

**CALCULATION OF Ba⁺ AND Ba WITH DIFFERENT
MBPT PARAMETERS. APPLICATION TO THE
ISOTOPE SHIFT.**

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ABSTRACT. My current calculations of Ba and Ba⁺ show strong dependence of the results on the choice of the MBPT parameters. Here I want to summarize different calculations and try to draw some conclusions about the choice of parameters and the overall reliability of the calculations.

After that I calculate isotope shift (both volume shift and specific mass shift) for Ba and Ba⁺.

1. BASIS SETS

- All calculations are in V^{N-2} approximation.
- Basis sets include following valence Dirac-Fock orbitals: 6,7sp, 5,6d, and 4f.
- CI basis set [13sp12d11f9g] is formed from B -splines [15/6]. It is diagonalized for V^{N-2} potential.
- Initial MBPT basis set (Ns=126) [16sp15d14fg12h] is also mostly formed from the same set of B -splines. Exceptions are: 14,15spdf and 12g.
- Used here set of B -splines does not allow longer basis set. In order to test the saturation of the MBPT, I generated two basis sets from the set Ns=126 using Auto mode. Ns=159 includes 3 extra shells spdfgh and Ns=192 includes 6 extra shells.

Dependence of the results on the parameter Ns are studied below.

2. EXTRAPOLATION TO $L \rightarrow \infty$

2.1. **Self-energy corrections.** It is known (see [1, 2]) that contribution of the partial wave l to σ operator scales as $1/(l+a)^4$, with a of the order of unity [the first term of the expansion gives $a = \frac{1}{2}$, but following term can change a]. That means that if σ_L is calculated on the basis set with $l_{\max} = L$, we can expect that

$$\sigma_L = \sigma_\infty - A/(L+a)^3. \quad (1)$$

This extrapolation ansatz is included in the new version of `sgc` code. Each matrix element of σ is calculated for $L = L_{\max}, L_{\max} - 1, L_{\max} - 2$ and σ_∞ is found using extrapolation ansatz (1).

In principle, it is possible to find all 3 parameters in (1). However, equations for a are of a high order and instead of solving them Subroutine `D_inf` tries several variants: $a = 0, \pm 1/2, \pm 1$. The number of tried variants is given by the global variable `K_inf=1,3,5`, while `K_inf=0` means that no extrapolation is done.

`K_inf` is another parameter, which influences the results.

2.2. Screening corrections. For two-electron diagrams there are always angular selection rules which eliminate contributions of the partial waves with $l > L_1$. Parameter L_1 depends on the quantum numbers of the valence orbitals and on the l_{\max} for the core. If $L_1 > L_{\max}$, we can try to extrapolate from L_{\max} to L_1 .

Assume that contribution of the p.w. l to the screening matrix element R is $\sim C/l^s$. Then we can use the similar method as for σ . Comparing $R(L)$ for three values of L we can find s and C :

$$s = \log \frac{R(L_{\max}) - R(L_{\max} - 1)}{R(L_{\max} - 1) - R(L_{\max} - 2)} \bigg/ \log \frac{L_{\max} - 1}{L_{\max}}, \quad (2)$$

$$C = [R(L_{\max}) - R(L_{\max} - 1)] L_{\max}^s. \quad (3)$$

After that we can extrapolate R as follows:

$$R = R(L_{\max}) + \sum_{L=L_{\max}+1}^{L_1} \frac{C}{L^s}. \quad (4)$$

This algorithm is implemented in the `scrc` code. Extrapolation is switched on/off by the same parameter `K_inf`. Note, however, that extrapolations for σ and for R are different and we **must independently test extrapolation for R** . Also note that (2) requires positive expression under logarithm. Otherwise, no extrapolation is made.

3. ENERGY DEPENDENCE OF σ

There are several choices how to account for energy dependence of σ in the codes `sgc` and `conf`. Parameter `Kval` defines basic energies. Here we use `Kval=2` with the following energies for partial waves:

$$\varepsilon(0) = -0.28, \quad \varepsilon(1) = -0.22, \quad \varepsilon(2) = -0.31, \quad \varepsilon(3) = -0.13. \quad (5)$$

Below I compare results of the CI calculations with and without energy dependence in the `conf` code.¹ When energy dependence is included, I use actual valence energies truncated to two digits [i.e. no energy shift] and the first variant of the extrapolation.

¹To distinguish between these two variants I introduced parameter `K_e`.

4. HIGH ORDER TERMS (HOT) CORRECTIONS

In our previous calculations we saw that HOT corrections for Ba are large. Here I compare calculation with and without HOT corrections. The following screening coefficients are used:

$$C_0 = 0.99, \quad C_1 = 0.82, \quad C_2 = 1.00, \quad C_3 = 1.02, \quad C_4 = 1.16. \quad (6)$$

These coefficients were calculated by `src` code. Result of the averaging depends on the parameter `Nmax`:

Nmax	Multipolarity K				
	0	1	2	3	4
83	0.99	0.86	1.00	1.00	1.11
29	0.99	0.87	1.00	1.01	1.14
22	0.99	0.82	1.00	1.02	1.16

The value `Nmax=83` corresponds to the full valence space, and `Nmax=22` corresponds to the first valence shell. It is seen that coefficients C_K are rather stable and their dependence on `Nmax` is a smaller effect than HOT correction itself.

5. RESULTS AND DISCUSSION FOR Ba^+

Here I summarize the results of the calculations for different combinations of the parameters. The file `Ba_I_II.txt` includes more details. I calculate 12 levels of Ba^+ : $6s$, $5d_{3/2,5/2}$, $6p_{1/2,3/2}$, $7s$, $6d_{3/2,5/2}$, $4f_{5/2,7/2}$, and $7p_{1/2,3/2}$. Comparison with the experiment is done for the ε_{6s} and for 11 frequencies. The table below gives the error for the ground state energy, the averaged error,² and the maximum error for different calculations. I think that these three numbers give sufficient information on the quality of the calculations and on the dependence of the results on the choice of the parameters.

The initial set of parameters is: `Ns=159`, `K_inf=1`, `K_e=0`, `Khot=1`, where `K_e=0,1` corresponds to the energy-dependence of σ in the CI calculation. Typically I change only one parameter at a time. Only this parameter is listed in the table. The only exception is the last calculation where all parameters acquire maximum values. This calculation is marked as “full” and is the most elaborate. Theoretically, we expect it to be the most accurate.

²when errors are of different signs, the averaging is done for the absolute values and the averaged value is given without the sign.

Parameters	Errors (%)			Score
	ε_{6s}	Av.	max	
Ns = 126	-0.8	-3.0	-9.5	5.9
= 159	-1.0	-2.7	-6.2	6.4
= 192	-1.1	-2.2	-3.3	8.8
K_inf = 0	-0.8	-4.2	-15.2	4.9
= 1	-1.0	-2.7	-6.2	6.4
= 3	-0.9	-2.4	-4.5	7.8
= 5	-0.9	-2.1	-3.4	9.2
K_e = 0	-1.0	-2.7	-6.2	6.4
= 1	-0.6	-1.5	-3.0	11.9
Khot = 0	-2.2	-4.5	-9.2	3.7
= 1	-1.0	-2.7	-6.2	6.4
“full”	-0.7	2.2	+7.0	7.4
CI	+6.6	13.4	-47.7	1.0

5.1. **Discussion.** General conclusion: **all parameters significantly influence the results.** Most importantly, **the saturation of the basis set has not been reached.** Probably that means that the set of B -splines [15/6] used here is not adequate.

To compare the quality of different calculations I assigned the score which shows improvement compared to pure CI calculation:

$$\text{Score} = \frac{1}{3} \sum_{i=1}^3 \left| \frac{\text{Err}_{\text{CI},i}}{\text{Err}_i} \right|. \quad (7)$$

According to this score, the worst MBPT calculation is the one with no HOT corrections. For each parameter the quality of the calculation improves as parameter grows. However, when all parameters acquire their maximum values (“full” calculation), the score drops down to a moderate value 7.4.³ This is discouraging, because theoretically this calculation should be the best.

6. BA I

The following table lists results of the calculations of the lowest 8 even and 8 odd states of Ba I, i.e.

$$\text{Even levels : } ^1S_0[6s^2], ^3D_J[5d6s], ^1D_2[5d6s], ^3F_J[5d^2]; \quad (8)$$

$$\text{Odd levels : } ^3P_J[6s6p], ^1P_1[6s6p], ^3F_J[5d6p], ^1D_2[5d6p]. \quad (9)$$

Parameters for the basic calculation here are: **Ns=192**, **Khot=1**, **K_inf=1:1**, **K_e=0**, where two values for **K_inf** correspond to the one-electron and two-electron MBPT corrections.

³I checked, that screening coefficients (6) are the same for the basis set **Ns=192**.

Parameters	Errors (%)			Score
	E_{GS}	Av.	max	
$K_{inf} = 1:1$	-1.2	1.3	-2.8	7.9
= 5:1	-1.1	1.9	+3.9	6.2
= 1:0	-1.0	2.3	+5.2	5.6
$K_e = 0$	-1.2	1.3	-2.8	7.9
= 1	-1.4	3.1	+6.2	4.2
= 1*	-1.5	3.0	+5.8	4.2
CI	+6.8	12.5	-23.3	1.0

I used the same Eq. (7) to compare the accuracy of different calculations. It is seen that extrapolation to $L \rightarrow \infty$ for the screening corrections is important. The energy dependence is also important, but it does not improve the accuracy of the calculation. It is possible that energies (5) are not optimal, as they require extrapolation in positive direction. However, calculation marked with the star shows that another choice of these energies does not improve the accuracy.⁴

7. VOLUME SHIFT FOR BA II AND BA I

Volume shift coefficient K_{VS} is calculated as above with the CI basis sets `Ns=83` [`h_83_0.dat`, `h_83_p.dat`, and `h_83_m.dat`]. MBPT parameters for the final calculation are `Ns=192`, `Khot=1`, `K_inf=1:1`, `K_e=0`. Parameter `C_is` is chosen to be ± 0.1 .

Three MBPT basis sets were generated. In order to estimate the errors I did several auxiliary calculations. The pure CI calculation was done on the single basis [CI(val)] and using basis sets, which account for core relaxation [CI]. CI+MBPT calculations accounted for core relaxation. The one marked as [+II] did not include HOT corrections.

Experimental data for volume shift can be obtained using King plots (see problem 1.9 in [3]). This method gives the ratios of VS constants for different transitions. In the table below reference constants are marked with letters X , Y , and Z . These reference constants are in turn linked to each other by different experimental data. Thus, it is possible to leave single reference constant. However, this will lead to larger error bars and I did not do this.

⁴The energies for this calculation were chosen using the rule: $\varepsilon_i = E_k - \varepsilon_{6s}$, where E_k is the valence energy of the lowest level of the configuration [6s,i]. This rule gives following energies for the spd waves: -0.22, -0.17, -0.18.

Volume shift for Ba II

Level	K_{VS} (GHz/Fm ²)					
	CI(val)	CI	+II	+HOT	[4]	[5]
$6s_{1/2}$	3.20	3.41	4.47	4.18	3.89	4.10
$5d_{3/2}$	0.00	-1.10	-1.01	-1.30	-1.22	
$5d_{5/2}$	0.00	-1.03	-0.96	-1.22	-1.15	
$6p_{1/2}$	0.07	-0.12	-0.09	-0.15	-0.15	-0.11
$6p_{3/2}$	0.00	-0.19	-0.18	-0.22	-0.23	-0.24
$7s_{1/2}$	1.05	1.10	1.26	1.22		
$6d_{3/2}$	0.00	-0.23	-0.16	-0.23		
$6d_{5/2}$	0.00	-0.23	-0.17	-0.22		
$4f_{5/2}$	0.00	-0.08	-1.51	-1.02		
$4f_{7/2}$	0.00	-0.09	-1.12	-0.77		
$7p_{1/2}$	0.02	-0.05	-0.04	-0.05		
$7p_{3/2}$	0.00	-0.07	-0.07	-0.08		

Volume shift for Ba I

Level	K_{VS} (GHz/Fm ²)			
	CI(val)	CI	+II	+HOT
$6s^2$ 1S_0	4.29	4.61	6.51	6.08
$5d6s$ 3D_1	1.98	1.46	2.40	1.96
3D_2	1.98	1.46	2.41	1.99
3D_3	2.01	1.54	2.48	2.07
1D_2	1.62	1.03	1.73	1.36
$5d^2$ 3F_2			-1.34	-1.75
3F_3			-1.33	-1.71
3F_4			-1.30	-1.68
$6s6p$ $^3P_0^o$	2.35	2.35	3.28	3.01
$^3P_1^o$	2.34	2.33	3.26	2.98
$^3P_2^o$	2.31	2.29	3.23	2.98
$^1P_1^o$	2.11	2.03	2.80	2.61
$5d6p$ $^3F_2^o$	0.07	-0.85	-0.87	-1.14
$^3F_3^o$	0.06	-0.84	-0.87	-1.12
$^1D_2^o$	0.04	-0.94	-0.92	-1.17
$^3F_4^o$	0.01	-0.84	-0.88	-1.12

Comparison with experimental data for volume shift in transitions

Transition	K_{VS}	Reference
Ba I		
$^1S_0(6s^2) - ^3P_1(6s6p)$	X	[6]
$^1S_0(6s^2) - ^1P_1(6s6p)$	$1.176(9) \times X$	[6]
" - "	$1.122 \times X$	this work
" - "	$0.8075(16) \times Z$	[4]
" - "	$0.778 \times Z$	this work
$^3D_3(6s5d) - ^1D_2(6p5d)$	$1.053(11) \times X$	[6]
" - "	$1.047 \times X$	this work
$^3D_3(6s5d) - ^3F_3(6p5d)$	$1.043(11) \times X$	[6]
" - "	$1.030 \times X$	this work
$^3D_1(6s5d) - ^1D_2(6p5d)$	$1.029(17) \times X$	[6]
" - "	$1.014 \times X$	this work
Ba II		
$6s_{1/2} - 6p_{1/2}$	$1.471(44) \times X$	[6]
" - "	$1.400 \times X$	this work
" - "	$0.975(3) \times Z$	[4]
" - "	$0.984 \times Z$	this work
$6s_{1/2} - 6p_{3/2}$	Z	[4]
$5d_{3/2} - 6p_{1/2}$	$-0.251(1) \times Z$	[4]
" - "	$-0.261 \times Z$	this work
$5d_{3/2} - 6p_{3/2}$	$-0.2312(6) \times Z$	[4]
" - "	$-0.245 \times Z$	this work
" - "	$1.0465(10) \times Y$	[7]
" - "	$1.073 \times Y$	this work
$5d_{5/2} - 6p_{3/2}$	$-0.222(1) \times Z$	[4]
" - "	$-0.228 \times Z$	this work
" - "	Y	[7]

8. NORMAL AND SPECIFIC MASS SHIFT FOR BA II AND BA I

Specific mass shift (SMS) is calculated in a similar way. The main difference is that SMS corrections explicitly enter the MBPT diagrams. Here the parameter `C.is` is chosen to be ± 0.001 . I check the relative size of the next term of the Taylor expansion:

$$\frac{E(C_{is}) - 2E(0) + E(-C_{is})}{E(C_{is}) - E(-C_{is})} \quad (10)$$

For the CI calculation this ratio is typically smaller than 1%. However, for the CI+MBPT calculation it is typically few percent and much larger for small values of K_{SMS} .⁵

⁵More details in the file `Ba_SMS.xls`.

Specific mass shift for Ba II

Level	K_{SMS} (GHz · amu)				H_{eff} (HOT)
	CI			Full	
	Core	1e	Full		
$6s_{1/2}$	881.5	-1745.2	-863.7	-297.6	
$5d_{3/2}$	2203.4	-3782.0	-1578.6	-1049.2	
$5d_{5/2}$	2073.3	-3643.0	-1569.7	-1032.8	
$6p_{1/2}$	418.0	-725.3	-307.3	-145.4	
$6p_{3/2}$	421.3	-595.5	-174.2	-3.5	
$7s_{1/2}$	279.8	-515.8	-236.0	-48.3	
$6d_{3/2}$	387.6	-607.4	-219.7	-91.3	
$6d_{5/2}$	390.3	-622.6	-232.4	-105.0	
$4f_{5/2}$	233.4	-327.4	-94.0	-1622.3	
$4f_{7/2}$	241.2	-337.1	-95.9	-1251.6	
$7p_{1/2}$	181.3	-290.0	-108.8	-44.2	
$7p_{3/2}$	153.7	-225.3	-71.6	-6.8	

Specific mass shift for Ba I

Level	K_{SMS} (GHz · amu)				H_{eff} (HOT)	
	CI			Full		
	Core	1e	2e			
$6s^2$ 1S_0	1254.5	-2535.4	101.0	-1179.9	-444.5	
$5d6s$	3D_1	2130.1	-3925.9	80.5	-1715.2	-998.0
	3D_2	2099.2	-3893.3	78.4	-1715.8	-1003.5
	3D_3	2027.2	-3823.7	78.5	-1718.0	-1006.1
$5d^2$	1D_2	1908.9	-3548.5	51.3	-1588.3	-1012.4
	3F_2					-1398.9
	3F_3					-1405.9
	3F_4					-1408.6
$6s6p$	$^3P_0^o$	962.2	-1894.7	-86.9	-1019.5	-814.4
	$^3P_1^o$	963.6	-1867.0	-90.8	-994.3	-784.5
	$^3P_2^o$	964.8	-1794.5	-101.9	-931.6	-716.4
	$^1P_1^o$	1089.0	-2058.4	142.7	-826.7	-221.2
$5d6p$	$^3F_2^o$	1819.8	-3239.8	-53.7	-1473.7	-1057.3
	$^3F_3^o$	1769.4	-3142.6	-65.4	-1438.6	-1045.0
	$^1D_2^o$	1732.1	-3064.6	-67.4	-1399.9	-917.3
	$^3F_4^o$	1887.6	-3316.6	30.0	-1398.9	-1012.6

Relativistic corrections to SMS for Ba II. NRU corresponds to non-relativistic SMS operator applied to upper component; NRB — non-relativistic operator applied to both components; R — relativistic operator.

Level	K_{SMS} (GHz · amu)			H_{eff} R
	DF			
	NRU	NRB	R	
$6s_{1/2}$	-863.7	-809.4	-919.8	-373.3
$5d_{3/2}$	-1574.5	-1533.1	-1618.8	-1084.4
$5d_{5/2}$	-1568.2	-1530.3	-1633.0	-1115.1
$6p_{1/2}$	-308.6	-329.1	-233.1	-69.0
$6p_{3/2}$	-171.4	-184.4	-174.1	-10.1
$7s_{1/2}$	-236.0	-219.0	-253.5	-67.4
$6d_{3/2}$	-232.7	-226.2	-237.3	-105.7
$6d_{5/2}$	-226.5	-220.4	-239.3	-111.1
$4f_{5/2}$	-94.0	-88.6	-101.9	-1716.7
$4f_{7/2}$	-95.0	-89.5	-103.0	-1333.1
$7p_{1/2}$	-121.1	-129.1	-91.7	-26.8
$7p_{3/2}$	-68.1	-73.3	-69.1	-5.0

Relativistic corrections to NMS for Ba II. NRU corresponds to non-relativistic NMS operator applied to upper component; NRB - non-relativistic operator applied to both components; R - relativistic operator.

Level	K_{NMS} (GHz · amu)				H_{eff} R	$\frac{K_{\text{NMS}}}{K_{\text{NMS}}^{\text{R}}}$
	DF					
	NRU	NRB	R			
$6s_{1/2}$	1333.1	1490.7	1229.3	1347.4	1.003	
$5d_{3/2}$	1026.3	942.0	1123.3	1287.4	1.018	
$5d_{5/2}$	1009.2	929.0	1122.8	1280.9	1.025	
$6p_{1/2}$	991.4	992.8	935.8	1000.9	1.001	
$6p_{3/2}$	912.7	911.1	915.6	974.5	1.004	
$7s_{1/2}$	637.1	688.4	602.5	630.4	0.998	
$6d_{3/2}$	531.4	515.0	546.7	572.7	1.003	
$6d_{5/2}$	523.4	507.5	545.5	571.0	1.007	
$4f_{5/2}$	453.3	445.4	465.4	437.6	0.825	
$4f_{7/2}$	454.0	446.4	466.2	452.2	0.871	
$7p_{1/2}$	516.6	517.2	494.9	514.1	0.998	
$7p_{3/2}$	486.1	485.6	487.0	504.9	1.000	

Relativistic correction to SMS for Ba I.

Level		K_{SMS} (GHz · amu)			H_{eff}
		NRU	NRB	R	
$6s^2$	1S_0	-1180.1	-1108.8	-1252.5	-731.9
$5d6s$	3D_1	-1714.6	-1646.2	-1786.9	-1249.2
	3D_2	-1715.2	-1647.7	-1789.1	-1259.2
	3D_3	-1717.4	-1651.1	-1799.1	-1276.8
	1D_2	-1588.1	-1535.5	-1650.5	-1288.5
$5d^2$	3F_2				-1652.9
	3F_3				-1672.2
	3F_4				-1689.0
$6s6p$	$^3P_0^o$	-1019.7	-996.3	-1006.7	-1236.2
	$^3P_1^o$	-994.4	-969.4	-997.1	-1213.1
	$^3P_2^o$	-931.7	-902.2	-973.3	-1197.0
	$^1P_1^o$	-826.8	-792.5	-861.0	-174.3
$5d6p$	$^3F_2^o$	-1473.2	-1453.6	-1463.6	-1137.3
	$^3F_3^o$	-1438.1	-1417.1	-1456.5	-1169.7
	$^1D_2^o$	-1398.7	-1373.1	-1436.1	-1072.8
	$^3F_4^o$	-1399.4	-1376.5	-1447.5	-1176.7

Relativistic correction to NMS for Ba I.

Level		K_{SMS} (GHz · amu)			
		CI		H_{eff}	
$6s^2$	1S_0	1876.4	0.99	2044.7	1.00
$5d6s$	3D_1	1696.2	1.00	1929.3	1.02
	3D_2	1696.3	1.00	1927.0	1.02
	3D_3	1697.1	1.00	1923.0	1.02
	1D_2	1679.9	1.00	1888.4	1.02
$5d^2$	3F_2			1750.3	1.04
	3F_3			1747.2	1.04
	3F_4			1743.1	1.04
$6s6p$	$^3P_0^o$	1714.6	0.99	1822.7	0.98
	$^3P_1^o$	1709.8	0.99	1817.5	0.98
	$^3P_2^o$	1699.2	0.99	1804.8	0.98
	$^1P_1^o$	1603.8	1.00	1747.7	1.00
$5d6p$	$^3F_2^o$	1526.1	1.00	1696.4	1.00
	$^3F_3^o$	1520.4	1.00	1683.4	1.00
	$^1D_2^o$	1512.4	1.00	1684.1	1.01
	$^3F_4^o$	1514.2	1.00	1671.9	1.01

Comparison with experimental data for SMS shift in transitions

Transition	K_{SMS} (GHz·amu)		
	Ref.[8]	CI	H_{eff}
Ba I			
$^1S_0(6s^2) - ^3P_1(6s6p)$	-244(9)	-256	481
$^1S_0(6s^2) - ^1P_1(6s6p)$	-338(9)	-392	-558
$^3D_3(6s5d) - ^3F_3(6p5d)$	-328(9)	-343	-107
$^3D_3(6s5d) - ^1D_2(6p5d)$	-338(19)	-363	-204
Ba II			
$6s_{1/2} - 6p_{1/2}$	-610(56)	-680	-371
$5d_{5/2} - 6p_{3/2}$	-1342(9)	-1458	-1197

9. BIBLIOGRAPHY ON IS IN BA

Calculation of IS in Ba II was done by Berengut et al. [4]. One can find several references to the experiment there too (see refs. [15 – 18]). More experimental data for Ba I and II is in [8]. More theory is in [5]. In ref. [7] the J -dependence of the IS is measured for $5d \rightarrow 6p$ transition in Ba II. State dependent volume isotope shift analysis of the low lying states of Ba I and Ba II was done in [6].

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