Space-time variation of the fine structure constant and evolution of isotope abundances

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- Why α-variation and evolution of isotope abundances are linked

- Atomic theory of the α-variation and isotope shifts

- Analysis of the transitions used in astrophysical search for α-variation

- Anchors and Probes

- Conclusions

Astrophysical search for α-variation

Suppose that the fine structure constant α can vary in space-time. Then, for a distant quasar all atomic frequencies will be shifted:

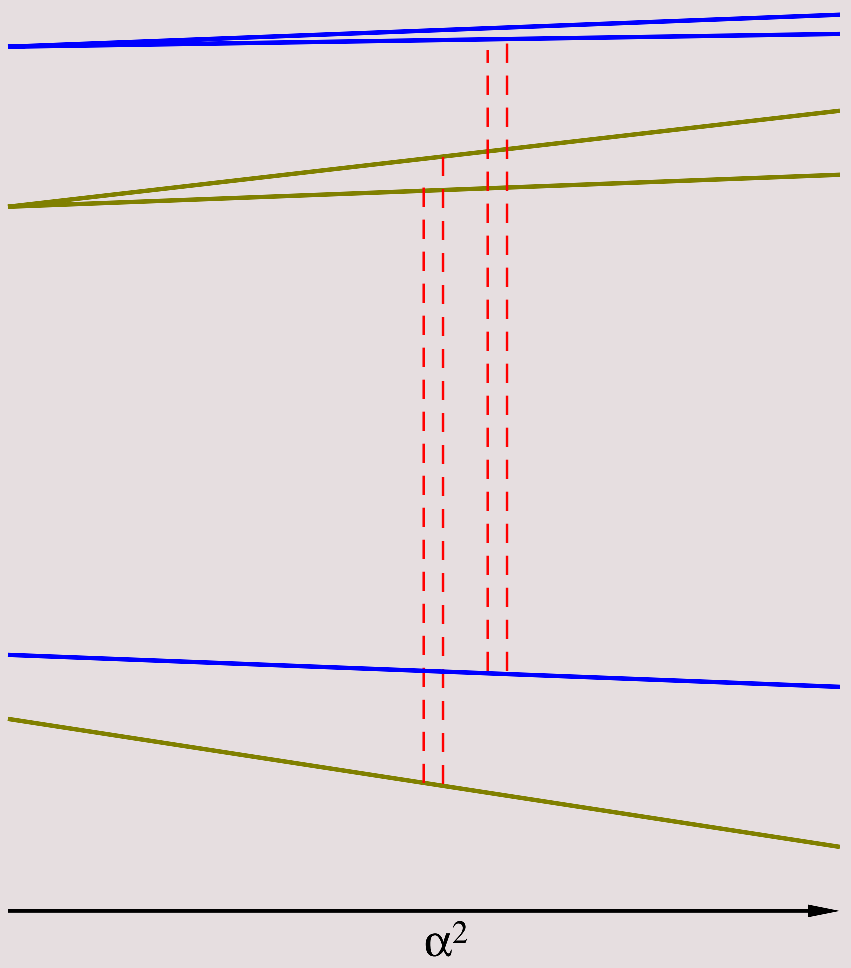
$$\begin{aligned} \omega_i &= \omega_{i,0} + q_i x + \ldots, \\ x &\equiv (\alpha/\alpha_0)^2 - 1, \quad \alpha \equiv e^2/(\hbar c), \end{aligned}$$

where $\alpha_0 = 1/137\ldots$ and $\omega_{i,0}$ are the laboratory values.

The light from the distant objects is red-shifted because of the expansion of the Universe. We can exclude cosmological red shift by taking the ratios of the frequencies:

$$\frac{\omega_i}{\omega_k} = \left(\frac{\omega_i}{\omega_k}\right)_0 \left(1 + \left(\frac{q_i\omega_k - q_k\omega_i}{\omega_i\omega_k}\right)_0 x\right).$$

Many-multiplet method



In many-multiplet method all available lines are compared to each other in order to determine α. That allows to:

(1) Increase statistics.

(2) Increase the effect by taking into account all line shifts rather than multiplet splittings.

(3) Average systematic errors caused by possible isotope shifts [!?]

What is known about α-variation?

Recent observations for the quasar spectra at distances of $\sim 10^{10}$ light years by Murphy *et al.* indicated that in the past α was slightly smaller. At least two other groups are also looking for such deviations in the spectra of distant quasars, but their results are consistent with non-varying α:

$$\frac{\Delta\alpha}{\alpha} = 10^{-5} \times \begin{cases} -0.57(11) & \text{Murphy } \textit{et al.} \quad (2003) \\ -0.04(19)(27)_{\text{sys}} & \text{Quast } \textit{et al.} \quad (2004) \\ -0.06(6) & \text{Srianand } \textit{et al.} \quad (2004) \end{cases}$$

These frequency shifts are of the same order of magnitude as typical isotope shifts. Therefore, possible changes in isotope abundances can be one of the sources of systematic errors in the search for α-variation.

Atomic calculations of q and mass shift (MS)

To find q_i we make a fully relativistic calculation of atomic frequencies for sufficiently small values of $x = (\alpha/\alpha_0)^2 - 1$:

$$q_i \approx 4\,[\omega_i(x = 1/8) - \omega_i(x = -1/8)]\,.$$

Because of the nuclear recoil effect atomic frequencies depend on the nuclear mass M. If it is changed by δM, the atomic frequency is changed too:

$$\omega_i = \omega_{i,0} + k_{i,\mathrm{MS}}\,\frac{\delta M}{M^2}.$$

There are two contributions to k_{MS}. Normal mass shift is associated with the substitution of the electron mass m with the reduced mass $\mu = mM/(m+M)$.

Specific mass shift (SMS) is described by the two-electron operator:

$$H_{\mathrm{SMS}} = \frac{1}{M} \sum_{i>k} \vec{p}_i \cdot \vec{p}_k,$$

where $\vec{p}_i$ is the momentum of the electron i and M is nuclear mass. This operator is similar to the Breit operator, which describes relativistic corrections to Coulomb interaction.

H_{SMS} is added to the many-electron Hamiltonian:

$$H_\lambda = H_0 + \lambda\, M\, H_{\mathrm{SMS}}.$$

The eigenvalue problem for this Hamiltonian is solved for $+\lambda$ and for $-\lambda$. Then, k_{SMS} is given by:

$$k_{\mathrm{SMS}} \approx \frac{E_{+\lambda} - E_{-\lambda}}{2\lambda}.$$

There is strong similarity in calculations of the coefficients q *and* k_{SMS}*!*

Ion	Transition			ω_0	q		k_{MS}		$\Delta\omega_\alpha$	$\Delta\omega_1$	$\Delta\omega_2$
				(cm^{-1})	(cm^{-1})		(cm$^{-1}\cdot$ amu)			(10^{-3}cm^{-1})	
O II	$^4S^o_{3/2}[2s^22p^3]$	→	$^4P_{5/2}[2s2p^4]$	119873	346		—		−4	—	0
		→	$^4P_{3/2}[2s2p^4]$	120000	489		—		−6	—	0
		→	$^4P_{1/2}[2s2p^4]$	120083	574		—		−7	—	0
Mg I	$^1S_0[3s^2]$	→	$^1P^o_1[3s3p]$	35051	86		14.5	(0.3)	−1	5	−8
Mg II	$3s_{1/2}$	→	$3p_{1/2}$	35669	120		32.1	(0.4)	−1	10	−16
		→	$3p_{3/2}$	35761	211		32.1	(0.2)	−2	10	−16
Al II	$^1S_0[3s^2]$	→	$^3P_0[3s3p]$	37393	146	(15)	—		−2	—	0
		→	$^3P_1[3s3p]$	37454	211	(20)	—		−2	—	0
Si II	$^2P^o_{1/2}[3s^23p]$	→	$^2D_{3/2}[3s3p^2]$	55309	520	(30)	63	(15)	−6	8	−9
		→	$^2S_{1/2}[2s^24s]$	65495	50	(30)	−13	(20)	−1	−2	2
Ti II	$^4F_{3/2}[3d^24s]$	→	$^4F^o_{3/2}[3d^24p]$	30837	541	(50)	20	(4)	−6	−2	1
		→	$^4F^o_{5/2}[3d^24p]$	30959	673	(70)	20	(4)	−8	−2	1
Cr II	$^6S_{5/2}[3d^5]$	→	$^6P^o_{3/2}[3d^44p]$	48399	−1360	(150)	−63	(40)	16	−2	1
		→	$^6P^o_{5/2}[3d^44p]$	48491	−1280	(150)	−63	(40)	15	−2	1
		→	$^6P^o_{7/2}[3d^44p]$	48632	−1110	(150)	−63	(40)	13	−2	1

Ion	Transition			ω_0	q		k_{MS}		$\Delta\omega_\alpha$	$\Delta\omega_1$	$\Delta\omega_2$
				(cm^{-1})	(cm^{-1})		(cm$^{-1}\cdot$ amu)		(10^{-3}cm^{-1})		
Mn II	$^7S_3[3d^54s]$	→	$^7P^o_2[3d^54p]$	38366	869	(90)	—		−10	—	0
		→	$^7P^o_3[3d^54p]$	38543	1030	(100)	—		−12	—	0
		→	$^7P^o_4[3d^54p]$	38807	1276	(100)	—		−15	—	0
		→	$^7P^o_2[3d^44s4p]$	83255	−3033	(300)	—		35	—	0
		→	$^7P^o_3[3d^44s4p]$	83376	−2825	(300)	—		32	—	0
		→	$^7P^o_4[3d^44s4p]$	83529	−2556	(300)	—		29	—	0
Fe II	$^6D_{9/2}[3d^64s]$	→	$^6D^o_{9/2}[3d^64p]$	38459	1330	(150)	60	(20)	−15	−4	2
		→	$^6D^o_{7/2}[3d^64p]$	38660	1490	(150)	60	(20)	−17	−4	2
		→	$^6F^o_{11/2}[3d^64p]$	41968	1460	(150)	63	(20)	−17	−4	2
		→	$^6F^o_{9/2}[3d^64p]$	42115	1590	(150)	63	(20)	−18	−4	2
		→	$^6P^o_{7/2}[3d^64p]$	42658	1210	(150)	60	(20)	−14	−4	2
		→	$^6P^o_{7/2}[3d^54s4p]$	62172	−1300	(300)	−67	(40)	15	4	−2
Ni II	$^2D_{5/2}[3d^9]$	→	$^2F^o_{7/2}[3d^84p]$	57080	−700	(250)	−77	(50)	8	−4	18
		→	$^2D^o_{5/2}[3d^84p]$	57420	−1400	(250)	−77	(50)	16	−4	18
		→	$^2F^o_{5/2}[3d^84p]$	58493	−20	(250)	−77	(50)	0	−4	18
Zn II	$4s_{1/2}$	→	$4p_{1/2}$	48481	1584	(25)	70.3	(2.3)	−18	3	−24
		→	$4p_{3/2}$	49355	2490	(25)	69.3	(2.3)	−28	3	−24
Ge II	$4p_{1/2}$	→	$5s_{1/2}$	62403	−607		−0.7	(2.3)	7	0	0

How to eliminate MS effect in α-variation search?

Consider two transitions of the same element:

$$\begin{aligned} \omega_i &= \omega_{i,0} + q_i x + k_i \frac{\delta M}{M^2}, \\ \omega_j &= \omega_{j,0} + q_j x + k_j \frac{\delta M}{M^2}, \end{aligned}$$

If we know coefficients k accurately, we can eliminate M-dependence by taking combination:

$$k_j\omega_i - k_i\omega_j = (k_j\omega_i - k_i\omega_j)_0 + (k_j q_i - k_i q_j)x.$$

Similarly, if we know coefficients q accurately, we can eliminate α-dependence:

$$q_j\omega_i - q_i\omega_j = (q_j\omega_i - q_i\omega_j)_0 + (q_j k_i - q_i k_j)\frac{\delta M}{M^2}.$$

$\Rightarrow$ *High precision atomic calculations are necessary!*

Anchors and probes

In the search for variation of α and/or isotope abundances it is convenient to have “anchor” lines, which are not sensitive to the variation of both parameters. In the Table there is only one such line for Si II:

$$A_I = \omega\left({}^2P^o_{1/2} \rightarrow {}^2S_{1/2}\right)_{\text{Si II}} = 65495 \text{ cm}^{-1}.$$

It is preferable to have more than one anchor. However, all other lines have either relatively large q, or k_{MS}, or both.

Aluminum, oxygen and manganese ions have only one stable isotope each. Assuming that calculated values for q are accurate, we can eliminate α-dependence by using frequency combinations. For ^{16}O and ^{27}Al following anchors can be formed:

$$\begin{aligned}
A_{II} &= 0.62 \cdot \omega\left({}^4S^o_{3/2} \rightarrow {}^4P_{5/2}\right)_{\text{O II}} \\
&- 0.38 \cdot \omega\left({}^4S^o_{3/2} \rightarrow {}^4P_{1/2}\right)_{\text{O II}} = 29650\ \text{cm}^{-1}, \\
A_{III} &= 0.59 \cdot \omega\left({}^1S_0 \rightarrow {}^3P_0\right)_{\text{Al II}} \\
&- 0.41 \cdot \omega\left({}^1S_0 \rightarrow {}^3P_1\right)_{\text{Al II}} = 6781\ \text{cm}^{-1}, \\
A_{IV} &= 0.68 \cdot \omega\left(3s_{1/2} \rightarrow 3p_{1/2}\right)_{\text{Al III}} \\
&- 0.32 \cdot \omega\left(3s_{1/2} \rightarrow 3p_{3/2}\right)_{\text{Al III}} = 19465\ \text{cm}^{-1}.
\end{aligned}$$

For ^{55}Mn we can take several combinations of frequencies, such as:

$$\begin{aligned}
A_{V} &= 0.67 \cdot \omega\left({}^7S_3 \rightarrow {}^7P^o_4[3d^5 4p]\right)_{\text{Mn II}} \\
&+ 0.33 \cdot \omega\left({}^7S_3 \rightarrow {}^7P^o_4[3d^4 4s 4p]\right)_{\text{Mn II}} = 53699\ \text{cm}^{-1}.
\end{aligned}$$

Isotope Probes

We can form several combinations, which can be used as “probes” of isotope abundances for Mg, Si, and Zn. For example,

$$\begin{aligned} P_I &= 0.64 \cdot \omega \left(3s_{1/2} \rightarrow 3p_{1/2}\right)_{\text{Mg II}} \\ &- 0.36 \cdot \omega \left(3s_{1/2} \rightarrow 3p_{3/2}\right)_{\text{Mg II}} = 9740\,\text{cm}^{-1} \end{aligned}$$

is insensitive to α-variation and can serve as a probe of the abundances of Mg isotopes in a distant astrophysical object.

By analogy with Mg II it is possible to form combinations for the fine structure doublets in Si IV and Zn II:

$$\begin{aligned} P_{II} &= 0.71 \cdot \omega \left(3s_{1/2} \rightarrow 3p_{1/2}\right)_{\text{Si IV}} \\ &- 0.29 \cdot \omega \left(3s_{1/2} \rightarrow 3p_{3/2}\right)_{\text{Si IV}} = 30381\,\text{cm}^{-1} \\ P_{III} &= 0.61 \cdot \omega \left(4s_{1/2} \rightarrow 4p_{1/2}\right)_{\text{Zn II}} \\ &- 0.39 \cdot \omega \left(4s_{1/2} \rightarrow 4p_{3/2}\right)_{\text{Zn II}} = 10423\,\text{cm}^{-1} \end{aligned}$$

For many the other transitions there is strong correlation between parameters q and k_{MS}. This correlation does not allow to exclude dependence on α. The only exception is Ni II, where the transition with the frequency 58493 cm^{-1} is insensitive to α-variation and two other transitions have different parameters q. That gives us two more probes of isotope abundances:

$$\begin{aligned}
P_{IV} &= \omega\left({}^2D_{5/2} \rightarrow {}^2F^o_{5/2}\right)_{\text{Ni II}} \\
&= 58493\ \text{cm}^{-1}; \\
P_{V} &= 0.667 \cdot \omega\left({}^2D_{5/2} \rightarrow {}^2F^o_{7/2}\right)_{\text{Ni II}} \\
&- 0.333 \cdot \omega\left({}^2D_{5/2} \rightarrow {}^2D^o_{5/2}\right)_{\text{Ni II}} \\
&= 18952\ \text{cm}^{-1};
\end{aligned}$$

Probes for α-variation, insensitive to isotope shifts.

Ion	ω cm^{-1}	q cm^{-1}	Frequency combinations
O II	119873	346	$\omega({}^4S^o_{3/2} \rightarrow {}^4P_{5/2})$
	120000	489	$\omega({}^4S^o_{3/2} \rightarrow {}^4P_{3/2})$
	120083	574	$\omega({}^4S^o_{3/2} \rightarrow {}^4P_{1/2})$
Al II	37393	146	$\omega({}^1S_0 \rightarrow {}^3P_0)$
	36454	211	$\omega({}^1S_0 \rightarrow {}^3P_1)$
Mn II	38366	869	$\omega({}^7S_3 \rightarrow {}^7P_2[3d^5 4p])$
	38543	1030	$\omega({}^7S_3 \rightarrow {}^7P_3[3d^5 4p])$
	38807	1276	$\omega({}^7S_3 \rightarrow {}^7P_4[3d^5 4p])$
	83255	-3033	$\omega({}^7S_3 \rightarrow {}^7P_2[3d^4 4s 4p])$
	83376	-2825	$\omega({}^7S_3 \rightarrow {}^7P_3[3d^4 4s 4p])$
	83529	-2556	$\omega({}^7S_3 \rightarrow {}^7P_4[3d^4 4s 4p])$
Ni II	170	-350	$1/2 \cdot \omega({}^2D_{5/2} \rightarrow {}^6D^o_{5/2})$
			$-1/2 \cdot \omega({}^2D_{5/2} \rightarrow {}^6F^o_{7/2})$
	537	690	$1/2 \cdot \omega({}^2D_{5/2} \rightarrow {}^6F^o_{5/2})$
			$-1/2 \cdot \omega({}^2D_{5/2} \rightarrow {}^6D^o_{5/2})$
Zn II	437	453	$1/2 \cdot \omega(4s_{1/2} \rightarrow 4p_{3/2})$
			$-1/2 \cdot \omega(4s_{1/2} \rightarrow 4p_{1/2})$
Ge II	62403	-607	$\omega(4p_{1/2} \rightarrow 5s_{1/2})$

Fe II

For Fe II there is strong correlation between the factors q and k_{MS}. That allows to form several combinations of frequencies suitable as anchors. It could be possible to make anchors from practically any pair of lines in Fe II which include the line 62172 cm^{-1}.

Isotope dependence for Fe II is rather weak and we can not form the isotope probes from the currently used lines.

We also can not eliminate isotope dependence to form ideal α-variation probes. That means that it may be impossible to get significant improvement of sensitivity to α-variation using only Fe II lines

Additional problem here is in the low accuracy of the current calculations for Fe II.

Sensitivity to the isotope abundances

Let us estimate typical sensitivity to the frequency shifts in modern astrophysical studies. The work of Quast *et al.*(2003) is based on the analysis of the lines of Fe II, where $|q| \approx 1300$ cm^{-1}. That allows to estimate their statistical accuracy

$$\Delta\omega \approx 0.005 \text{ cm}^{-1}.$$

We will use this estimate of the accuracy for the frequency shifts in modern astrophysical observations to find the sensitivity to the isotope abundances.

We need to specify how isotope abundances are changed. We assume that the intensity of the line of the leading isotope is transferred to the next to the leading one. If there are two comparable weaker lines, we assume that they are equally increased. Within this model we calculate the shifts of the centers of gravity of the lines and the resulting shift of the probe. Comparison of this shift to the modern frequency sensitivity gives us the sensitivity to the isotope abundances.

Mg has three stable isotopes $A = 24$, 25, and 26 with abundances $79 : 10 : 11$. Suppose that in the early universe it was $(79 - x) : (10 + x/2) : (11 + x/2)$. Ignoring the volume shift, we can estimate corresponding shifts of the center of gravity of the probe P_I:

$$\delta P_I \; = \; -0.27\frac{3k_{\mathrm{MS}}\,x}{200A^2} \approx 0.00023\,x \text{ cm}^{-1}.$$

For Si and Zn there are also two comparable admixtures to the leading isotope. If we assume $(92-x):(5+x/2):(3+x/2)$ abundances for Si and $(49-y):0:(28+y/2):4:(19+y/2):0:1$ abundances for Zn, we get:

$$\begin{aligned}\delta P_{II} &= -0.43\frac{3k_{\mathsf{MS}}\,x}{200\,28^2} \approx 0.00074\,x\ \mathrm{cm}^{-1},\\ \delta P_{III} &= -0.22\frac{3k_{\mathsf{MS}}\,y}{100\,64^2} \approx 0.00011\,y\ \mathrm{cm}^{-1}.\end{aligned}$$

Ni has only one dominant admixture to the leading isotope, so we assume $(68-x):0:(26+x):1:4:0:1$ abundances for Ni. That gives:

$$\begin{aligned}\delta P_{IV} &= -\frac{2k_{\mathsf{MS}}\,x}{100\,58^2} \approx 0.00046\,x\ \mathrm{cm}^{-1},\\ \delta P_{V} &= -0.33\frac{2k_{\mathsf{MS}}\,x}{100\,58^2} \approx 0.00015\,x\ \mathrm{cm}^{-1}.\end{aligned}$$

Comparing dependence of the probes on isotope variation with current experimental sensitivity we see that it is possible to detect:

- 22% change in abundance of the isotope ^{24}Mg,
- 7% changes in abundances of the dominant isotope ^{28}Si,
- 45% change for the dominant isotope ^{64}Zn, and
- 11% change in abundance of the isotope ^{58}Ni.

Method of effective operators for valence electrons

In quantum mechanics the many-electron system is described by the following equations:

$$\begin{array}{lcrcl} \text{spectrum} & : & H\boldsymbol{\Psi}_n & = & E_n\boldsymbol{\Psi}_n, \\ \text{observables} & : & A_{m,n} & = & \langle\boldsymbol{\Psi}_m|A|\boldsymbol{\Psi}_n\rangle, \end{array} \tag{1}$$

where H is all-electron Hamiltonian and $\boldsymbol{\Psi}$ is all-electron wave function.

Instead of solving (1) we use many-body perturbation theory (MBPT) to form effective operators for valence electrons and use configuration-interaction (CI) to solve the valence equation:

$$\begin{array}{rcl} H_{\mathsf{eff}}(E_n)\boldsymbol{\Phi}_n & = & E_n\boldsymbol{\Phi}_n, \\ A_{m,n} & = & \langle\boldsymbol{\Phi}_m|A_{\mathsf{eff}}|\boldsymbol{\Phi}_n\rangle. \end{array} \tag{2}$$

CI+MBPT formalism

We devide all-electron space into valence subspace and complimentary subspace and introduce corresponding projectors P and $Q = 1 - P$.

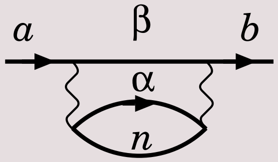
All-electron Schrödinger equation is equivalent to the system:

$$\begin{aligned} \Psi = P\Psi + Q\Psi \equiv \Phi + \chi, \\ H_{\text{eff}}(E)\Phi = E\Phi, \end{aligned}$$

where

$$\begin{aligned} H_{\text{eff}}(E) &\equiv PHP + \Sigma(E), \\ \Sigma(E) &\equiv PHQ\,R_Q(E)\,QHP, \\ R_Q(E) &\equiv (E - QHQ)^{-1}\,. \end{aligned}$$

Linked diagrams for self-energy operator Σ



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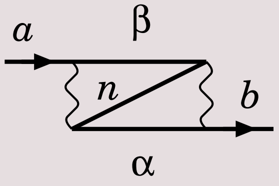

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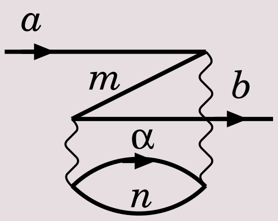

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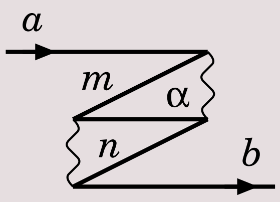

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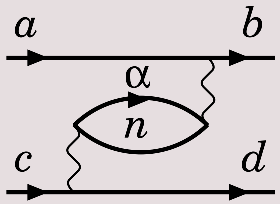

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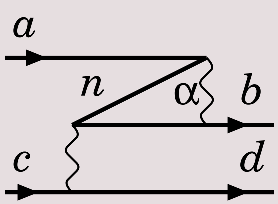

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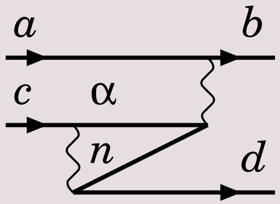

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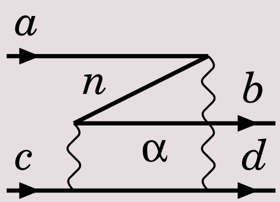

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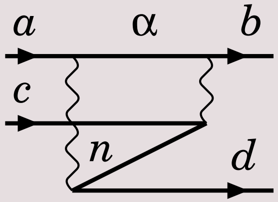

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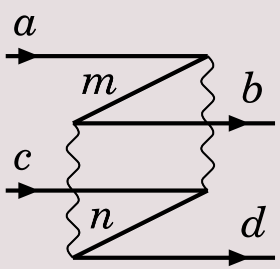

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Comparison with experiment of the SMS for ^{26}Mg and ^{24}Mg.

Calculations are done within frozen-core (FC) approximation and with effective valence Hamiltonian. We assume that the field shift is negligible.

Transition			SMS (MHz)		
			Expt.	H_{FC}	H_{eff}
$^1S_0(3s^2)$	→	$^3P^o_1(3s3p)$	1530[*]	1208	1570
$^1S_0(3s^2)$	→	$^1P^o_1(3s3p)$	−436[†]	−739	−394
"		"	−458[‡]		
$^3P^o_0(3s3p)$	→	$^3S_1(3s4s)$	−1416[§]	−1348	−1387
$^3P^o_1(3s3p)$	→	$^3S_1(3s4s)$	−1409[§]	−1345	−1385
$^3P^o_2(3s3p)$	→	$^3S_1(3s4s)$	−1407[§]	−1340	−1378
$^3P^o_0(3s3p)$	→	$^3D_1(3s3d)$	−1316[†]	−1368	−1293
$^3P^o_1(3s3p)$	→	$^3D_2(3s3d)$	−1314[†]	−1365	−1291
$^3P^o_2(3s3p)$	→	$^3D_3(3s3d)$	−1315[†]	−1360	−1284

[*] Sterr *et al.*, 1993

[†] Hallstadius, 1979

[‡] Le Boiteux *et al.*, 1988

[§] Hallstadius and Hansen, 1978

Conclusions

- In order to improve experimental sensitivity to α-variation and eliminate systematic errors caused by the isotope effects the high accuracy atomic calculations are necessary. One way to improve the accuracy of the theory is to use the method of effective operators for valence electrons.

- As a byproduct of the α-variation surveys one can get information about isotope abundances in the early Universe.

- The new experiments and independent calculations of the IS are highly desirable.