square charge radii differences from several sources, taking ^{138}Ba as the reference isotope. The aim of this table is to illustrate the difficulties in reducing uncertainties in the nuclear rms charge radii. The first pair of columns is obtained with the semiempirical formula

$$R_{\text{rms}} = \langle r^2\rangle^{1/2} = 0.836A^{1/3} + 0.570\ \text{fm}, \quad \text{if A} > 9, \tag{14}$$

and is compared with the values compiled by Angeli [35] and Angeli and Marinova [36]. The positive sign of $\delta\langle r^2\rangle$ (according to the convention $\delta\langle r^2\rangle^{A,A'} = \langle r^2\rangle^{A} - \langle r^2\rangle^{A'}$ with $A > A'$) indicates that the neutron-deficient isotopes of barium have smaller rms radii than ^{138}Ba.

The remaining two pairs of columns report the $\delta\langle r^2\rangle^{138,A}$ values deduced using different techniques. Bekk *et al.* [5] measured IS by laser-induced resonance fluorescence on an atomic beam of a sample of barium. In continuity of the work by Nowicki *et al.* [4], they connected their IS measurement of the $^1S_0 - {}^1P_1^o$ transition in Ba I to the data of Fischer *et al.* [2] on the $\lambda = 493.4$ nm transition of Ba II via a King plot. Thanks to the electronic factor F and SMS value deduced in [2], Bekk *et al.* [5] were able to get their own F factor. They deduced the NMS through the relation

$$\delta\nu_{\text{NMS}}^{A,A'} \simeq \left(\frac{m_e}{M'} - \frac{m_e}{M}\right)\nu_{\text{exp}} \tag{15}$$

and, assuming that $\delta\nu_{\text{SMS}} = (0 \pm 1)\delta\nu_{\text{NMS}}$ [4], obtained the nuclear mean-square charge radius values. As pointed out by the authors themselves, the latter approximation is the major source of the uncertainties in $\delta\langle r^2\rangle$. Baird *et al.* [6] combined their own results with other optical data and electronic x-ray measurements. Muonic x-ray measurements of the nuclear charge radii and $\delta\langle r^2\rangle$ values were presented by Shera *et al.* [37]. By comparing IS data on the $^1S_0 - {}^1P_1^o$ transition with the muonic $\delta\langle r^2\rangle$ values, Shera *et al.* extracted the electronic factor. Grundevik *et al.* [7] reevaluated the SMS values in the Ba I and Ba II resonance transitions and obtained results strongly consistent with [5]. On their side, van Wijngaarden and Li [10] used the procedure proposed by [4] on their new IS measurements. Using the electronic factor of Fischer *et al.* [2], they deduce a new value of the variation of the nuclear mean-square $\delta\langle r^2\rangle$ in very good agreement with [4].

It is noteworthy that in some cases the rms charge radius $\langle r^2\rangle^{1/2}$ decreases when the number of neutrons increases along the isotope chain. This will never be reflected when using the semiempirical formula, (14), whose values increase monotonically. Therefore, in the present paper, this approach will be left aside when rms charge radii are needed, in favor of data from the literature such as Angeli (and Marinova)'s compilations [35,36]. In addition, Table I demonstrates the difficulties in isolating the nuclear rms radius and sheds light on the remaining large uncertainties in the $\delta\langle r^2\rangle$ nuclear data for these systems.

B. Some well-known transitions

The resonance transition $6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$ is maybe the most well-known in barium and is, together with the intercombination line $6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$, a good starting point of our analysis. ^{138}Ba is the most abundant isotope of barium on Earth, with its 82 neutrons, and as such is often chosen as the pivot; the IS relative to isotope 138 are given from $A = 137$ to $A = 134$ in Table II. Some details behind these measurements are given in Sec. I. The values of Arroe [1], originally given in cm^{-1}, were converted so that the given error bars of $\pm 0.7 \times 10^{-3}$cm^{-1} become ± 21 MHz.

The negative signs indicate that the isotope ^{138}Ba has the lowest line frequency for each $^{138,A'}$Ba isotope pair ($A' < 138$). Assuming the dominance of the FS, these isotopes behave in the most current way, considering the density reduction with electronic excitations (i.e., $\delta\nu_{\text{FS}}^{A,A'} < 0$ with $A > A'$). The consistency between experiments is rather good.

Neugart *et al.* [39] and Mueller *et al.* [9] reported IS measurements for the neutron-rich isotopes ^{139}Ba to ^{144}Ba

TABLE II. Experimental measurements of isotope shifts for the transitions $6s^2\,{}^1S_0 - 6s6p\,{}^1P_1^o$ and $6s^2\,{}^1S_0 - 6s6p\,{}^3P_1^o$ (in GHz).

	^{138}Ba	^{137}Ba	^{136}Ba	^{135}Ba	^{134}Ba
			$6s^2\,{}^1S_0 - 6s6p\,{}^1P_1^o$		
Ref. [10] (1995)	0.0	−0.21515(16)	−0.12802(39)	−0.25929(17)	/
Ref. [5] (1979)	0.0	−0.2150(7)	−0.1289(5)	−0.2609(7)	−0.1430(5)
Ref. [6] (1979)	0.0	−0.2147(5)	−0.1275(13)	−0.2587(7)	−0.1428(12)
Ref. [1] (1950)	0.0	−0.16(2)	−0.066(20)	−0.22(2)	−0.13(2)
			$6s^2\,{}^1S_0 - 6s6p\,{}^3P_1^o$		
Ref. [8] (1983)	0.0	−0.1834(10)	−0.1092(10)	−0.2199(10)	−0.1223(25)

and the mean-square nuclear charge radii $\delta\langle r^2\rangle$ have been estimated following the procedure of Bekk *et al.* [5], in which the unknown SMS is taken to be of the order of the NMS. These results are presented in Table III. The relativistic coupled-cluster approach has been used by Mårtensson-Pendrill and Ynnerman [40] to calculate an electronic F factor that allowed the authors to revise the values of nuclear charge radii using optical ISs for ${}^{122-148}$Ba and muonic results for the stable isotopes ${}^{114-138}$Ba. Muonic results $\delta\langle r^2\rangle_\mu$ were used to derive a K_{SMS} parameter, itself used to extract $\delta\langle r^2\rangle_{\text{opt}}$. The error bars reflect the uncertainty in the SMS, in F, and in the optical data. The agreement within the three sets of of $\delta\langle r^2\rangle$ is quite satisfactory.

1. Mass shift calculation

The results of our calculations for the mass factors of transitions $6s^2\,{}^1S_0 - 6s6p\,{}^1P_1^o$ and $6s^2\,{}^1S_0 - 6s6p\,{}^3P_1^o$ are reported in Table IV. For each transition, the first column of data gives the value of the $\widetilde{K}_{\text{MS}}$ parameters (in GHz u), and the second column is the value of the MS (in MHz) for the isotopic pair ^{138,136}Ba [i.e., multiplying the $\widetilde{K}_{\text{MS}}$ parameter by the mass factor $(1/M_{138} - 1/M_{136})$]. Nuclear masses (M) are calculated by subtracting the mass of the electrons and the binding energy from the atomic mass (M_{atom}), using the formula

$$M(A,Z) = M_{\text{atom}}(A,Z) - Zm_e + B_{\text{el}}(Z), \qquad (16)$$

where the total electronic binding energy (expressed in eV) is estimated using [41,42]

$$B_{\text{el}}(Z) = 14.4381\,Z^{2.39} + 1.55468 \times 10^{-6} Z^{5.35}. \qquad (17)$$

Atomic masses are provided in [43].

Table IV illustrates the large correlation effects on the transition MSs. The 8SrD values are unfortunately not converged, while getting close to the available computational resources. However, a comparison of the MS with the IS values in Table II reveals that the contribution of the MS is small and represents only 5% of the total IS value for the resonance transition but reaches around 20% for the transition ${}^1S_0 - {}^3P_1^o$. In consequence, for both lines one expects a much larger contribution of the FS. For the latter, single excitations are known to be important and the addition of three more layers (9S–11S) was possible. Furthermore, one observes a much greater stability and better convergence of the transition parameter $\Delta\widetilde{K}_{\text{MS}}$ for the spin-forbidden transition (with a 0.5% difference between the $10S$ and the $11S$ values) than for the resonance transition suffering from oscillations, even in the largest calculations. Actually, the values of $\widetilde{K}_{\text{MS}}$ for the ${}^1P_1^o$ and ${}^1S_0$ levels are so close that the slightest change in the level parameter strongly affects the transition parameter $\Delta\widetilde{K}_{\text{MS}}$. The accuracy of the latter is therefore hard to evaluate but its reliability is discussed further in relation to the $\delta\langle r^2\rangle$ values that can be deduced from the experimental IS (see Table VI). Behind the value of the mass parameter $\Delta\widetilde{K}_{\text{MS}} = -61.22$ GHz u for the transition λ_1 hides the sum of $\Delta\widetilde{K}_{\text{NMS}} = 362.51$ GHz u and $\Delta\widetilde{K}_{\text{SMS}} = -423.74$ GHz u. Looking at them, it seems that the approximation $\delta\nu_{\text{SMS}} = (0 \pm 1)\delta\nu_{\text{NMS}}$ proposed by Nowicki *et al.* [4] is not senseless.

2. Field shift calculation

The level FS in Ba I is around $10^{-4} E_{\text{h}}$ for both state $6s^2\,{}^1S_0$ and state $6s6p\,{}^1P_1^o$, while the transition FS is $10^{-8} E_{\text{h}}$; a good accuracy is not easy to reach, especially for a total binding

TABLE III. Experimental measurements of neutron-rich isotope shifts for the transitions $6s^2\,{}^1S_0 - 6s6p\,{}^1P_1^o$ (in GHz) and their related difference in nuclear mean-square radii from the reference isotope ^{138}Ba.

	^{141}Ba	^{140}Ba	^{139}Ba
		$6s^2\,{}^1S_0 - 6s6p\,{}^1P_1^o$	
Ref. [39]	1.505(8)	1.075(6)	0.473(6)
Ref. [9]	1.505(5)	1.075(3)	0.473(3)
	$\delta\langle r^2\rangle^{138,141}$	$\delta\langle r^2\rangle^{138,140}$	$\delta\langle r^2\rangle^{138,139}$
Ref. [39] (1981)	−0.395(13)	−0.281(9)	−0.124(5)
Ref. [9] (1983)	−0.395	−0.281	−0.124
Ref. [40] (1992)	−0.440(1)(13)(1)	−0.314(1)(9)(1)	−0.1381(5)(41)(9)
Ref. [36] (2013)	−0.410	−0.292	−0.129

TABLE IV. Values of the $\Delta\widetilde{K}_{\mathrm{MS}}$ parameter for the $6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$ and $6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$ transitions (in GHz u) and values of the MS (in MHz) for the ^{138,136}Ba pair.

	$6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$			$6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$		
	$\Delta\widetilde{K}_{\mathrm{MS}}$	→	MS	$\Delta\widetilde{K}_{\mathrm{MS}}$	→	MS
DHF	296.65	→	−31.68	242.69	→	−25.92
6SrD	−393.26	→	42.00	−125.10	→	13.36
7SrD	−21.81	→	2.33	−203.07	→	21.69
8SrD	37.28	→	−3.98	−183.89	→	19.64
9S	61.66	→	−6.58	−184.19	→	19.67
10S	−59.65	→	6.37	−180.10	→	19.23
11S	−61.22	→	6.54	−179.14	→	19.13

energy around $-8000E_{\mathrm{h}}$. In that respect, the formalism, (9), is more reliable in view of the extreme difficulty of obtaining highly converged total energies. Furthermore, the perturbative approach offers the freedom to explore and seek the best nuclear mean-square radius.

Table V gives a chronological list of the experiments and calculations performed so far to determine the electronic F factor of the $6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$ and $6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$ transitions. In the second half of the table the results of our calculations are presented, starting from DHF to our most correlated model.

To our knowledge, it is the first time that such a highly correlated model has been used on barium. This could be an explanation for the fact that our values present some differences from the literature. For the ${}^1S_0 - {}^1P_1^o$ transition, our estimation is in favor of a large F factor, in line with Bekk *et al.* [5] and Kunold *et al.* [44]. For the spin-forbidden line, our F factor value is larger (around 37%) than any others available in the literature. The FS parameters listed in Table V have converged within 0.1% for both transitions.

TABLE V. Comparison of different theoretical and experimental determinations of the electronic F factor.

	F (GHz/fm^2)	
	$6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$	$6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$
Theory		
Ref. [8]	−2.34	−2.34
Ref. [16]	−2.99	−2.55
Ref. [30]	−2.996	−2.546
Ref. [17]	−2.998	−2.544
Ref. [40]	−3.39(10)	
Experiment		
Ref. [5]	−3.929	
Ref. [37]	−3.04(26)	
Ref. [16]		−2.59(22)
Ref. [44]	−3.99(65)	
	GRASP2K	
This work		
DHF	−3.48	−2.76
⋮	⋮	⋮
10S	−3.95	−3.49
11S	−3.95	−3.49

TABLE VI. Extraction of $\delta\langle r^2\rangle$ values (in fm^2) using experimental IS values (in MHz) from the literature and our electronic factors MS (in MHz) and F (in GHz fm^2).

	$\delta\langle r^2\rangle = (\mathrm{IS} - \mathrm{MS})/F$		
	$(\mathrm{IS}_{\mathrm{exp}} - \mathrm{MS})/F$	→	$\delta\langle r^2\rangle^{138,A}$
	$6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$		
^{141}Ba	$(1505(8) + 9.48)/-3.95$	→	−0.3832(20)
^{140}Ba	$(1075(6) + 6.37)/-3.95$	→	−0.2736(15)
^{139}Ba	$(473(6) + 3.21)/-3.95$	→	−0.1205(15)
^{137}Ba	$(-215.15(16) - 3.24)/-3.95$	→	0.0553(0)
^{136}Ba	$(-128.02(39) - 6.54)/-3.95$	→	0.0341(1)
^{135}Ba	$(-259.29(17) - 9.88)/-3.95$	→	0.0681(0)
^{134}Ba	$(-143.0(5) - 13.3)/-3.95$	→	0.0395(13)
	$6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$		
^{137}Ba	$(-183.4(1.0) - 9.49)/-3.49$	→	0.0553(3)
^{136}Ba	$(-109.2(1.0) - 19.13)/-3.49$	→	0.0368(3)
^{135}Ba	$(-219.9(1.0) - 28.90)/-3.49$	→	0.0714(3)
^{134}Ba	$(-122.3(2.5) - 38.83)/-3.49$	→	0.0462(7)
	$6s^2\,{}^1S_0{-}6p^2\,{}^3P_0$		
^{137}Ba	$(-331.7(5.0) - 21.49)/-7.09$	→	0.0498(7)
^{136}Ba	$(-199.0(3.0) - 43.33)/-7.09$	→	0.0342(4)
^{135}Ba	$(-396.1(5.9) - 65.45)/-7.09$	→	0.0651(8)
^{134}Ba	$(-219.0(9.9) - 88.94)/-7.09$	→	0.0433(14)

3. $\delta\langle r^2\rangle^{A,A'}$ extraction

Thanks to the $\Delta\widetilde{K}_{\mathrm{MS}}$ parameters in Table IV, the electronic F factors in Table V, and formula (11), we propose to isolate the values of $\delta\langle r^2\rangle$ that would reproduce the total measured IS value (see Tables II and III). These values are reported in the last column of Table VI. For the transition $6s^2\,{}^1S_0{-}6s6p\,{}^1P_1^o$, one uses the IS values of van Wijngaarden and Li, which appear to be the most precise experimental values. It is possible to double-check the consistency of our results by extracting the $\delta\langle r^2\rangle$ values from the experimental IS of the other transition, i.e., $6s^2\,{}^1S_0{-}6s6p\,{}^3P_1^o$ [7]. These results are presented in Table VI and look really promising. Error bars on $\delta\langle r^2\rangle^{138,A}$ reflect the uncertainty in the IS measurements. The $\delta\langle r^2\rangle^{138,137}$ values obtained from these two transitions differ by less than 1%. The $\delta\langle r^2\rangle^{138,136}$ and $\delta\langle r^2\rangle^{138,135}$ values resulting from the two lines agree within 8% to 5%, respectively. However, the $\delta\langle r^2\rangle^{138,134}$ values reveal a discrepancy of 17%.

The ISs of the $6s^2\,{}^1S_0{-}6p^2\,{}^3P_0$ transition listed in Table VI are taken from the work of Jitschin and Meisel [45]. They resolved the IS for several highly excited states, using Doppler-free two-photon laser spectroscopy. They needed the relevant electronic F factors to extract the $\delta\langle r^2\rangle$ values and the only response was from Olsson *et al.* [17]. Based on the correlation model detailed in Sec. III, we calculated the IS parameters of the $6p^2\,{}^3P_0$ state. The errors bars are sensitively larger than for the two other experiments. However, the consistency among the three independent sets gives us confidence in the reliability

TABLE VII. Values of the electronic F factor (in GHz/fm^2) and of the $\Delta\widetilde{K}_{\rm MS}$ parameter (in GHz u) for the $6s5d\,{}^3D_1$–$6s6p\,{}^1P_1^o$ and $6s5d\,{}^3D_2$–$6s6p\,{}^1P_1^o$ transitions.

	F (GHz/fm^2)		$\Delta\widetilde{K}_{\rm MS}$ (GHz u)	
	${}^3D_1-{}^1P_1^o$	${}^3D_2-{}^1P_1^o$	${}^3D_1-{}^1P_1^o$	${}^3D_2-{}^1P_1^o$
DHF	0.31	0.31	937.12	962.56
⋮	⋮	⋮	⋮	⋮
10S	0.75	0.74	−284.34	−324.09
11S	0.76	0.74	−311.99	−294.94

of our electronic parameters ($K_{\rm MS}$ and F), which is the original point of this section.

Let us refer to Table I in order to compare these newly extracted values with the available ones. The $\delta\langle r^2\rangle$ values from the semiempirical formula as well as results of Baird *et al.* [6] are both out of range but there are some nice agreements with other experiments. The results of Bekk *et al.* [5] and Grundevik *et al.* [7] seem to be confirmed, especially for $\delta\langle r^2\rangle^{138,137} \simeq 0.055$ fm^2, but not for $\delta\langle r^2\rangle^{138,136}$, for which our results are closer to van Wijngaarden and Li's value [10] ($\delta\langle r^2\rangle^{138,136} = 0.034$ fm^2). The $\delta\langle r^2\rangle^{138,135}$ is more disputable, but let us just emphasize that our result is closer to van Wijngaarden and Li's as well as the value obtained by Mårtensson-Pendrill and Ynnerman, $\delta\langle r^2\rangle^{138,135} = 0.0728(15)(22)(2)$ fm^2 [40]. The discrepancy found for $\delta\langle r^2\rangle^{138,134}$ forbids us from drawing any further conclusions. All our results for neutron-rich isotopes confirm the deductions of Neugart *et al.* [39] and Mueller *et al.* [9] within 3% (see Table III).

V. THE ISSUES OF THE ${}^1P_1^o - {}^3D_{1,2}$ TRANSITIONS

The level scheme of barium also exhibits low-lying $6s5d\,{}^1D_2$, ${}^3D_1$, and ${}^3D_2$ metastable states. However, the transitions $6s5d\,{}^3D_1$–$6s6p\,{}^1P_1^o$ and $6s5d\,{}^3D_2$–$6s6p\,{}^1P_1^o$ are far less studied and the first measurements of their IS were performed by Dammalapati *et al.* [19]. The latter are listed in Table VIII using ^{138}Ba as the pivot. Those authors also measured shifts of other pairs, reporting $\delta\nu_{\rm IS}^{136,134} = -84.8(8)$ MHz and $-80(1)$ MHz for the transitions ${}^1P_1^o - {}^3D_1$ and ${}^1P_1^o - {}^3D_2$, respectively, and $\delta\nu_{\rm IS}^{137,135} = -75.3(5)$ MHz for the resonance line frequency.

Following the computational procedure described in Sec. III, the F and $\widetilde{K}_{\rm MS}$ parameters have been calculated and are listed in Table VII.

It first appears that the electronic F factor is much smaller and the $\Delta\widetilde{K}_{\rm MS}$ parameter larger than for the three transitions considered above (see Table IV). The MS value is $\delta\nu_{\rm MS}^{138,136} = 33.32$ MHz, while the frequency FS is $\delta\nu_{\rm FS}^{138,136} = 25.74$ MHz [using $\delta\langle r^2\rangle^{138,136} = 0.034(3)$ fm^2]. The difference between the two most elaborated calculations of the values listed in Table VII is around 9% for the two $\Delta\widetilde{K}_{\rm MS}$ parameters and 0.5% for both electronic F factors. The error bars of the IS values calculated with the present electronic factors can be estimated at about 10% for both transitions, taking the uncertainty of the $\delta\langle r^2\rangle^{138,136}$ value into account.

Table VIII compiles the results of Dammalapati *et al.* with our predictions using the $\delta\langle r^2\rangle^{138,A}$ values of other authors. The underlined data are obtained with the $\delta\langle r^2\rangle$ values that look the most reliable on the basis of the ${}^{3,1}P_1^o - {}^1S_0$ transitions.

Table VIII reports much interesting information. Most of our values are in complete contradiction with the results of Dammalapati *et al.* The pair ^{138,137}Ba is consistent, but only for the ${}^3D_2 - {}^1P_1^o$ transition. It is true that as regards the proximity of the two levels $6s5d\,{}^3D_{1,2}$, it is rather strange that the IS, $\delta\nu_{\rm IS}^{138,137} = 114$ MHz, for one transition is reduced by a factor of 2 for the second one. All the $\delta\nu_{\rm IS}^{138,136}$ and $\delta\nu_{\rm IS}^{138,134}$ values show signs opposite to ours, regardless of the $\delta\langle r^2\rangle^{138,A}$ used.

TABLE VIII. Experimental measurements of isotope shifts for the transitions $6s5d\,{}^3D_1$–$6s6p\,{}^1P_1^o$ and $6s5d\,{}^3D_2$–$6s6p\,{}^1P_1^o$ (in MHz) from [19] compared with the isotope shifts calculated with the mean-square radii differences available in the literature and our electronic factors.

	^{138}Ba	^{137}Ba	^{136}Ba	^{135}Ba	^{134}Ba
		$6s5d\,{}^3D_1$–$6s6p\,{}^1P_1^o$			
Dammalapati *et al.* [19]	0.0	114(4)	−59.3(6)	39(4)	−144.1(10)
Present work, using the $\delta\langle r^2\rangle$ of:					
Baird *et al.* [6]	0.0	67.2	79.5	132.1	139.5
Bekk *et al.* [5]		$\underline{61.2}$	64.4	110.1	107.7
Shera *et al.* [37]		71.0	66.6	116.9	106.2
Grundevik *et al.* [7]		$\underline{61.2}$	65.1	110.9	110.0
van Wijngaarden *et al.* [10]		53.6	$\underline{59.1}$	99.5	
		$6s5d\,{}^3D_2$–$6s6p\,{}^1P_1^o$			
Dammalapati *et al.* [19]	0.0	69(3)	−63(1)		−143(1)
Present work, using the $\delta\langle r^2\rangle$ of:					
Baird *et al.* [6]	0.0	65.0	76.5	127.2	134.0
Bekk *et al.* [5]		$\underline{59.1}$	61.7	105.8	103.0
Sherra *et al.* [37]		68.7	63.9	112.5	101.5
Grundevik *et al.* [7]		$\underline{59.1}$	62.5	106.6	105.2
van Wijngaarden *et al.* [10]		51.8	$\underline{56.6}$	95.5	

TABLE IX. Extraction of the $\Delta\widetilde{K}_{\mathrm{MS}}$ that would be necessary to reproduce the experimental results of Dammalapati *et al.* [19], combining our theoretical F factor with the $\delta\langle r^2\rangle$ and nuclear masses from the literature: $\Delta\widetilde{K}_{\mathrm{MS}} = (\delta\nu_{\mathrm{IS}} - F\delta\langle r^2\rangle)/(1/M - 1/M')$.

	$\mathrm{IS}_{\mathrm{exp}}$ (MHz)	F (GHz/fm^2)	$\delta\langle r^2\rangle$ (fm^2)	$(1/M - 1/M')$ (u^{-1})	→	$\Delta\widetilde{K}_{\mathrm{MS}}$ (GHz u)
			$6s5d\,^3D_1$–$6s6p\,^1P_1^o$			
$^{138-137}$Ba	114(4)	0.76	0.055	−0.000053	→	−1366.4
$^{138-136}$Ba	−59.3(6)	0.76	0.035	−0.000107	→	803.4
$^{138-135}$Ba	39(4)	0.76	0.072	−0.000161	→	96.1
$^{138-134}$Ba	114.1(1.0)	0.76	0.040	−0.000217	→	−386.7
$^{136-134}$Ba	−84.8(8)	0.76	0.005	−0.000110	→	805.6
$^{137-135}$Ba	−75.3(5)	0.76	0.017	−0.000108	→	813.8
			$6s5d\,^3D_2$–$6s6p\,^1P_1^o$			
$^{138-137}$Ba	69(3)	0.74	0.055	−0.000053	→	−536.9
$^{138-136}$Ba	−63(1)	0.74	0.035	−0.000107	→	831.6
$^{138-135}$Ba	/					
$^{138-134}$Ba	−143(1)	0.74	0.040	−0.000217	→	795.8
$^{136-134}$Ba	−80(1)	0.74	0.005	−0.000110	→	761.1

However, $\delta\nu_{\mathrm{IS}}^{138,136}$ are consistent on the absolute scale. As for $\delta\nu_{\mathrm{IS}}^{138,134}$, its determination suffers from our incapacity to discriminate between correct and incorrect $\delta\langle r^2\rangle^{138,134}$ values.

In order to circumvent the problem, Table IX presents the ΔK_{MS} values that would reproduce the experimental results of Dammalapati *et al.* [19]. In order to do so, we trusted the values of our F factors and adopted the most reliable $\delta\langle r^2\rangle$ and the nuclear masses from the literature. This was done with the help of the formula $\Delta K_{\mathrm{MS}} = (\mathrm{IS} - F\delta\langle r^2\rangle)/(1/M_{138} - 1/M')$. For the comparison, we deduced a value for $\delta\langle r^2\rangle^{136,134}$ by making the difference $\delta\langle r^2\rangle^{136,134} = \delta\langle r^2\rangle^{138,134} - \delta\langle r^2\rangle^{138,136} = 0.005\ \mathrm{fm}^2$, as well as $\delta\langle r^2\rangle^{137,135} = \delta\langle r^2\rangle^{138,135} - \delta\langle r^2\rangle^{138,137} = 0.017\ \mathrm{fm}^2$.

In theory, the ΔK_{MS} parameter is isotope independent and its value should be identical for a given transition. Table IX clearly reveals the incompatibility of the ΔK_{MS} values within a given transition.

VI. CONCLUSION

The analysis of the $6s^2\,^1S_0$–$6s6p\,^{3,1}P_1^o$ and $6s^2\,^1S_0$–$6p^2\,^3P_0$ transitions gave us confidence in our theoretical calculations of the IS electronic factors. At the end of their study of $6s5d\,^3D_{1,2}$–$6s6p\,^1P_1^o$ transitions, Dammalapati *et al.* [19] suggest that "the nuclear spin gives rise to an additional contribution to the IS" for odd isotopes. On the basis of the present results—and also the observation of discrepancies for even isotopes—their statement is open to doubt. Complementary investigations would be very valuable. For instance, further investigation of the convergence of the *ab initio* parameters would be welcome to confirm our predictions of large MS found for these transitions. The convergence of the electronic parameters with respect to more elaborate correlation models should be investigated to refine the estimation of the accuracy of our electronic parameters. Unfortunately, the present calculations have reached the limits of the current computational resources. Study of other transitions could provide more reliable data on the change in the nuclear mean-square radii between isotopes. As an extension of the present study, many investigations remain possible. A possibility would be to reinvestigate the Ba II system, which also presents many experimental studies [46,47] but few relativistic calculations [2]. Another interesting track would be to (re)investigate experimentally ISs of transitions involving the $6s5d\,^3D_J$ levels.

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