

Isotope mass shift for two-electron atoms II

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Accurate calculations of the isotope shift for atomic transitions can not be made without accounting for the core-valence correlations. Specific mass shift (SMS) is described by the two-electron operator and is most difficult to calculate. Here we develop a method for SMS calculations which accounts for both valence and core-valence correlations. In addition we study the role of relativistic corrections to SMS operator. Our calculations of the SMS for several transitions in Mg I are in good agreement with the experiment.

Introduction

The accurate knowledge of the isotope shift (IS) is important for many spectroscopic studies. IS consists of the field shift (also known as volume shift) and the mass shift. The latter in turn is a sum of normal mass shift (NMS) and specific mass shift (SMS). NMS is a result of the dependence of the electron reduced mass on the nuclear mass and it is immediately derived from experimental transition frequency. Field shift depends on the nuclear radius. It is described by a simple one-electron operator and can be relatively easily calculated, provided nuclear radius is known. NMS is described by the two-electron operator and is most difficult to calculate.

Recently there was significant progress in calculating SMS for atoms with one valence electron [1, 2]. On the other hand, accurate SMS calculations for many-electron atoms are still missing. Recent calculation of SMS for Mg I [3] is not very accurate. In that calculation valence correlations are accounted for by means of the configuration interaction (CI) method and core-valence correlations are neglected. Therefore, we can expect that core-valence correlations are important for SMS calculations. That is in agreement with the results for one-electron atoms [2].

SMS calculations are usually made within finite-field method when perturbation is added to the Hamiltonian with some scaling parameter λ . Atomic energies E_n are then calculated for several values of λ and derivatives $\partial E_n / \partial \lambda |_{\lambda=0}$ are found by numerical differentiation. This method allows straightforward generalization to account for the core-valence correlations in a same way as it was done in [4, 5], where an effective valence Hamiltonian was formed within second order many body perturbation theory (MBPT). Effective Hamiltonian is used then to make valence CI and corresponding method is called CI+MBPT.

The two-electron non-relativistic SMS operator depend on the electron momenta \mathbf{p}_i :

$$\lambda H_{\text{SMS}} = \lambda \sum_{i < j} \mathbf{p}_i \cdot \mathbf{p}_j. \quad (1)$$

A more accurate relativistic form of the SMS operator was derived in [6]. It is shown there that for the optical spectra of light atoms, considered here, the difference

between non-relativistic and relativistic SMS operators is on the scale of few percent. That allows us to use (1) in this work.

It is technically easy to add operator (1) to the Coulomb two-electron interaction. After that all calculations are made exactly as they are done without SMS operator. Usually we do three calculations for $\lambda = 0, \pm 0.005$ and find SMS coefficient k_{SMS} for level n as

$$k_{\text{SMS}}^n = 100 \cdot (E_{\lambda=0.005}^n - E_{\lambda=-0.005}^n). \quad (2)$$

In previous valence CI calculations [3] it was checked that this choice of λ is sufficiently small to neglect nonlinear terms and convenient from numerical point of view. However, here we found that for CI+MBPT calculations the non-linear in λ corrections are often much larger. We can estimate their relative size by looking at the ratios:

$$c_{\text{nl}}^n = 2 \cdot \frac{E_{\lambda=0.005}^n - 2E_{\lambda=0}^n + E_{\lambda=-0.005}^n}{E_{\lambda=0.005}^n - E_{\lambda=-0.005}^n}. \quad (3)$$

For the frozen-core CI calculations the size of the non-linear corrections given by Eq. (3) is of the order of few percent. That justifies usage of the linear approximation (2). However, MBPT corrections for Ca appear to be much more non-linear. That means that chosen value of λ is too large here. Because of that we repeat calculations for $\lambda = \pm 0.001$ and then use 4-point expression for k_{SMS} instead of Eq. (2):

$$k_{\text{SMS}}^n = \frac{25}{6} \cdot (-E_{\lambda=0.005}^n + 125E_{\lambda=0.001}^n - 125E_{\lambda=-0.001}^n + E_{\lambda=-0.005}^n). \quad (4)$$

For the CI calculation the values obtained with Eq. (2) and Eq. (4) are always very close, but the difference becomes noticeable for some CI+MBPT calculations. Below we first make calculations for $\lambda = 0, \pm 0.005$. Then we use (3) to estimate non-linear terms. If necessary, we do additional calculations for $\lambda = \pm 0.001$.

Mg II and Mg I

CI+MBPT calculations are usually done with the help of two basis sets. The shorter one includes orbitals 1 – 12s, 2 – 12p, 3 – 12d, and 4 – 9f ([12spd9f]) and is used

TABLE I: Specific mass shift constants k_{SMS} for Mg II. Results correspond to the Dirac-Fock (DF) and second order effective Hamiltonians. Results of Berengut *et al.* are given for comparison. NR₁, NR₂, and R correspond to the non-relativistic and relativistic forms of the SMS operator. Non-relativistic operator is applied either to upper component of the Dirac function (NR₁), or to both (NR₂).

Level	$k_{\text{SMS}}(\text{GHz} \cdot \text{amu})$						
	H_{DF}		H_{eff}		[2]		
	NR ₁	NR ₂	R	NR ₁	NR ₂	R	NR ₁
$3s_{1/2}$	-174.1	-172.4	-176.4	100.0	102.1	97.0	83
$3p_{1/2}$	-405.9	-406.8	-400.9	-286.5	-287.2	-281.4	-296
$3p_{3/2}$	-400.3	-401.1	-400.2	-280.9	-281.6	-281.1	-290
$3d_{3/2}$	-31.6	-31.2	-32.3	45.4	45.9	44.6	-296
$3d_{5/2}$	-99.9	-99.9	-99.9	-98.8	-98.8	-98.9	-290
$4s_{1/2}$	-100.6	-100.6	-100.6	-99.5	-99.5	-99.6	
$4p_{1/2}$	-141.2	-141.6	-139.5	-98.8	-99.0	-97.1	
$4p_{3/2}$	-139.4	-139.7	-139.4	-97.0	-97.2	-97.0	

for valence CI. This basis set was already used in [3]. The longer basis set [17spd12f9gh] is used for intermediate summations in second order MBPT diagrams (see [5] for details). Core orbitals in both basis sets are the solutions of the Dirac-Fock equations for the core.

For one-electron ion Mg II our method is equivalent to that used in [2], so we first calculate Mg II to test our codes and basis sets. Results of this calculation are listed in Table I. Note the huge difference between Dirac-Fock and MBPT calculations. Experimentally SMS shifts are usually observed in optical transitions. The differences between two approximations become slightly less dramatic for this case.

There is reasonably good agreement between our MBPT calculation and that of Berengut *et al.* [2]. These two calculations are done in the similar approximations, so the comparison can serve as a test of the codes. Comparison with [6] is more physically informative as there a different method was used. Tupitsyn *et al.* used relativistic form of the SMS operator and made a large-scale CI, which included both core and valence excitations. For the $3s_{1/2} \rightarrow 3p_{3/2}$ transition they obtained [6]:

$$k_{\text{SMS}}(3p_{3/2}) - k_{\text{SMS}}(3s) = \begin{cases} -416 & [6], \text{NR}_2, \\ -406 & [6], \text{R}, \end{cases} \quad (5)$$

which has to be compared with

$$k_{\text{SMS}}(3p_{3/2}) - k_{\text{SMS}}(3s) = \begin{cases} -373 & \text{ref. [2],} \\ -381 & \text{this work, NR}_1, \\ -384 & \text{this work, NR}_2, \\ -378 & \text{this work, R.} \end{cases} \quad (6)$$

We see that the error from using operator (1) is smaller than the errors associated with the approximations in treatment of the electron correlations.

On the next step we calculate neutral Mg as a two-electron atom. Valence part of this calculation is practically identical to [3]. In previous CI+MBPT calculation

TABLE II: Relativistic corrections to constants k_{SMS} and k_{NMS} for Mg II. Results correspond to the Dirac-Fock (DF) and second order effective Hamiltonians.

Transition	$\delta k_{\text{SMS}}^{\text{rel}}$		$\delta k_{\text{NMS}}^{\text{rel}}$	
	CI	H_{eff}	CI	H_{eff}
$3s_{1/2} \rightarrow 3p_{1/2}$	7.3	8.1	0.3	1.0
$\rightarrow 3p_{3/2}$	2.4	2.8	1.1	1.8
$\rightarrow 3d_{3/2}$	1.7	2.2	1.1	1.7
$\rightarrow 3d_{5/2}$	2.3	2.9	1.4	2.2
$\rightarrow 4s_{1/2}$	2.3	2.9	1.5	2.3
$\rightarrow 4p_{1/2}$	4.0	4.7	1.1	1.9
$\rightarrow 4p_{3/2}$	2.3	2.9	1.4	2.2

TABLE III: Calculations of the spectrum (in cm^{-1}) and specific mass shift constants k_{SMS} (in $\text{GHz} \cdot \text{amu}$) for the levels of Mg I. Results are given for the valence calculation in the frozen-core approximation (H_{FC}) and for calculation with the effective Hamiltonian (H_{eff}). Here we neglect the energy-dependence of the operator H_{eff} .

Level	Spectrum			k_{SMS}	
	H_{FC}	H_{eff}	Exper. ^a	H_{FC}	H_{eff}
$^1S_0(3s^2)$	0.0	0.0	0.0	-192	205.4
$^3S_1(3s4s)$	40415.2	41121.0	41197.4	-149	140.0
$^1S_0(3s4s)$	42698.8	43450.0	43503.3	-179	114.4
$^1D_2(3s3d)$	45128.6	46303.2	46403.1	-544	-279.7
$^3D_1(3s3d)$	46990.0	47923.6	47957.1	-143	118.7
$^3D_2(3s3d)$	46990.0	47923.6	47957.0	-143	118.7
$^3D_3(3s3d)$	46990.0	47923.6	47957.0	-143	118.7
$^3P_0^o(3s3p)$	20908.7	21768.2	21850.4	-570	-284.7
$^3P_1^o(3s3p)$	20929.1	21789.4	21870.5	-569	-284.1
$^3P_2^o(3s3p)$	20969.7	21832.7	21911.2	-567	-281.9
$^1P_1^o(3s3p)$	34490.9	35041.5	35051.3	38	328.8
$^3P_0^o(3s4p)$	47276.6	48096.3	47841.1	-213	70.0
$^3P_1^o(3s4p)$	47279.9	48100.1	47844.4	-213	70.4
$^3P_2^o(3s4p)$	47286.7	48107.1	47851.2	-212	70.4

^aExperimental data taken from the NIST web page [9]

of Mg the V^N approximation was used [7, 8], while here we use V^{N-2} approximation. Table III presents results of our calculations for the spectrum and for the SMS coefficients.

Again we see that k_{SMS} calculated in CI+MBPT approximation differs strongly from the frozen-core calculation. That means that SMS is much more sensitive to the core-valence correlations than the energy, where these correlations account only for few percent corrections.

Now we can use results from Table III to calculate SMS corrections to the transition frequencies, where experimental data is available. That is done in Table IV.

We see that CI+MBPT method provide significantly better agreement with the experiment in comparison with valence CI. The improvement is particularly noticeable for the transitions from the ground state. That is not surprising as core-valence correlations are stronger for the ground state. Again the difference between CI and CI+MBPT calculations is less dramatic for the transitions than for the individual levels.

TABLE IV: Comparison with experiment of the SMS for several transitions between ^{26}Mg and ^{24}Mg . When we extract SMS from the total experimental isotope shift, we assume that the field shift is negligible.

Transition	SMS (MHz)		
	Expt.	H_{FC}	H_{eff}
$^1S_0(3s^2) \rightarrow ^3P_1^o(3s3p)$	1530(0) ^a	1208	1570
$^1S_0(3s^2) \rightarrow ^1P_1^o(3s3p)$	-436(21) ^b	-739	-394
"	-458(31) ^c		
$^3P_0^o(3s3p) \rightarrow ^3S_1(3s4s)$	-1416(6) ^d	-1348	-1387
$^3P_1^o(3s3p) \rightarrow ^3S_1(3s4s)$	-1409(5) ^d	-1345	-1385
$^3P_2^o(3s3p) \rightarrow ^3S_1(3s4s)$	-1407(7) ^d	-1340	-1378
$^3P_0^o(3s3p) \rightarrow ^3D_1(3s3d)$	-1316(15) ^b	-1368	-1293
$^3P_1^o(3s3p) \rightarrow ^3D_2(3s3d)$	-1314(3) ^b	-1365	-1291
$^3P_2^o(3s3p) \rightarrow ^3D_3(3s3d)$	-1315(4) ^b	-1360	-1284

^aSterr *et al.*, 1993 [10]

^bHallstadius, 1979 [11]

^cLe Boiteux *et al.*, 1988 [12]

^dHallstadius and Hansen, 1978 [13]

Ca II

For Ca we use CI basis set [12spd11fg] and MBPT basis set [16spd15fg16h]. Orbitals of the MBPT basis set are diagonalized for V^{N-2} field, which means that we use V^{N-2} version of MBPT. In the CI basis set for Ca I the valence orbitals $4s, 4p, 3d$ and $5s$ correspond to V^N approximation.

Note that previous calculations of Ca I within CI+MBPT method were done in V^N approximation [5, 7]. The advantage of the latter is a better starting approximation. On the other hand, the former leads to a simpler version of the MBPT, is more stable, and gives comparable final accuracy [14]. Ca presents much more difficult case than Mg because of the low-lying $3d$ shell. To improve the accuracy for the spectrum, we include energy-dependent corrections to the effective Hamiltonian as suggested in [4].

Table V presents our results for Ca II. We see that $3d$ -shell is very sensitive to core-valence correlations. The difference between SMS coefficients obtained with and without energy-dependent corrections to the effective Hamiltonian is relatively small and does not lead to a significant improvement of the agreement with the experiment (see Table VI). Our results for the transitions to or from $3d$ -shell are in a poor agreement with calculations of Berengut *et al.* [2]. The reason for this discrepancy is not clear.

As in the case of Mg we make three calculations for $\lambda = 0, \pm 0.005$. For the frozen-core calculations the size of the non-linear corrections given by Eq. (3) is 3% at most. In contrast to that, in the CI+MBPT approximation some of the coefficients c_{nl}^n are about unity. That means that chosen value of λ is too large here. Because of that we repeat calculations for $\lambda = \pm 0.001$ and then use expression (4) for k_{SMS} .

Table VI shows that there is obvious problem with

TABLE V: Spectrum (in cm^{-1}) and SMS coefficients (in $\text{GHz} \cdot \text{amu}$) for Ca II. CI+MBPT calculations are done with energy-dependent effective Hamiltonian $H_{\text{eff}}(E)$ and without energy-dependent corrections. Experimental data are taken from [15].

Level	Spectrum			k_{SMS}		
	H_{FC}	$H_{\text{eff}}(E)$	Exper.	H_{FC}	H_{eff}	$H_{\text{eff}}(E)$
$4s_{1/2}$	0	0	0	500	132	143
$3d_{3/2}$	18822	13111	13650	2498	1908	1949
$3d_{5/2}$	18846	13195	13711	2493	1916	1942
$4p_{1/2}$	23403	25511	25192	299	168	166
$4p_{3/2}$	23603	25747	25414	284	152	152
$5s_{1/2}$	49019	52591	52167	125	-13	
$4d_{3/2}$	54406	57258	56839	453	220	
$4d_{5/2}$	54423	57281	56859	451	222	
$5p_{1/2}$	57036	61022	60535	112	58	
$5p_{3/2}$	57109	61104	60613	107	51	

TABLE VI: SMS for several transitions in Ca II. Experimental data are taken from [2].

Transition	SMS ($\text{GHz} \cdot \text{amu}$)				
	Expt.	H_{FC}	H_{eff}	$H_{\text{eff}}(E)$	[2]
$4s_{1/2} \rightarrow 4p_{1/2}$	-9(6)	-202	36	23	13
$4s_{1/2} \rightarrow 4p_{3/2}$	-9(12)	-217	20	9	-3
$4s_{1/2} \rightarrow 3d_{3/2}$	2199(30)	1998	1776	1806	2008
$4s_{1/2} \rightarrow 3d_{5/2}$	2167(6)	1992	1784	1799	1999
$3d_{3/2} \rightarrow 4p_{1/2}$	-2169(3)	-2200	-1740	-1783	-1994
$3d_{3/2} \rightarrow 4p_{3/2}$	-2171(2)	-2214	-1757	-1797	-2011
$3d_{5/2} \rightarrow 4p_{3/2}$	-2173(3)	-2209	-1765	-1790	-2002

CI+MBPT calculation as it does not match the experiment and calculation of Berengut *et al.* We study several possible sources of errors by making several additional calculations, which are summed in Table VII.

- We use non-relativistic operator (1) with relativistic Dirac-Fock orbitals. Accurate relativistic form of the SMS operator is more complicated [6] and usually supposed to be unnecessary for calculations of light atoms. One of the ways to estimate the error caused by the operator 1 is to calculate contribution of the lower components of the Dirac-Fock orbitals to the SMS coefficients.
- Incompleteness of the basis set is another possible source of errors. This error can be estimated by repeating calculations with a longer basis set, say [19spd18fg19h].
- Table V shows that energy-dependence of the effective Hamiltonian leads to a noticeable corrections to the SMS coefficients. Usually we calculate MBPT diagrams at Hartree-Fock energies and extrapolate them to the final energy. For $4s$ and $3d$ states the difference $E - E_0$ is rather large and extrapolation error can be significant. It is possible to reduce this error by calculating diagrams for the energies, which are closer to the final ones.

TABLE VII: Coefficients k_{SMS} for Ca II in different approximations: (1) is the initial CI+MBPT calculation; (2) corresponds to similar calculation, but SMS matrix elements include contributions of the lower components of Dirac-Fock orbitals; (3) calculation with expended basis set; (4) the same as (3), but MBPT diagrams are calculated for the energies, which are close to the final Brueckner ones; (5) the same as (4), but with energy-dependent corrections; (6) the same as (4), but with scaling coefficients. All calculations are done for $\lambda = \pm 0.001$.

	(1)	(2)	(3)	(4)	(5)	(6)
$4s_{1/2}$	132	132	134	144	141	195
$3d_{3/2}$	1909	1911	1913	1982	1947	2061
$3d_{5/2}$	1917	1913	1918	1974	1938	2054
$4p_{1/2}$	168	168	166	168	164	182
$4p_{3/2}$	152	152	152	150	150	166
$5s_{1/2}$	-13	-13	-13	11	-5	25
$4d_{3/2}$	220	220	218	242	235	263
$4d_{5/2}$	222	224	222	242	235	263
$5p_{1/2}$	58	58	58	60	56	65
$5p_{3/2}$	51	52	52	54	52	61

- In Ref. [2] semi-empirical scaling of the self-energy operator was used to account for the high order corrections: $\hat{\sigma}_{lj}(E) \rightarrow f_{lj} * \hat{\sigma}_{lj}(E)$, where scaling factors f_{lj} were chosen to match the experimental spectrum. MBPT corrections to k_{SMS} are large and scaling can lead to large corrections. We made calculation of SMS coefficients with following scaling coefficients: $f_{0,1/2} = 0.8763$, $f_{1,1/2} = 0.9017$, $f_{1,3/2} = 0.9054$, $f_{2,3/2} = 0.8848$, and $f_{2,5/2} = 0.8865$.

Table VII shows that coefficients k_{SMS} are sensitive to the details of the approximations used. The differences between test calculations (1) — (6) are sufficient to explain the difference between this work and calculations of Berengut *et al.* for $s \rightarrow p$ transitions, but can account for only about 30% of the differences for the $s \rightarrow d$ and $p \rightarrow d$ transitions. Thus, we conclude that there may be some unknown sources of errors, which appear to be more important for the d -wave.

Ca I

Results of our calculations for Ca I are presented in Table VIII. CI+MBPT calculations of the spectrum are done for energy-dependent effective Hamiltonian, which leads to a better agreement with the experimental spectrum [15]. CI calculations of the SMS coefficients are done for $\lambda = \pm 0.005$. Non-linear corrections, estimated

with the help of Eq. (3) appear to be between 1% and 6%.

CI+MBPT calculations of the SMS coefficients are done with the help of Eq. (4). That requires four calculations for $\lambda = \pm 0.001, \pm 0.005$. In these calculations

TABLE VIII: Spectrum (in cm^{-1}) and SMS coefficients (in $\text{GHz} \cdot \text{amu}$) for Ca I. CI+MBPT calculations of the spectrum are done with energy-dependent effective Hamiltonian $H_{\text{eff}}(E)$. Experimental data are taken from [15]. SMS calculations with H_{eff} are done with Eqs. (2) and (4).

Level	Spectrum			k_{SMS}	
	H_{FC}	$H_{\text{eff}}(E)$	Exper.	H_{FC}	H_{eff}
$^1S_0(4s^2)$	0	0	0	664	119 123
$^3D_1(4s3d)$	24201	19706	20335	1783	1396 1401
$^3D_2(4s3d)$	24202	19726	20349	1782	1394 1399
$^3D_3(4s3d)$	24204	19756	20371	1780	1389 1393
$^1D_2(4s3d)$	23853	21313	21850	1566	1460 1466
$^3S_1(4s5s)$	30151	31647	31540	504	74 78
$^1S_0(4s5s)$	31894	33454	33317	539	98 101
$^3P_0^o(4s4p)$	13511	15330	15158	744	600 609
$^3P_1^o(4s4p)$	13560	15385	15210	742	597 605
$^3P_2^o(4s4p)$	13658	15496	15316	736	591 599
$^1P_1^o(4s4p)$	23056	23726	23652	450	-118 -108
$^3F_2^o(3d4p)$	37741	35195	35730	1902	1819 1642
$^3F_3^o(3d4p)$	37787	35284	35819	1898	1677 1682
$^3F_4^o(3d4p)$	37847	35373	35897	1893	1666 1669
$^1D_2^o(3d4p)$	38740	35344	35835	1986	1450 1639
$^3P_0^o(4s5p)$	35142	36492	36548	550	496 485
$^3P_1^o(4s5p)$	35151	36499	36555	550	501 489
$^3P_2^o(4s5p)$	35170	36523	36575	549	499 489
$^1P_1^o(4s5p)$	35659	36662	36732	638	437 459
$^3D_1^o(3d4p)$	42113	37612	37748	2257	1732 1721
$^3D_2^o(3d4p)$	42125	37646	37752	2249	1717 1724
$^3D_3^o(3d4p)$	42149	37697	37757	2257	1716 1722
$^1F_3^o(3d4p)$	44748	39924	40538	2210	1856 1861

we neglect energy-dependence of the effective Hamiltonian.

Experimental results for Ca I are summed in Table IX, where SMS is given for a number of optical transitions. Experimental papers usually give total mass shift which is the sum of NMS and SMS. NMS constant form the transition with the frequency ν is given by the following expression:

$$k_{\text{NMS}} = -\frac{\nu}{1823}, \quad (7)$$

where the value 1823 refers to the ratio of the atomic mass unit to the electron mass. Note that there is reasonable agreement between two experimental results [16, 17] for the $^1S_0(4s^2) \rightarrow ^1P_1^o(4s4p)$ transition.

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[2] J. C. Berengut, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **68**, 022502 (2003).

TABLE IX: Comparison with the experiment of the SMS for several transitions in Ca I.

Transition	SMS (GHz · amu)			
	Expt.	H_{FC}	H_{eff}	
$^1S_0(4s^2) \rightarrow ^3P_1^o(4s4p)$	210.56(14) ^a	77	478	482
$^1S_0(4s^2) \rightarrow ^1P_1^o(4s4p)$	-26.94(31) ^a	-214	-237	-231
”	-26.47(12) ^b			
$^1S_0(4s^2) \rightarrow ^1S_0(4s5s)$	-22.01(14) ^a	-126	-21	-22
$^1S_0(4s^2) \rightarrow ^1P_1^o(4s5p)$	243.(12) ^c	-27	318	336
$^3P_2^o(4s4p) \rightarrow ^3S_1(4s5s)$	-294.5(9) ^a	-232	-516	-521
$^1D_2(3d4s) \rightarrow ^1F_3^o(3d4p)$	322.6(12) ^a	664	396	395

^aSee Palmer *et al.*, 1984 [16] and references therein.

^bNörtershäuser *et al.*, 1998 [17].

^cMortensen *et al.*, 2004 [18].

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