Sensitivity of microwave molecular transitions and atomic FIR transitions from quasar spectra to variation of fundamental constants

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Abstract: Microwave and far infrared (FIR) spectra posses higher sensitivity to possible variation of fundamental constants, than optical and UV spectra. Molecular rotational lines and, particularly, inversion line of ammonia are sensitive to variation of proton-to-electron mass ratio, while fine-structure lines of C I, C II, N II, and O I, O III are sensitive to variation of fine-structure constant. Comparing apparent redshifts of these lines one can place stringent limits on time-variation of fundamental constants at extremely high redshifts, up to z~10.

1. Introduction

The problem of variability of fundamental physical constants has a long history starting 70 years ago with publications by Milne [1] and Dirac [2]. The review of its current status is given in [3]. Recent achievements in laboratory studies of the time-variation of fundamental constants are described, for example, in Ref. [4], and the most stringent bound on the time-variation of the fine-structure constant is recently published in Ref. [5]. The variability of the dimensionless physical constants is considered in the framework of the theories of fundamental interactions beyond the Standard Model, such as string and *M* theories, Kaluza-Klein theories, quintessence theories, etc. In turn, the experimental physics and observational astrophysics offer possibilities to probe directly the temporal changes in the physical constants on a short timescale and on a scale comparable with the total age of the Universe respectively.

The constants which can be probed from astronomical spectra are the proton-to-electron mass ratio, $\mu = m_p/m_e$, the fine-structure constant, $\alpha = e^2/(\hbar c)$, or different combinations of μ, α, and the nuclear gyromagnetic ratio g_n (the latter defines frequencies of the hyperfine transitions). Reported in the literature optical data concerning the relative variation of constants $\delta\mu/\mu$ and $\delta\alpha/\alpha$ at redshifts $z \sim 1$–3 are controversial at the level of a few ppm (1ppm = 10^{-6}). Such a spread indicates to the presence of some unaccounted systematics. We can state, however, that a conservative upper limit on the hypothetical variability of these constants on the timescale of few billion years from optical observations is 10^{-5}. Since hyperfine structure of optical lines is usually not resolved, observations in the optical range do not constrain time-variation of g_n. Some of the limits, which follow from the observations at microwave and FIR ranges will be discussed below. A more comprehensive discussion is given in Refs. [3,4].

Astronomical estimates of the dimensionless physical constants are based on the comparison of the line centers in the absorption/emission spectra of astronomical objects and the corresponding laboratory values. In practice, in order to disentangle the line shifts caused by the motion of the object and by the putative effect of the variability of constants, lines with different sensitivities to the variation of fundamental constants should be used. The accuracy of the method depends on the linewidths and the respective sensitivity coefficients. If different elements are involved in the analysis, an additional source of errors due to the so-called Doppler noise arises. The Doppler noise is caused by non-identical spatial distributions of different species, which, in turn, causes different velocity distributions. It introduces offsets which can mimic or obliterate real signals. For this reason the lines of a single species arising exactly from the same atomic or molecular level are desired. If this is not possible, the lines with highest sensitivities should be used to suppress the systematic errors from the Doppler noise. In this contribution we argue that microwave and far infrared (FIR) spectra of quasars present certain opportunities to reach these goals and obtain stringent bounds on the time-variation of fundamental constants.

2. Sensitivity coefficients to the variation of fundamental constants

The observed linewidth Γ in astrophysical spectra is usually determined by the Doppler broadening effect, i.e.

$$\frac{\Gamma}{\omega} = \frac{\Delta v}{c}, \tag{1}$$

where Δv is the velocity dispersion, c is the speed of light, and ω is the transition frequency. For extragalactic observations the typical values of Δv are about 1 – 10 km/s, which means that:

$$\frac{\Gamma}{\omega} \sim 10^{-5}. \tag{2}$$

Therefore, the typical accuracy of the frequency measurements for a sufficiently strong single line does not depend on a waveband and is on the order of $\delta\omega/\omega \sim 10^{-5}$. When we are looking for variation of fundamental constants, we can increase sensitivity by either averaging over large number of lines from different species, or by looking for lines with highest sensitivity to the variation of fundamental constants. The dimensionless sensitivity coefficients can be defined as:

$$\frac{\delta\omega}{\omega} = K_\alpha \frac{\delta\alpha}{\alpha} + K_\mu \frac{\delta\mu}{\mu} + K_g \frac{\delta g_n}{g_n}. \tag{3}$$

When the line with sensitivity coefficients given by Eq.(3) is observed, the apparent redshift z′ may differ from the actual redshift if either of the fundamental constants has changed during the time, which has passed since the transition happened:

$$\frac{z' - z}{1 + z'} = -K_\alpha \frac{\delta\alpha}{\alpha} - K_\mu \frac{\delta\mu}{\mu} - K_g \frac{\delta g_n}{g_n}. \tag{4}$$

Now if we observe two lines with different sensitivities, the apparent redshifts will differ by

$$\frac{\delta z'}{1 + z'} = -\Delta K_\alpha \frac{\delta\alpha}{\alpha} - \Delta K_\mu \frac{\delta\mu}{\mu} - \Delta K_g \frac{\delta g_n}{g_n}. \tag{5}$$

Obviously, from the observation of one pair of lines it is impossible to distinguish between variation of different constants. Thus, we rewrite Eq.(5) in terms of the variation of a following combination of fundamental constants:

$$\frac{\delta z'}{1 + z'} = -\frac{\delta F}{F}, \qquad F = \alpha^{\Delta K_\alpha} \mu^{\Delta K_\mu} g_n^{\Delta K_g}. \tag{6}$$

In order to study the time-variation of α, μ, or g_n we should maximize either ΔK_α, ΔK_μ, or ΔK_g. The summary of the sensitivity coefficients for different wavebands is presented in Table 1. These coefficients are calculated in the assumption, that atomic energy unit (27.2 eV) is independent of the fundamental constants. This assumption is only a matter of convenience, because, as one can see from Eq.(6), only the differences in sensitivities are important.

Table 1. Sensitivity coefficients for different wavebands

Transition	K_α	K_μ	K_g
Optical and UV range			
typical E1-transition in atom	10^{-2} - 10^{-1}	10^{-3}	10^{-7}
electronic transition in light molecule	10^{-2}	10^{-2}	10^{-7}
Microwave and FIR range			
fine-structure M1-transition	2	0.0	0.0
vibrational transition	0.0	−0.5	0.0
rotational transition	0.0	−1.0	0.0
hyperfine transition (21-cm line in hydrogen)	2.0	−1.0	1.0
18-cm Λ-doublet line in OH	−2	−3	10^{-1}
1.25-cm inversion line in NH_3	0.0	−4.5	0.0

Table 1 shows that typical sensitivities in the optical and UV ranges are very small. This is due to the fact that the dominant part of the transition energy in these bands corresponds to the non-relativistic electronic energy. In atomic units this energy does not depend on fundamental constants. Relativistic corrections to the transition energy are of the order of $(\alpha Z)^2$, where Z is the atomic number. The finite nuclear mass changes optical frequencies in atoms only via isotope effects, which are of the order of μ^{-1}. Optical spectra

of molecules consist of vibrational and rotational bands and because of that are more sensitive to μ-variation. The dependence on the third constant g_n enters only via the hyperfine structure, which is of the order of $(\alpha Z)^2 \mu g_n$.

It follows from Table 1 that sensitivity coefficients in microwave and FIR ranges are several orders of magnitude larger, than in optical and UV ranges. It is also important that there are lines of different types here, and sensitivity coefficients change drastically from one type to another. For example, the splitting between the components of the Λ-doublet of the ground $\Pi_{3/2}$ state in the OH molecule appears in the 3rd order in Coriolis interaction and is extremely sensitive to both fundamental constants [6,7]. The inversion line in ammonia corresponds to the tunneling transition of three hydrogen atoms from one minimum of a double-well potential to another. The tunneling frequency exponentially depends on the reduced mass for the respective vibrational mode and is, therefore, extremely sensitive to μ-variation [8,9]. The Λ-doublet OH line and NH_3 inversion line from the object *B*0218+357 were recently used to place very stringent bounds on the variation of constants at the redshift $z = 0.68$ [7,9]:

$$\delta F/F = (3.5 \pm 4.0) \times 10^{-6} \text{ , where } F = \alpha^{3.14} \mu^{1.57} g_n \text{ ,} \tag{7a}$$

$$\delta \mu/\mu = (0.6 \pm 1.9) \times 10^{-6} \text{ .} \tag{7b}$$

The reference lines were the 21 cm hydrogen hyperfine transition and rotational lines of OH, HCO^+, and HCH respectively.

The idea to use microwave lines to place limits on the variation of fundamental constants is not new. In 1996 Varshalovich & Potekhin compared apparent redshifts of rotational and optical lines to place following bound at $z = 1.9$ [10]: $\delta\mu/\mu = (70 \pm 100) \times 10^{-6}$. Later Murphy et al [11] compared redshifts of 21 cm hydrogen line and a number of rotational lines for the object *B*0218+357 at $z = 0.68$ to get the bound on variation of the product $F' = \alpha^2 g_n$:

$$\delta F'/F' = (1.6 \pm 5.4) \times 10^{-6}. \tag{7c}$$

We want to emphasize once again, that Refs. [7,9,11] analyzed different microwave lines of the same object *B*0218+357 at $z = 0.68$, namely rotational lines of several molecules including OH, HCO^+, and HCN, the Λ-doublet OH line, the 21 cm hydrogen line, and 1.2 cm inversion line of ammonia. It is clear from Table 1, that simultaneous analysis of all these lines allow to have a *complete* experiment, i.e. to study all three fundamental constants relevant to atomic physics and place three model-independent limits on their time-variation. As a first step, we can combine the bounds (7a) – (7c) from Refs. [7,9,11] to get following result for the deviations of all three constants for $z = 0.68$ from their present values:

$$\begin{cases} \delta\mu/\mu = (0.6 \pm 1.9) \times 10^{-6}, \\ \delta\alpha/\alpha = (0.9 \pm 6.4) \times 10^{-6}, \\ \delta g_n/g_n = (0 \pm 17) \times 10^{-6}. \end{cases} \tag{8}$$

We see that these bounds are rather strict and comparable, or even stronger, than bounds obtained from optical spectra. It would be extremely interesting to reanalyze all existing microwave spectra of the object *B*0218+357 to get more accurate and consistent bounds on the variation of constants. Of course, it would be also extremely interesting to get new high precision data for this object for a dedicated and comprehensive analysis.

Another interesting example where FIR lines were used to place bounds on time-variation at very high redshifts is discussed in Ref. [12]. The fine-structure [C II] 158 μm line was compared to the rotational CO line. Both lines were observed in emission for the quasars J1148+5251 and BR 1202-0725 with respective redshifts $z = 6.42$ and $z = 4.69$. The absence of the meaningful differences in apparent redshifts allowed to place bounds on the variation of the parameter $F'' = \alpha^2 \mu$:

$$\begin{cases} \delta F''/F'' = (0.1 \pm 1.0) \times 10^{-4}, z = 6.42, \\ \delta F''/F'' = (1.4 \pm 1.5) \times 10^{-4}, z = 4.69. \end{cases} \tag{9}$$

Note that $z = 6.42$ corresponds to the look-back time of approximately 12.9 Gyr, which constitutes 93% of the age of the Universe.

3. Using transitions in the same species to reduce Doppler noise

We already mentioned above that in order to reduce systematic errors from the Doppler noise it is desirable to compare redshifts for transitions in the same species (atom, ion, or molecule). Moreover, it is the best to use transitions from the same level. Otherwise, the lines can form in the parts of the gas clouds with different temperatures. Of course, Eqs. (5,6) are still applicable and we need transitions with different sensitivities. This requirement usually hampers usage of the lines of the same nature. For example, all rotational lines have very close sensitivities. Small differences may be caused by the non-adiabatic corrections, hyperfine structure, etc.

It seems that one can enhance such small differences by taking proper combinations of frequencies. Let us consider, for example, the Λ-doublet transition in OH. In fact, due to the hyperfine structure on hydrogen, there are four lines with the frequencies, which differ by few percent. Consider two hyperfine components of the Λ-doublet with frequencies ω_1 and ω_2. The hyperfine contribution to these frequencies is small, on the order of few percent, so the sensitivity coefficients are close to the values from Table 1. On the other hand, the difference frequency $\omega_- = \omega_1 - \omega_2$ depends only on the hyperfine contribution to the transition energy and has respective sensitivity coefficients (i.e. 2, −1, 1). Thus, we can compare "transitions" ω_- and, say, $\omega_+ = \omega_1 + \omega_2$, which have sensitivities of hyperfine and Λ-doublet transitions respectively [6,7]. An obvious drawback of this scheme is following: the frequency ω_- is small, but the corresponding linewidth is the same as for ω_+. Thus, the relative accuracy with which we know ω_- is lower and we do not gain from the enhanced sensitivity (actual situation is even less favorable, because the largest frequency ω_- corresponds to two weak transitions with $\Delta F \neq 0$). Similar argument holds for the inversion transition in NH_3, where there are also rotational and hyperfine structures [9]. On the other hand, both OH and NH_3 molecules have normal rotational spectrum, which can be used as a reference for the Λ-doublet and inversion lines. This way we can have large ΔK_μ (and also large ΔK_α and ΔK_g for the case of OH), normal relation (2) between linewidths and frequencies, and reduced Doppler noise.

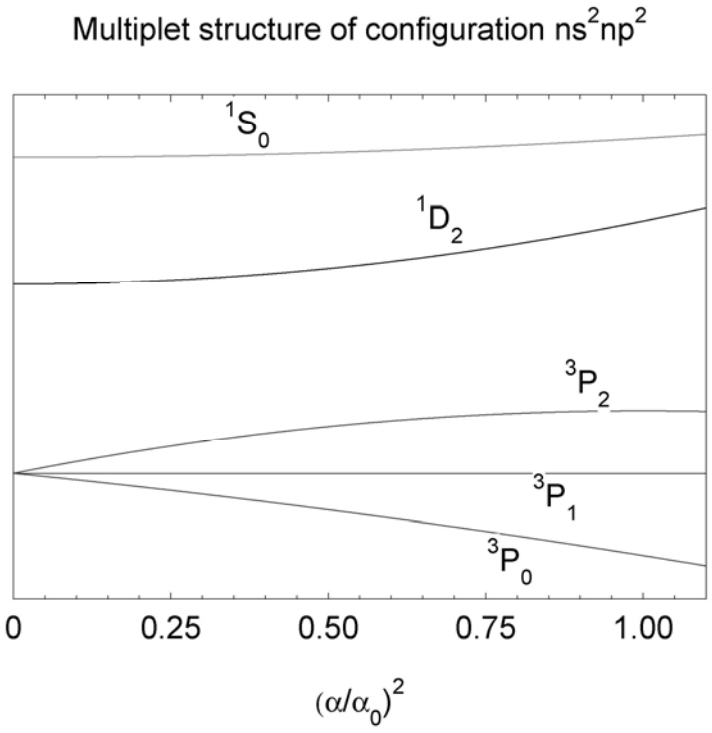

Fig. 1. Dependence of the structure of electronic states of ions with configuration ns^2np^2, such as C I, O III, Ar V, etc. on α^2 (not to scale). Levels $^3P_2$ and $^3P_0$ interact with levels $^1D_2$ and $^1S_0$ respectively via non-diagonal spin-orbit interaction. This interaction leads to the violation of the Landé-rule for the fine-structure intervals and also changes the slopes of the curves (i.e. sensitivity coefficients).

Let us consider now the fine-structure transitions in atomic ions in more detail. Note that such transition in C I was used to obtain bounds (9) at large redshifts. Here we focus on the case, where electronic ground state multiplet produce more than one fine-structure line. For example, the ground state of C I ion is ^3P_J, where J=0,1,2, and there are two fine-structure transitions with ΔJ=1. To a first approximation the fre-

quencies of these transitions obey the Landé-rule, i.e. $\omega_{2,1}/\omega_{1,0} = 2$ (see Ref. [13] for details). According to Table 1 both fine-structure transitions have sensitivity coefficients $K_\alpha = 2$. However, in the next order in relativistic corrections, the Landé-rule does not hold. Simultaneously the values of sensitivity coefficients K_α start to deviate from 2 (see Fig. 1). For the ions with the ground state ^3P_J and intermediate values of nuclear charge Z, $10 < Z < 50$, there is a simple relation between the violation of the Landé-rule and the difference in sensitivity of two fine-structure transitions [14]:

$$\Delta K_\alpha \equiv K_\alpha(2,1) - K_\alpha(1,0) = \frac{\omega_{2,1}}{\omega_{1,0}} - 2\,. \tag{10}$$

This expression allows to estimate ΔK_α without serious calculations using only experimental fine-structure frequencies. Some results of such estimates are presented in Table 2. One can see, that in several cases, such as Ar III and Ca V, the factor ΔK_α is on the order of unity. Thus, it is possible to use two infrared fine-structure transitions in the same ion to study α-variation without noticeable loss in sensitivity and significantly reducing Doppler noise.

Table 2. Differences in sensitivity coefficients for fine-structure transitions in light ions.

Ion	Transition *a*			Transition *b*			ΔK_α
	(J_a,J_a')	λ_a (μm)	ω_a (cm^{-1})	(J_b,J_b')	λ_b (μm)	ω_b (cm^{-1})	
C I	(1,0)	609.1	16.40	(2,1)	370.4	27.00	−0.016
O I	(0,1)	145.5	68.73	(1,2)	63.2	158.27	0.042
Si I	(1,0)	129.7	77.11	(2,1)	68.5	146.05	−0.11
S I	(0,1)	56.3	177.59	(1,2)	25.3	396.06	0.23
Ti I	(2,3)	58.8	170.13	(3,4)	46.1	216.74	−0.090
Fe I	(2,3)	34.7	288.07	(3,4)	24.0	415.93	0.17
	(1,2)	54.3	184.13	(2,3)	34.7	288.07	0.086
	(0,1)	111.2	89.94	(1,2)	54.3	184.13	0.048
N II	(1,0)	205.3	48.70	(2,1)	121.8	82.10	−0.032
Fe II	(5/2,7/2)	35.3	282.89	(7/2,9/2)	26.0	384.79	0.12
	(3/2,5/2)	51.3	194.93	(5/2,7/2)	35.3	282.89	0.074
	(1/2,3/2)	87.4	114.44	(3/2,5/2)	51.3	194.93	0.044
O III	(1,0)	88.4	113.18	(2,1)	51.8	193.00	−0.054
Ne III	(0,1)	36.0	277.67	(1,2)	15.6	642.88	0.11
S III	(1,0)	33.5	298.69	(2,1)	18.7	534.39	−0.21
Ar III	(0,1)	21.9	458.05	(1,2)	9.0	1112.18	0.42
Fe III	(2,3)	33.0	302.7	(3,4)	22.9	436.2	0.16
	(1,2)	51.7	193.5	(2,3)	33.0	302.7	0.086
	(0,1)	105.4	94.9	(1,2)	51.7	193.5	0.038
Ne V	(1,0)	24.3	411.23	(2,1)	14.3	698.24	−0.12
Mg V	(0,1)	13.5	738.7	(1,2)	5.6	1783.1	0.41
Ca V	(0,1)	11.5	870.9	(1,2)	4.2	2404.7	0.76
Na VI	(1,0)	14.3	698	(2,1)	8.6	1161	−0.37
Fe VI	(5/2,3/2)	19.6	511.3	(7/2,5/2)	14.8	677.0	−0.11
	(7/2,5/2)	14.8	677.0	(9/2,7/2)	12.3	812.3	−0.13
Mg VII	(1,0)	9.0	1107	(2,1)	5.5	1817	−0.36
Si VII	(0,1)	6.5	1535	(1,2)	2.5	4030	0.62
Ca VII	(1,0)	6.2	1624.9	(2,1)	4.1	2446.5	−0.55
Fe VII	(3,2)	9.5	1051.5	(4,3)	7.8	1280.0	−0.17
Si IX	(1,0)	3.9	2545.0	(2,1)	2.6	3869	−0.48

Relation (10) can be easily generalized for other ground state multiplets, such as ^3F_J in Ti I, or ^6D_J in Fe II [14]:

$$\Delta K_\alpha \equiv K_\alpha(J,J-1) - K_\alpha(J-1,J-2) = 2\frac{J-1}{J}\frac{\omega_{J,J-1}}{\omega_{J-1,J-2}} - 2\,. \tag{11}$$

Again, as in Eq. (10), the right hand side vanishes when $\omega_{J,J-1}/\omega_{J-1,J-2} = J/J-1$, i.e. when Landé-rule is fulfilled. For light ions with $Z \le 10$, such as C I, O I,III, or Ne III,V, the fine-structure intervals significantly depend on the magnetic interaction between valence electrons, and Eqs. (10,11) do not work. For these ions one has to use more complicated expression, which can be derived from Eq. (5.197) in Ref. [13]. This method was used for light ions with $Z \le 10$ from Table 2. For these ions the differences in sensitivities ΔK_α of fine-structure transitions are much smaller, than for heavier ions as they roughly scale as Z^2. Note that

fine-structure transition frequency also grows with Z and for the heavier ions with larger values of ΔK_α typically corresponds to the infrared range, rather than to FIR.

4. Conclusions

In this contribution we discussed how to use the lines from microwave and FIR ranges to study time-variation of fundamental constants. We demonstrated that these lines possess several advantages compared to spectroscopic lines from optical and UV ranges. In particular:

1. Microwave and FIR lines have higher sensitivity to time-variation of fundamental constants.
2. Lines of different nature (fine-structure, hyperfine, rotational, Λ-doublet, inversion, etc.) are sensitive to different combinations of fundamental constants. If several lines of different types are observed for one object, it is possible to make a *complete* experiment, i.e. to determine in a model-independent way the time-variation of all three constants, α, μ, and g_n.
3. Some fine-structure and rotational lines are observed in emission for extremely high redshifts, up to $z \approx 10$. This allows to probe fundamental constants at very early epochs of the evolution of the Universe, which is impossible in optical and UV ranges.
4. Observing lines of the same species one can significantly reduce Doppler noise and suppress systematic errors caused by non-identical special distribution of different species in cold molecular gas clouds. For example, one can use 18 cm Λ-doublet line in combination with rotational OH lines. Similarly, the 1.2 cm inversion line can be used in combination with rotational ammonia lines. In principle, it is even possible that these lines correspond to the same initial state. Of course, it depends on the observability of desired rotational lines for a given high redshifted object.
5. We have shown that infrared and FIR fine-structure lines in ions have different sensitivities to α-variation and can be also used in pairs to reduce Doppler noise. The frequency of the fine-structure transitions and the absolute values of ΔK_α grow with Z. For light ions, where the fine-structure transitions are in FIR range, $|\Delta K_\alpha| << 1$. For heavier ions the fine-structure transitions are in infrared range, and $|\Delta K_\alpha| \sim 1$.
6. Existing data on microwave and FIR lines already allows to place very stringent bounds on time-variation of all three constants. These bounds are comparable, or better than the ones obtained in optical range. New generation of instruments will allow to raise sensitivity by at least one order of magnitude and to study objects with even higher redshifts.

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