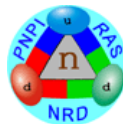


Search for space-time variation of the fine structure constant α and m_p/m_e using molecules

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Collaborators

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Plan of the talk

- 1 Experimental search for time-variation of fundamental constants
 - Astrophysics: quasar absorption spectra
 - Atomic clocks
 - Geophysics: Oklo natural nuclear reactor, Gabon
- 2 Molecular spectra
 - Optical transitions
 - Microwave transitions
 - Inversion spectrum of ammonia
- 3 Conclusions
 - Publications
 - Appendix

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:

$$\begin{aligned}\omega_j &= \omega_{j,0} + q_j x + \dots, \\ x &\equiv (\alpha/\alpha_0)^2 - 1, \quad \alpha \equiv e^2/(\hbar c),\end{aligned}$$

where $\alpha_0 = 1/137 \dots$ and $\omega_{j,0}$ are the laboratory values. The light from the distant objects is red-shifted because of the expansion of the Universe. We can account for that by taking ratios of the frequencies:

$$\frac{\omega_j}{\omega_k} = \left(\frac{\omega_j}{\omega_k} \right)_0 \left[1 + \left(\frac{q_j}{\omega_{j,0}} - \frac{q_k}{\omega_{k,0}} \right) x \right].$$

Astrophysical results for 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. Other groups are also looking for such deviations in the spectra of distant quasars, but their results (at 3σ -level) are consistent with non-varying α :

$$\frac{\Delta\alpha}{\alpha} = 10^{-5} \times \begin{cases} -0.57(11) & \text{Murphy } et al. (2003) & 0.2 < z < 3.7 \\ -0.04(19)(27) & \text{Quast } et al. (2004) & z = 1.15 \\ -0.06(6) & \text{Srianand } et al. (2004) & 0.4 < z < 2.3 \\ +0.54(25) & \text{Levshakov } et al. (2007) & z = 1.84 \end{cases}$$

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.

Laboratory tests

If we have two atomic clocks their frequencies are likely to have different dependence on α and on m_p/m_e . By comparing these frequencies at different times we can look for time-variation of a certain combination x of α and m_p/m_e , $x \equiv \alpha^\nu (m_p/m_e)^\mu$.

- Typical time scale of such experiments is of the order of one year, compared to 10^{10} years in astrophysics.
- Typical accuracy of the frequency measurements is about 10^9 – 10^{10} times higher than in astrophysics.
- No isotope effects and other systematic effects are well controlled.
- Laboratory tests are complementary to astrophysical tests because they measure \dot{x}/x , not $\Delta x/x$.

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Laboratory limits

Results of several most recent laboratory experiments based on comparison of pairs of atomic clocks.

Group, year		Limit	Clocks used	
		$10^{15} \times \dot{\alpha}/\alpha \text{ yr}^{-1}$		
Fortier <i>et al.</i>	(2007)	-0.55 ± 0.95	^{133}Cs	$^{199}\text{Hg}^+$
Peik <i>et al.</i>	(2006)	-0.26 ± 0.39	$^{171}\text{Yb}^+$	$^{199}\text{Hg}^+$
Cingöz <i>et al.</i>	(2006)	-2.7 ± 2.6	^{163}Dy	^{162}Dy
Fischer <i>et al.</i>	(2004)	-0.9 ± 2.9	H	$^{199}\text{Hg}^+$
		$10^{15} \times \dot{x}/x \text{ yr}^{-1}, x = g_{\text{nuc}} m_e/m_p$		
Fortier <i>et al.</i>	(2007)	3.0 ± 5.7	^{133}Cs	$^{199}\text{Hg}^+$

Oklo reactor

It is generally recognized that some 1.8 billion years ago a natural nuclear reactor operated in Oklo uranium mine in Gabon.

In 1976 Shlyakhter realized that some of the involved nuclear reactions depended on the resonances between nuclear and electronic transitions. He concluded that when Oklo reactor was operational α should be very close to its present value.

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Limits on time-variation from Oklo

In the most recent analyzes of data from Oklo the following limits were obtained:

$$\frac{\dot{\alpha}}{\alpha} = 10^{-18} \text{yr}^{-1} \times \begin{cases} +3 \pm 10 & \text{Gould } et al. (2006) \\ -5 \pm 35 & \text{Petrov } et al. (2006) \end{cases}$$

These result depends on a number of assumptions. In particular, it is assumed that strong coupling constant did not change in time, which is unlikely if α was changing.

Flambaum and Shuryak argue that Oklo does not allow to place any restriction on α -variation. Instead they place the limit on $X_s \equiv m_s/\Lambda_{\text{QCD}}$:

$$\left| \dot{X}_s / X_s \right| \leq 10^{-18} \text{yr}^{-1}$$

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Electronic, vibrational, and rotational structures

It is well known that mass ratio $\mu = m_p/m_e$ determines relative scales of electronic, vibrational, and rotational intervals in molecular spectra: $E_{el} : E_{vib} : E_{rot} \sim 1 : \mu^{-1/2} : \mu^{-1}$.

This relation was used in many astrophysical surveys of optical spectra of H_2 , which placed increasingly stringent limits on time-variation of μ . However, the most recent publication by Reinhold *et al.* [PRL, **96**, 151101 (2006)] suggests non-zero variation at 3.5σ level:

$$\delta\mu/\mu = (20 \pm 6) \times 10^{-6},$$

at the time scale of approximately 12 Gyr. Assuming linear variation with time this result translates into

$$\dot{\mu}/\mu = (-17 \pm 5) \times 10^{-16} \text{ yr}^{-1}.$$

Sensitivity coefficients

Sensitivity coefficient K to time-variation of fundamental constant \mathcal{A} is defined as

$$\frac{\delta\omega}{\omega} = K \frac{\delta\mathcal{A}}{\mathcal{A}}$$

In optical transitions in molecules typical sensitivity coefficients for both α and μ are:

$$K = \text{few} \times 10^{-2}$$

In microwave region, the fine-structure transitions, the rotational transitions, or the inversion transition in NH_3 can have

$$K \geq 1$$

Fine-structure of C^+ versus rotational transition in CO

Fine-structure line of C^+ is sensitive to α with $K = 2$, while CO rotational lines are sensitive to μ with $K = -1$.

Comparing redshifts for these two lines we test time-variation of the parameter $F = \alpha^2 \mu$.

Fine-structure line of C^+ and (6 – 5) line of CO were observed by [Maiolino *et al.* \(2005\)](#) and [Bertoldi *et al.* \(2003\)](#) for the quasar with $z = 6.42$ (lookback-time ~ 14 Gyr):

$$\begin{aligned} C^+ : z_{fs} &= 6.4189 \pm 0.0006, \\ CO (6 - 5) : z_{rot} &= 6.4189 \pm 0.0006. \end{aligned}$$

This gives:

$$\left| \frac{\Delta F}{F} \right| \leq 1.1 \times 10^{-4}.$$

18 cm⁻¹ λ -doublet line in OH molecule

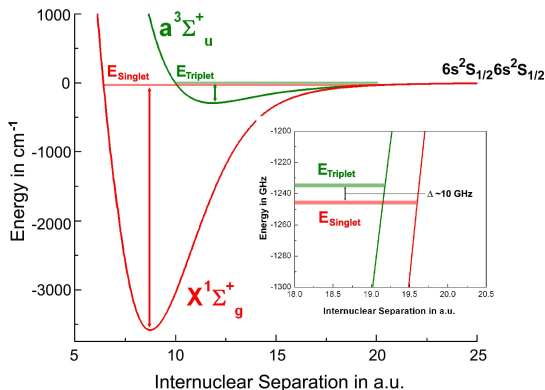
The 18 cm⁻¹ OH lines are seen from very distant objects, up to redshifts $z \approx 0.765$. These lines correspond to the ground state λ -doublet with $\lambda = 1$. Frequency of this transition roughly scales as μ^{-2} Ry.

One can compare frequencies of OH lines with 21 cm⁻¹ hyperfine hydrogenic lines, which scale as $\alpha^2 \mu^{-1} g_p$. This method allows to put a limit on the time-variation of the parameter $x = g_p (\alpha^2 \mu)^{1.57}$ [Kanekar *et al.*, 2005]:

$$\Delta x/x = (0.44 \pm 0.36 \pm 1.0) \times 10^{-5}.$$

Laboratory experiment with Cs₂ [David DeMille]

Ultra cold Cs₂ molecules can be obtained by photo-association in atomic trap. Cs₂ has very narrow forbidden transition



${}^3\Sigma_u^+ \rightarrow {}^1\Sigma_g^-$. The frequency of this transition can be matched by $n \sim 10^2$ vibrational quanta:

$$\omega = \omega_{el} - n\omega_{vib} \approx 0.$$

Frequency ω is very sensitive to variation of μ : $\delta\omega = n\delta\omega_{vib}$.

Diatomic molecules with ground state ${}^2\Pi_{\Omega}$

Fine structure splitting between the states ${}^2\Pi_{1/2}$ and ${}^2\Pi_{3/2}$ depends on α :

$$\omega_f \sim \alpha^2 Z^2 \text{ Hartree,}$$

while vibrational frequency depends on the reduced mass $M_r m_p$:

$$\omega_v \sim (M_r \mu)^{-1/2} \text{ Hartree,} \quad \mu = m_p / m_e.$$

Choosing parameters Z and M_r we can satisfy the equation:

$$\omega = \omega_f - n\omega_v \approx 0, \quad n = 1, 2, \dots$$

Dependence on fundamental constants is given by:

$$\frac{\delta\omega}{\omega} \approx K \left(2 \frac{\delta\alpha}{\alpha} + \frac{1}{2} \frac{\delta\mu}{\mu} \right), \quad K \equiv \frac{\omega_f}{\omega} \gg 1.$$

Examples of molecules with ground state $^2\Pi$ and quasi-degeneracy between ω_f and ω_v from Huber & Herzberg

Molecule	ω_f	ω_v
Cl_2^+	645	645.6
CuS	433.4	415
SiBr	423.1	424.3

Sensitivity of the microwave transition to fundamental constants is given by:

$$\delta\omega = 2\omega_f \left(\frac{\delta\alpha}{\alpha} + \frac{1}{4} \frac{\delta\mu}{\mu} \right)$$

Assuming $\delta\alpha/\alpha \sim 10^{-15}$ and $\omega_f \sim 500 \text{ cm}^{-1}$, we get

$$\delta\omega \sim 3 \times 10^{-2} \text{ Hz.}$$

The line width for these transition is $\Gamma \sim 10^{-2} \text{ Hz.}$

Molecular ion HfF^+

The ion HfF^+ is considered by **Cornell's group in JILA** for the experiment to search for the electric dipole moment (EDM) of the electron.

In principle, EDM experiments and time-variation experiments are similar as both require **high precision frequency measurements.**

Molecular ion HfF^+

Recent calculation by [Petrov *et al.* \(2007\)](#) suggests that the ground state of this ion is $^1\Sigma^+$ and the first excited state $^3\Delta_1$ lies only 1633 cm^{-1} higher. \Rightarrow the levels ($^1\Sigma^+, v = 3$) and ($^3\Delta_1, v = 1$) are very close.

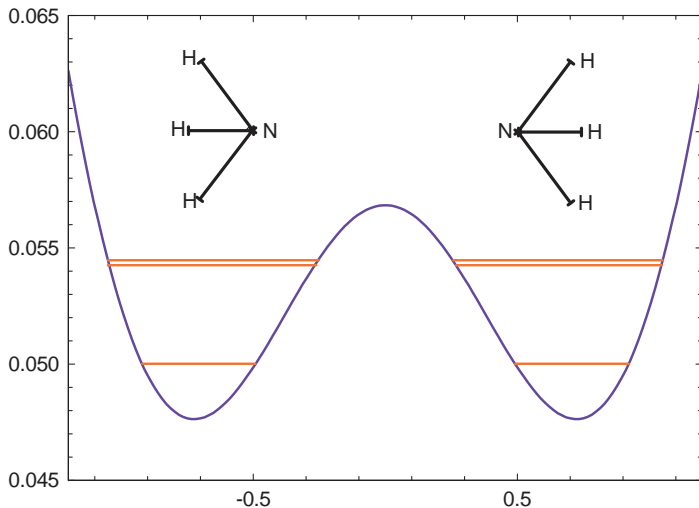
The very rough estimate for the transition ($^1\Sigma^+, v = 3$) \rightarrow ($^3\Delta_1, v = 1$) gives:

$$\frac{\delta\omega}{\omega} \approx \left(\frac{2q}{\omega} \frac{\delta\alpha}{\alpha} + \frac{\omega_{\text{el}}}{2\omega} \frac{\delta\mu}{\mu} \right) \approx \left(2000 \frac{\delta\alpha}{\alpha} + 80 \frac{\delta\mu}{\mu} \right),$$

$$\delta\omega \approx 20000 \text{ cm}^{-1} (\delta\alpha/\alpha + 0.04\delta\mu/\mu).$$

Assuming $\delta\alpha/\alpha \sim 10^{-15}$ we obtain $\delta\omega \sim 0.6 \text{ Hz}$.

Inversion mode of NH_3 molecule



Inversion spectrum of the first vibrational level

Molecular rotation leads to the centrifugal distortion of the potential curve. Because of that, the inversion splitting depends on the rotational angular momentum J and its projection on the molecular symmetry axis K :

$$\omega_{\text{inv}}(J, K) = \omega_{\text{inv}}^0 - c_1 [J(J+1) - K^2] + c_2 K^2 + \dots,$$

$$\omega_{\text{inv}}^0 \approx 23.787 \text{ GHz}, \quad c_1 \approx 151.3 \text{ MHz}, \quad c_2 \approx 59.7 \text{ MHz}.$$

Because of the dipole selection rule $\Delta K = 0$ the levels with $J = K$ are metastable and corresponding inversion lines are usually much narrower and easier to observe.

Inversion Hamiltonian

The inversion line can be approximately described by the following Hamiltonian:

$$H_{\text{inv}} = -\frac{1}{2M_1} \partial_x^2 + U(x)$$
$$U(x) = \frac{1}{2} kx^2 + b \exp(-cx^2),$$

where $k \approx 0.07598$ a.u., $b \approx 0.05684$ a.u., and $c \approx 1.3696$ a.u. Numerical integration of the Schrödinger equation gives the following result:

$$\frac{\delta\omega_{\text{inv}}}{\omega_{\text{inv}}} \approx -4.46 \frac{\delta\mu}{\mu}.$$

Analytical solution [Landau & Lifshitz]

In WKB approximation the inversion frequency is given by:

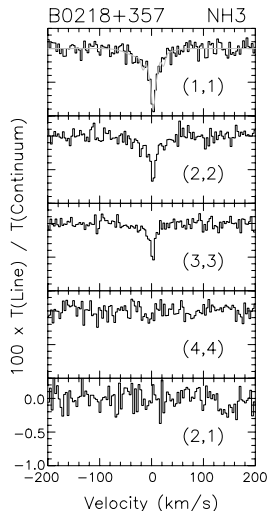
$$\begin{aligned}\omega_{\text{inv}} &= \frac{\omega_V}{\pi} \exp(-S) \\ &= \frac{\omega_V}{\pi} \exp\left(-\frac{1}{\hbar} \int_{-a}^a \sqrt{2M_1(U(x) - E)} dx\right), \\ \frac{\delta\omega_{\text{inv}}}{\omega_{\text{inv}}} &\approx -\frac{\delta\mu}{2\mu} \left(1 + S + \frac{S}{2} \frac{\omega_V}{U_{\text{max}} - E}\right) = -4.4 \frac{\delta\mu}{\mu}.\end{aligned}$$

Similar result was obtained for ND_3 by
 van Veldhoven *et al.* [Eur. Phys. J. D, **31**, 337 (2005)].

Ammonia lines in astrophysics

The most distant object, where inversion lines of NH_3 are seen is the galaxy B0218+357 at the redshift $z \approx 0.68466$, which corresponds to the look back time about 6 Gyr.

Fig. Inversion ammonia lines $\omega_{\text{inv}}(J, K)$ [Henkel *et al.* *Astronomy and Astrophysics*, **440**, 893 (2005)].



Redshifts of microwave lines for B0218+357

Rotational lines			
CO	$J = 1 \rightarrow 2$	red-shifted	0.68470
		blue-shifted	0.68463
CO, HCO ⁺ , HCN		average	0.68466(1)
Inversion lines of NH ₃			
NH ₃	$(J, K) = (1, 1)$	red-shifted	0.684679(3)
		blue-shifted	0.684649(15)
	$= (2, 2)$	red-shifted	0.684677(3)
		blue-shifted	0.684650(17)
	$= (3, 3)$	red-shifted	0.684673(3)
		blue-shifted	0.684627(33)
		average red-shifted	0.684676(3)
		average blue-shifted	0.684647(11)
H	$\lambda = 21$ cm	average	0.68466(4)

Limit on time-variation of μ from microwave lines in the spectrum of B0218+357

Using average redshifts of NH_3 inversion lines we can calculate the average deviation in respect to the average molecular redshift (0.68466(1)):

$$\Delta z_{\text{av}}^{\text{unweighted}} = (0.2 \pm 0.9) \times 10^{-5},$$

$$\Delta z_{\text{av}}^{\text{weighted}} = (0.6 \pm 0.9) \times 10^{-5}.$$

This gives the following estimate for variation of μ :

$$\frac{\delta\mu}{\mu} = 10^{-6} \times \begin{cases} 0.3 \pm 1.6 & \text{(unweighted),} \\ 1.1 \pm 1.5 & \text{(weighted).} \end{cases}$$

Final conservative limit covers the total interval between the minimal and maximal values for estimates above:

$$\delta\mu/\mu = (0.6 \pm 1.9) \times 10^{-6}.$$

Assuming linear time dependence we obtain

$$\dot{\mu}/\mu = (-1 \pm 3) \times 10^{-16} \text{ yr}^{-1}.$$

Previous astrophysical result [Reinhold *et al.*, PRL, **96**, 151101 (2006)] gives non-zero variation:

$$\delta\mu/\mu = (20 \pm 6) \times 10^{-6},$$

which translates into

$$\dot{\mu}/\mu = (-17 \pm 5) \times 10^{-16} \text{ yr}^{-1}.$$

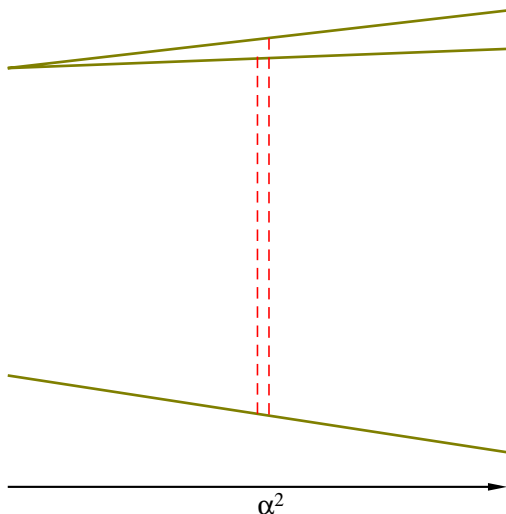
Conclusions

- Search for time-variation of α and $\mu = m_p/m_e$ allows to test theoretical models beyond the standard model.
- There is no decisive evidence of α - and/or μ -variation, but there are some hints for that from astrophysics.
- The most stringent limit on time-variation of μ follows from astrophysical spectra of ammonia.
- Laboratory tests are slightly less sensitive than astrophysical tests. Proposed experiments with cold diatomic molecules potentially have even higher sensitivity to time-variation of α and μ .
- Comparison of fine-structure line of C II with rotational line of CO allows to place limit on time-variation of $\alpha^2\mu$ at $z = 6.42$.

Publications

- V F Flambaum & M G Kozlov,
Phys.Rev.Lett. **98**, 240801 (2007);
arXiv: [0704.2301\[astro-ph\]](#).
- V F Flambaum & M G Kozlov,
Phys.Rev.Lett. **99**, 150801 (2007);
arXiv: [0705.0849\[physics.atom-ph\]](#).

Single multiplet method



Take a doublet (multiplet) line and measure the ratio:

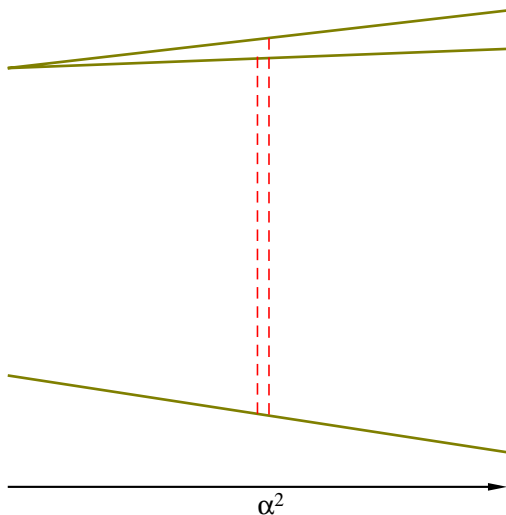
$$(\omega_1 - \omega_2)/(\omega_1 + \omega_2)$$

★ It does not depend on the redshift;

★ it is proportional to α^2 .

• Singlet lines with strong α -dependence are not used and for doublets only the splitting is used.

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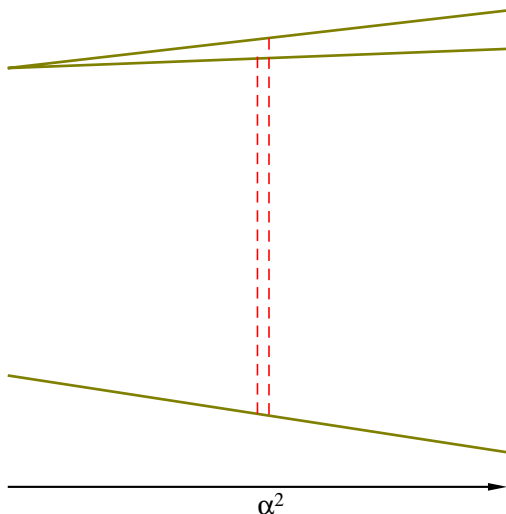
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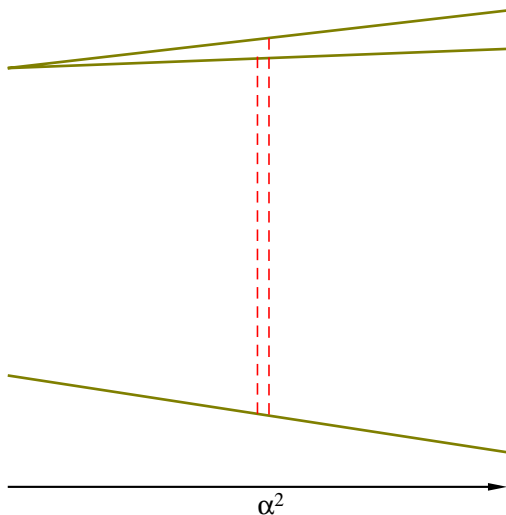
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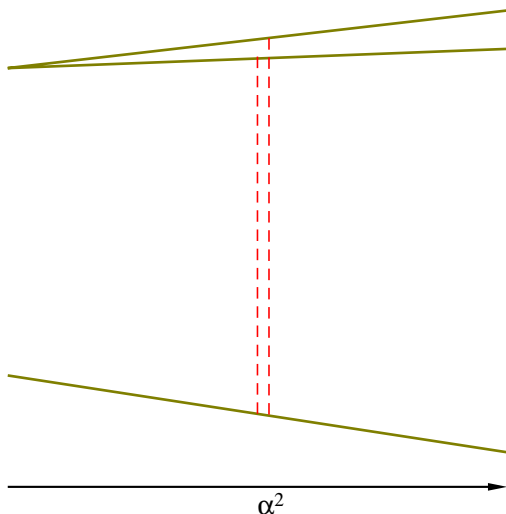
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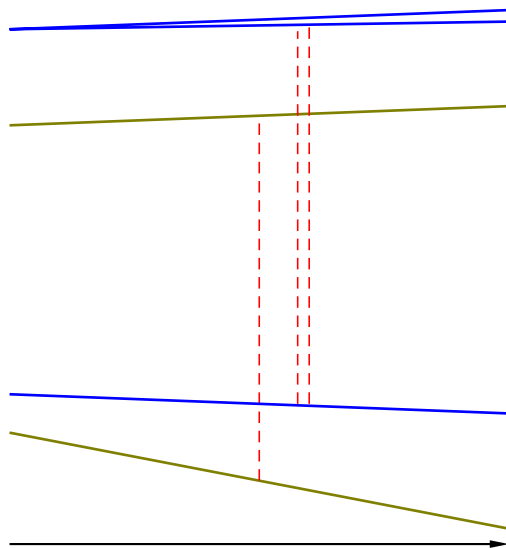
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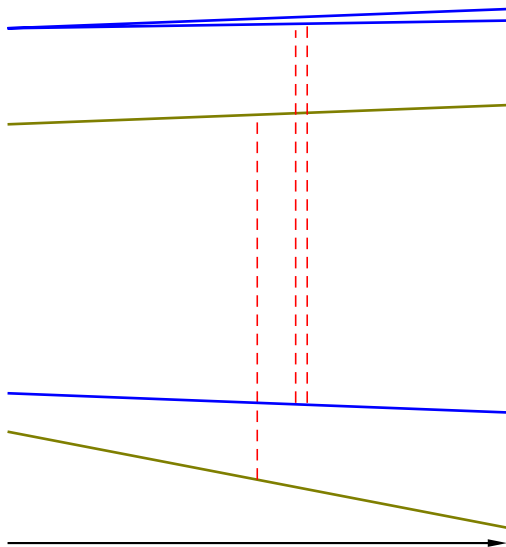
Many multiplet method



Take all lines and make a fit to find the redshift and α for each astrophysical object

- ★ higher statistics
 - ★ larger effects
 - possible systematics from isotope effects and from residual redshifts
- ⇒ requires large-scale averaging

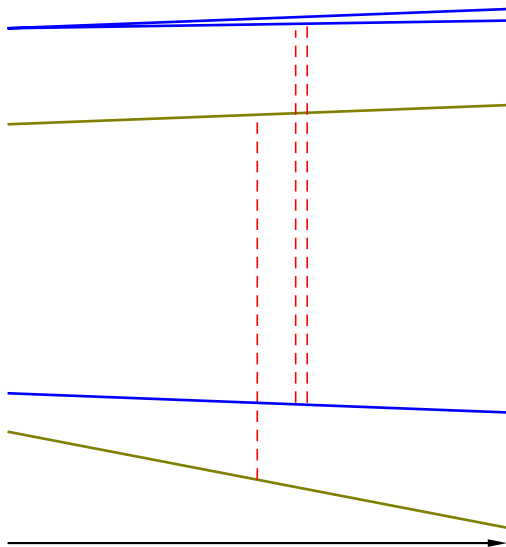
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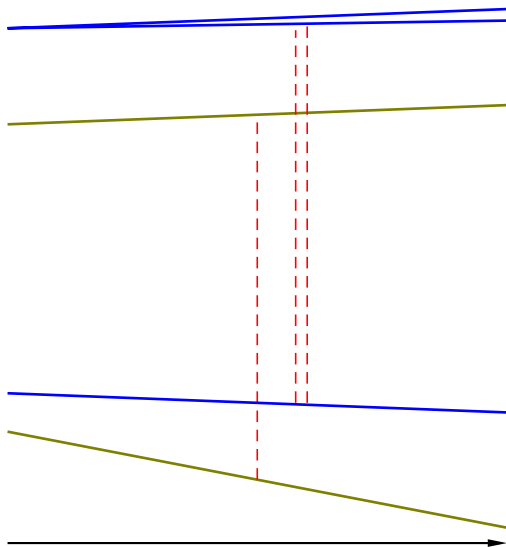
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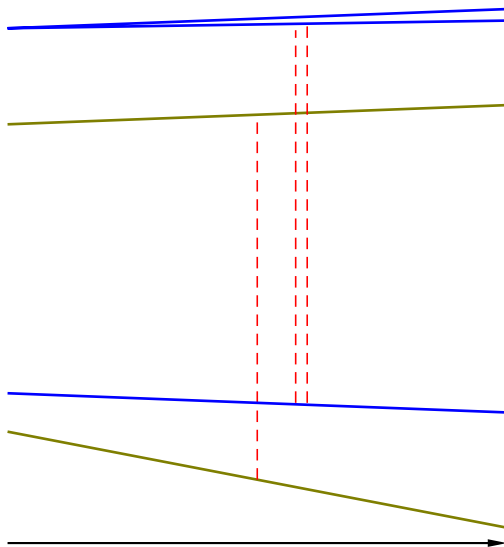
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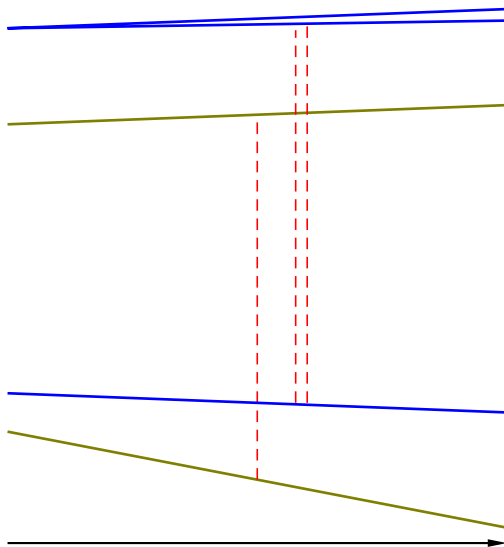


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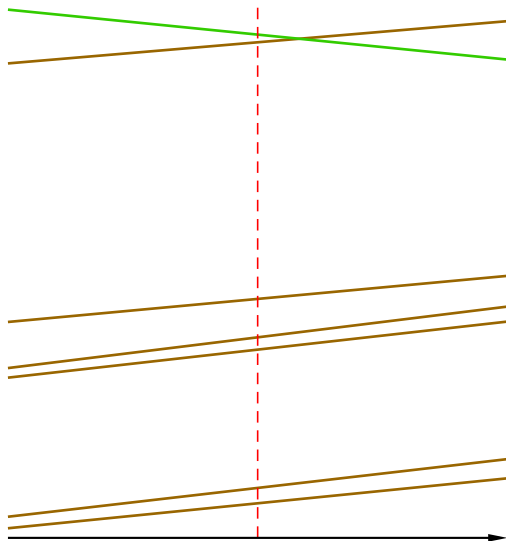
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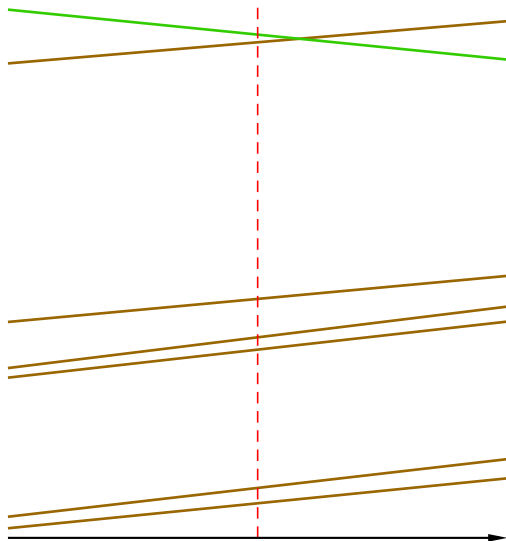
Single ion method using Fe II



Fe II ion:

- ★ strong lines
- ★ high abundance
- ★ large effects
- ★ q -factors of both signs!
- ★ relatively small isotope effects
- complicated electronic structure

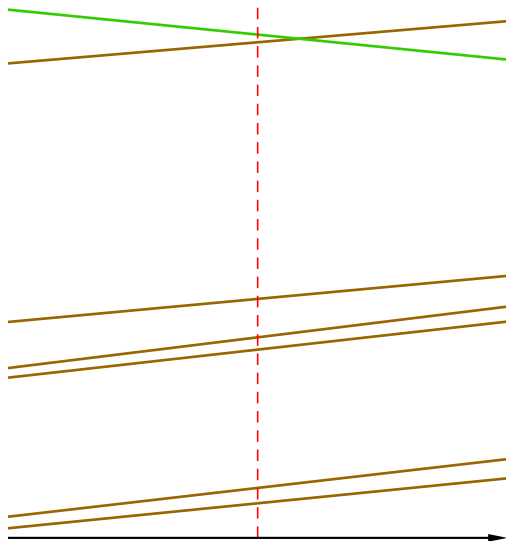
Single ion method using Fe II



Fe II ion:

- ★ strong lines
- ★ high abundance
- ★ large effects
- ★ q -factors of both signs!
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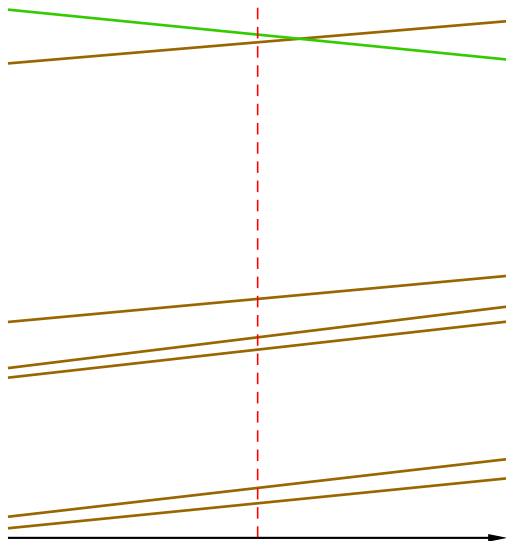
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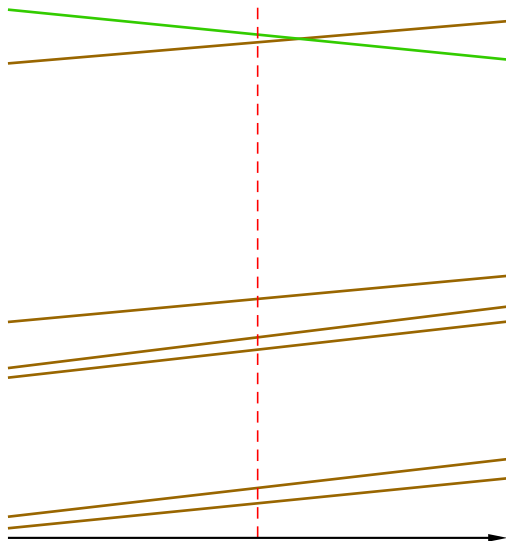
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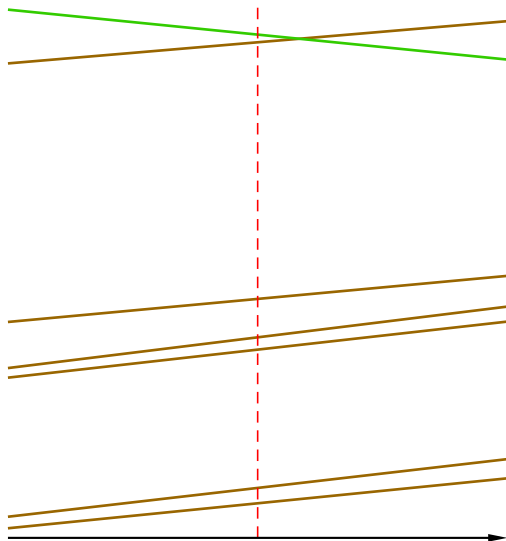
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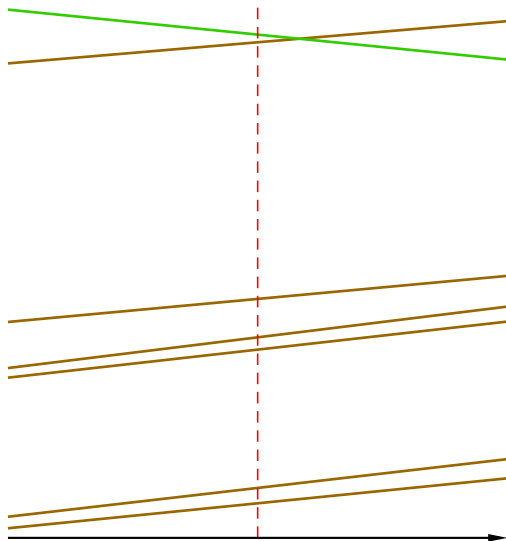
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