Mid- and far-infrared fine-structure-line sensitivities to hypothetical variability of the fine-structure constant

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Sensitivity coefficients to temporal variation of the fine-structure constant α for transitions between the fine-structure (FS) sublevels of the ground states of C I, Si I, S I, Ti I, Fe I, N II, Fe II, O III, S III, Ar III, Fe III, Mg V, Ca V, Na VI, Fe VI, Mg VII, Si VII, Ca VII, Fe VII, and Si IX are calculated. These transitions lie in the mid- and far-infrared regions and can be observed in spectra of high-redshift quasars and infrared bright galaxies with active galactic nuclei. Using FS transitions to study α variation over cosmological time scales allows one to improve the limit on $\Delta\alpha/\alpha$ by several times as compared to contemporaneous optical observations ($|\Delta\alpha/\alpha|<10^{-5}$), and to suppress considerably systematic errors of the radial velocity measurements caused by the Doppler noise. Moreover, the far infrared lines can be observed at redshifts $z\gtrsim 10$, far beyond the range accessible to optical observations ($z\lesssim 4$). We have derived a simple analytical expression which relates the FS intervals and the sensitivity of the FS transitions to the change of α.

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I. INTRODUCTION

The problem of variability of fundamental physical constants has a long history starting 70 years ago [1,2]. The review of its current status is given in Refs. [3,4]. Recent achievements in laboratory studies of the time-variation of fundamental constants are described, for example, in Refs. [5,6].

The variability of the dimensionless physical constants is usually considered in the framework of the theories of fundamental interactions such as string and *M* theories, Kaluza-Klein theories, quintessence theories, etc. In turn, the experimental physics and observational astrophysics offer possibilities to directly probe the temporal changes in the physical constants both locally and at early cosmological epochs comparable with the total age of the Universe ($T_U=13.8$ Gyr for the $H_0=70$ km s^{-1} Mpc^{-1}, $\Omega_m=0.3$, $\Omega_\Lambda=0.7$ cosmology). Here we discuss a possibility of using the ground state fine-structure (FS) transitions in atoms and ions to probe the variability of α at high redshifts, up to $z\sim 10$ ($\sim$96% of T_U).

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 proton gyromagnetic ratio g_p. The reported in the literature data concerning the relative values of $\Delta\mu/\mu$ and $\Delta\alpha/\alpha$ at $z\sim 1-3$ are controversial at the level of a few ppm (1 ppm$=10^{-6}$): $\Delta\mu/\mu=24\pm 6$ ppm [7] versus 0.6 ± 1.9 ppm [8] and $\Delta\alpha/\alpha=-5.7\pm 1.1$ ppm [9] versus -0.6 ± 0.6 ppm [10], -0.4 ± 1.9 ppm [11], and 5.4 ± 2.5 ppm [12]. Such a spread points unambiguously to the presence of unaccounted systematics. Some of the possible problems were studied in Refs. [13–16], but the revealed systematic errors cannot explain the full range of the observed discrepancies between the $\Delta\alpha/\alpha$ and $\Delta\mu/\mu$ values. We can state, however, that a conservative upper limit on the hypothetical variability of these constants is 10^{-5}.

Astronomical estimates of the dimensionless physical constants are based on the comparison of the line centers in the absorption and 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 constant variations should be employed. However, 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. It introduces offsets which can either mimic or obliterate a real signal. The evaluation of the Doppler noise is a serious problem [17–22]. For this reason lines of a single element arising exactly from the same atomic or molecular level are desired. This would provide reliable astronomical constraints on variations of physical constants.

In the present paper we propose to use the mid- and far-infrared FS transitions within the ground multiplets ^3P_J, ^5D_J, ^6D_J, ^3F_J, and ^4F_J of some of the most abundant atoms and ions, such as Si I, S I, Ti I, Fe I, Fe II, S III, Ar III, Fe III, Mg V, Ca V, Na VI, Fe VI, Mg VII, Si VII, Ca VII, Fe VII, and Si IX for constraining the variability of α. This approach has the following advantages. Most important is that each element provides two, or more FS lines which can be used independently—this considerably reduces the Doppler noise. The mid- and far-infrared FS transitions are typically more sensitive to the change of α than optical lines. For high redshifts ($z>2$), the far-infrared (FIR) lines are shifted into sub-mm range. The receivers at sub-mm wavelengths are of the heterodyne type, which means that the signal can be fixed at a high frequency stability ($\sim 10^{-12}$). In addition, FIR lines can be observed at early cosmological epochs ($z\gtrsim 10$) which are far beyond the range accessible to optical observations ($z\lesssim 4$).

II. ASTRONOMICALLY OBSERVED FS TRANSITIONS

The ground state FS transitions in mid- and far-infrared are observed in emission in the interstellar dense and cold molecular gas clouds, diffuse ionized gas in the star forming H II regions and in the "coronal" gas of active galactic nuclei (AGNs), and in the warm gas envelopes of the protostellar objects. Cold molecular gas clouds have been observed not only in our Galaxy, but also in numerous galaxies with redshifts $z>1$ up to $z=6.42$ [23] and often around powerful quasars and radio galaxies [24]. Recently the C II 158 μm line and CO low rotational lines were used to set a limit on the variation of the product $\mu\alpha^2$ at $z=4.69$ and 6.42 [21]. The FIR transitions in C I (370,609 μm) were detected at $z=2.557$ toward H1413+117 [25,26]. Four other observations of the C I 609 μm line were reported at $z=4.120$ (PSS 2322+1944) [27], at $z=2.285$ (IRAS F10214+4724) and $z=2.565$ (SMM J14011+0252) [26], and at $z=3.913$ (APM 08279+5255) [28].

In our Galaxy the most luminous protostellar objects are seen in the O I lines λ63, 146 μm [29] and in the FIR lines from intermediate ionized atoms O III, N III, N II, and C II, photoionized by the stellar continuum [30]. The lines of N II (122,205 μm) S III (19,34 μm), Fe III (23 μm), Si II (35 μm), Ne III (36 μm), O III (52,88 μm), N III (57 μm), O I (63,146 μm), and C II 158 μm [31–33], as well as Ne II (13 μm), S IV (11 μm), and Ar III (9 μm) [34] have been observed in the highly obscured ($A_v \simeq 21$ mag) massive star forming region G333.6–0.2. The FS transitions of N III, O III, Ne III, S III, Si II, N III, O I, C II, and N II are detected in numerous Galactic H II regions [35–37]. Compact and ultracompact H II regions are the sources of the FS lines of S III, O III, N III, Ne II, Ar III, and S IV [38,39]. Giant molecular clouds in the Orion Kleinmann-Low cluster [40], the Sgr B2 complex [41,42], the ρ Oph and σ Sco star-forming regions [43], and in the Carina nebular [44,45] emit the FIR lines of O I, N II, C II, Si II, O III, and N III.

Ions with low excitation potential $E_{ex}<50$ eV (N II, Fe II, S III, Ar III, Fe III) as well as ions with high excitation potential 50 eV $<E_{ex}\leq 351$ eV (O III, Ne III, Ne V, Mg V, Ca V, Na VI, Mg VII, Si VII, Ca VII, Fe VII, Si IX) are effectively produced by hard ionizing radiation and ionizing shocks in the gas surrounding active galactic nuclei. The FS emission lines of these ions have been detected with the Infrared Space Observatory (ISO) and the Spitzer Space Telescope (Spitzer) in Seyfert galaxies, 3C radio sources and quasars, and in ultraluminous infrared galaxies in the redshift interval from $z\sim 0.01$ up to $z=0.994$ [46–51].

The infrared FS lines of the neutral atoms Si I, S I, and Fe I have not been detected yet in astronomical objects, but these atoms were observed in resonance ultraviolet lines in two damped Lyα systems at $z=0.452$ [52] and $z=1.15$ [53] toward the quasars HE0000–2340 and HE0515–4414, respectively. The FIR lines are expected to be observed in extragalactic objects at a new generation of telescopes such as the Stratospheric Observatory for Infrared Astronomy (SOFIA), the Herschel Space Observatory originally called the Far Infrared and Submillimeter Telescope, and the Atacama Large Millimeter Array (ALMA) which open a new opportunity of probing the relative values of the fundamental physical constants with an extremely high accuracy ($\delta\sim 10^{-7}$) locally and at different cosmological epochs.

III. ESTIMATE OF THE SENSITIVITY COEFFICIENTS

In the nonrelativistic limit and for an infinitely heavy pointlike nucleus all atomic transition frequencies are proportional to the Rydberg constant $\mathcal{R}$. In this approximation, the ratio of any two atomic frequencies does not depend on any fundamental constants. Relativistic effects cause corrections to atomic energy, which can be expanded in powers of α^2 and $(\alpha Z)^2$, the leading term being $(\alpha Z)^2\mathcal{R}$, where Z is atomic number. Corrections accounting for the finite nuclear mass are proportional to $\mathcal{R}/(\mu Z)$, but for atoms they are much smaller than relativistic corrections. The finite nuclear mass effects form the basis for the molecular constraints to the m_p/m_e mass ratio variation [7,8,54–58].

Consider the dependence of an atomic frequency ω on α in the comoving reference frame

$$\omega_z = \omega + qx + \cdots, \quad x \equiv (\alpha_z/\alpha)^2 - 1. \tag{1}$$

Here ω and ω_z are the frequencies corresponding to the present-day value of α and to a change $\alpha \to \alpha_z$ at a redshift z. The parameter q (so-called q factor) is individual for each atomic transition [59].

If α is not a constant, the parameter x differs from zero and the corresponding frequency shift $\Delta\omega=\omega_z-\omega$ is given by

$$\Delta\omega/\omega = 2\mathcal{Q}(\Delta\alpha/\alpha), \tag{2}$$

where $\mathcal{Q}=q/\omega$ is the dimensionless sensitivity coefficient and $\Delta\alpha/\alpha \equiv (\alpha_z-\alpha)/\alpha$. Here we assume that $|\Delta\alpha/\alpha| \ll 1$.

If such a frequency shift takes place for a distant object observed at a redshift z, then an apparent change in the redshift $\Delta z=\tilde{z}-z$ occurs:

$$\Delta\omega/\omega = -\Delta z/(1+z) \equiv \Delta v/c, \tag{3}$$

where Δv is the Doppler radial velocity shift. If ω' is the observed frequency from a distant object, then the true redshift is given by

$$1+z = \omega_z/\omega', \tag{4}$$

whereas the shifted (apparent) value is

$$1+\tilde{z} = \omega/\omega'. \tag{5}$$

If we have two lines of the same element with the apparent redshifts $\tilde{z}_1$ and $\tilde{z}_2$ and the corresponding sensitivity coefficients $\mathcal{Q}_1$ and $\mathcal{Q}_2$, then

$$2\Delta\mathcal{Q}(\Delta\alpha/\alpha) = (\tilde{z}_1-\tilde{z}_2)/(1+z) = \Delta v/c, \tag{6}$$

where $\Delta v=v_1-v_2$ is the difference of the measured radial velocities of these lines, and $\Delta\mathcal{Q}=\mathcal{Q}_2-\mathcal{Q}_1$.

Relativistic corrections grow with atomic number Z, but for optical and uv transitions in light atoms they are small, i.e., $\mathcal{Q}\sim(\alpha Z)^2 \ll 1$. For example, Fe II lines have sensitivities $\mathcal{Q}\sim 0.03$ [60]. Other atomic transitions, used in astrophysical searches for α variation have even smaller sensitivi-

ties. The only exceptions are the Zn II λ2026 Å line, where $\mathcal{Q}\approx 0.050$ [59] and the Fe I resonance transitions considered in Ref. [61], where $\mathcal{Q}$ ranges between 0.03 and 0.09. One can significantly increase the sensitivity to α variation by using transitions between FS levels of one multiplet [62]. In the nonrelativistic limit $\alpha\to 0$ such levels are exactly degenerate. Corresponding transition frequencies ω are approximately proportional to $(\alpha Z)^2$. Consequently, for these transitions $\mathcal{Q}\approx 1$ and

$$\Delta\omega/\omega \approx 2\Delta\alpha/\alpha, \tag{7}$$

which implies that for any two FS transitions $\Delta\mathcal{Q}\approx 0$. In this approximation $\Delta\alpha/\alpha$ cannot be determined from Eq. (6).

We will show now that in the next order in $(\alpha Z)^2$ the $\mathcal{Q}$ factors of the FS transitions deviate from unity and $\Delta\mathcal{Q}$ in Eq. (6) is not equal to zero. In fact, for heavy atoms with $\alpha Z\sim 1$ it is possible to find FS transitions with $|\Delta\mathcal{Q}|\gg 1$ [62]. Here we focus on atoms with $\alpha Z\ll 1$, which are more important for astronomical observations. For such atoms $|\Delta\mathcal{Q}|<1$ and, as we will show below, there is a simple analytical relation between $\Delta\mathcal{Q}$ and experimentally observed FS intervals.

There are two types of relativistic corrections to atomic energy. The first type depends on the powers of αZ and rapidly grows along the periodic table. The second type of corrections depends on α and does not change much from atom to atom. Such corrections are usually negligible, except for the lightest atoms. Expanding the energy of a level of the FS multiplet $^{2S+1}L_J$ into (even) powers of αZ we have (see Ref. [63], Sec. 5.5)

$$E_{L,S,J} = E_0 + \frac{A(\alpha Z)^2}{2}[J(J+1) - L(L+1) - S(S+1)] + B_J(\alpha Z)^4 + \cdots, \tag{8}$$

where A and B_J are the parameters of the FS multiplet. Note, that in general, B_J depends on quantum numbers L and S, but we will omit L and S subscripts since they do not change the following discussion. In Eq. (8) we keep the term of the expansion $\sim(\alpha Z)^4$, but neglect the term $\sim\alpha^2$. This is justified only for atoms with $Z\gtrsim 10$. Therefore, the following discussion is not applicable to atoms of the second period. As long as these atoms are very important for astrophysics, we will briefly discuss them in the end of this section.

The strongest FS transitions are of $M1$ type. They occur between levels with $\Delta J=1$:

$$\omega_{J,J-1} = E_{L,S,J} - E_{L,S,J-1} = AJ(\alpha Z)^2 + (B_J - B_{J-1})(\alpha Z)^4. \tag{9}$$

In the first order in $(\alpha Z)^2$ we have the well known Landé rule $\omega_{J,J-1}=AJ(\alpha Z)^2$, which directly leads to Eq. (7). In the next order we get

$$\mathcal{Q}_{J,J-1} = 1 + \frac{B_J - B_{J-1}}{AJ}(\alpha Z)^2. \tag{10}$$

Let us consider the multiplet ^3P_J (i.e., the ground multiplet for Si I, S I, Ar III, Mg V, Ca V, Na VI, Mg VII, Si VII, Ca VII, and Si IX). For two transitions $\omega_{2,1}$ and $\omega_{1,0}$ Eq. (10) gives

$$\mathcal{Q}_{2,1} - \mathcal{Q}_{1,0} = \frac{B_2 - 3B_1 + 2B_0}{2A}(\alpha Z)^2. \tag{11}$$

At the same time, Eq. (9) gives the following expression for the frequency ratio:

$$\frac{\omega_{2,1}}{\omega_{1,0}} = 2 + \frac{B_2 - 3B_1 + 2B_0}{A}(\alpha Z)^2. \tag{12}$$

Comparison of Eqs. (11) and (12) leads to the final result

$$\Delta\mathcal{Q} = \mathcal{Q}_{2,1} - \mathcal{Q}_{1,0} = \frac{1}{2}\left(\frac{\omega_{2,1}}{\omega_{1,0}}\right) - 1. \tag{13}$$

In a general case of the $^{2S+1}L_J$ multiplet the difference between the sensitivity coefficients $\mathcal{Q}_{J,J-1}$ and $\mathcal{Q}_{J-1,J-2}$ is given by

$$\Delta\mathcal{Q} = \frac{J-1}{J}\left(\frac{\omega_{J,J-1}}{\omega_{J-1,J-2}}\right) - 1. \tag{14}$$

If two arbitrary FS transitions $\omega_{J_1,J_1'}$ and $\omega_{J_2,J_2'}$ of the $^{2S+1}L_J$ multiplet are considered, then the difference $\Delta\mathcal{Q}=\mathcal{Q}_{J_2,J_2'} - \mathcal{Q}_{J_1,J_1'}$ is expressed by

$$\Delta\mathcal{Q} = \frac{J_1(J_1+1) - J_1'(J_1'+1)}{J_2(J_2+1) - J_2'(J_2'+1)}\left(\frac{\omega_{J_2,J_2'}}{\omega_{J_1,J_1'}}\right) - 1. \tag{15}$$

This equation can be used also for $E2$ transitions with $\Delta J=2$ and for combination of $M1$ and $E2$ transitions.

It is to note that the derived values of $\Delta\mathcal{Q}$ for two FS transitions are expressed in terms of their frequencies, which are known from the laboratory measurements. Another point is that the right-hand side of Eq. (14) turns to zero when the frequency ratio equals $J/(J-1)$, i.e., when the Landé rule is fulfilled. Equations (13)–(15) hold only as long as we neglect corrections of the order of α^2 and $(\alpha Z)^6$ to Eq. (8), which is justified for the atoms in the middle of the periodic table, i.e., approximately from Na ($Z=11$) to Sn ($Z=50$).

Table I lists the calculated $\Delta\mathcal{Q}$ values for the most abundant atoms and ions observed in galactic and extragalactic gas clouds. The ions C I, Si I, N II, O III, Na VI, Mg VII, and Ca VII, have configuration ns^2np^2 and "normal" order of the FS sublevels. The ions Mg V, Si VII, S I, and Ca V have configuration ns^2np^4 and "inverted" order of the FS sublevels. However, Eq. (13) is applicable for both cases. We note that the FS lines of N II (122,205 μm) can be asymmetric and broadened due to hyperfine components, as observed in Refs. [40,42]. The hyperfine splitting occurs also in the FS lines of Na VI (8.6,14.3 μm).

Transition wavelengths and frequencies listed in Table I are approximate and are given only to identify the FS transitions. At present, many of them have been measured with a sufficiently high accuracy [64].

The iron ions Fe I, Fe II, Fe III, Fe VI, and Fe VII, have ground multiplets ^5D, ^6D, ^5D, ^4F, and ^3F, respectively. All these multiplets, except the last one, produce more than two FS lines, which can be used to further reduce the systematic errors. The sensitivity coefficients for transitions in iron and titanium from Table I are calculated with the help of Eq. (14).

TABLE I. The differences of the sensitivity coefficients $\Delta\mathcal{Q}$ of the FS emission lines within the ground multiplets ^3P_J, ^5D_J, ^6D_J, ^4F_J, and ^3F_J for the most abundant atoms and ions. The FS intervals for S I, Fe I–III, Ar III, Mg V, Ca V, and Si VII are inverted. The excitation temperature T_{ex} for the upper level is indicated. Transition wavelengths and frequencies (rounded) are taken from Ref. [64]. The values of $\Delta\mathcal{Q}$ for the ions C I, N II, and O III are calculated using Eq. (5.197) from Ref [63].

	Transition a				Transition b					
Atom/Ion	(J_a,J_a')	λ_a (μm)	ω_a (cm^{-1})	T_{ex} (K)	(J_b,J_b')	λ_b (μm)	ω_b (cm^{-1})	T_{ex} (K)	ω_b/ω_a	$\Delta\mathcal{Q}=\mathcal{Q}_b-\mathcal{Q}_a$
C I	(1,0)	609.1	16.40	24	(2,1)	370.4	27.00	63	1.646	−0.008
Si I	(1,0)	129.7	77.11	111	(2,1)	68.5	146.05	321	1.894	−0.053
S I	(0,1)	56.3	177.59	825	(1,2)	25.3	396.06	570	2.230	0.115
Ti I	(2,3)	58.8	170.13	245	(3,4)	46.1	216.74	557	1.274	−0.045
Fe I	(2,3)	34.7	288.07	1013	(3,4)	24.0	415.93	599	1.444	0.083
	(1,2)	54.3	184.13	1278	(2,3)	34.7	288.07	1013	1.565	0.043
	(0,1)	111.2	89.94	1407	(1,2)	54.3	184.13	1278	2.048	0.024
N II	(1,0)	205.3	48.70	70	(2,1)	121.8	82.10	188	1.686	−0.016
Fe II	(5/2,7/2)	35.3	282.89	961	(7/2,9/2)	26.0	384.79	554	1.360	0.058
	(3/2,5/2)	51.3	194.93	1241	(5/2,7/2)	35.3	282.89	961	1.451	0.037
	(1/2,3/2)	87.4	114.44	1406	(3/2,5/2)	51.3	194.93	1241	1.703	0.022
O III	(1,0)	88.4	113.18	163	(2,1)	51.8	193.00	441	1.705	−0.027
S III	(1,0)	33.5	298.69	430	(2,1)	18.7	534.39	1199	1.789	−0.105
Ar III	(0,1)	21.9	458.05	2259	(1,2)	9.0	1112.18	1600	2.428	0.214
Fe III	(2,3)	33.0	302.7	1063	(3,4)	22.9	436.2	628	1.441	0.081
	(1,2)	51.7	193.5	1342	(2,3)	33.0	302.7	1063	1.564	0.043
	(0,1)	105.4	94.9	1478	(1,2)	51.7	193.5	1342	2.039	0.019
Mg V	(0,1)	13.5	738.7	3628	(1,2)	5.6	1783.1	2566	2.414	0.207
Ca V	(0,1)	11.5	870.9	4713	(1,2)	4.2	2404.7	3460	2.761	0.381
Na VI	(1,0)	14.3	698	1004	(2,1)	8.6	1161	2675	1.663	−0.168
Fe VI	(5/2,3/2)	19.6	511.3	736	(7/2,5/2)	14.8	677.0	1710	1.324	−0.054
	(7/2,5/2)	14.8	677.0	1710	(9/2,7/2)	12.3	812.3	2879	1.200	−0.067
Mg VII	(1,0)	9.0	1107	1593	(2,1)	5.5	1817	4207	1.641	−0.179
Si VII	(0,1)	6.5	1535	8007	(1,2)	2.5	4030	5817	2.625	0.313
Ca VII	(1,0)	6.2	1624.9	2338	(2,1)	4.1	2446.5	5858	1.506	−0.247
Fe VII	(3,2)	9.5	1051.5	1513	(4,3)	7.8	1280.0	3354	1.217	−0.087
Si IX	(1,0)	3.9	2545.0	3662	(2,1)	2.6	3869	9229	1.520	−0.240

According to Table I, the absolute values of the difference $\Delta\mathcal{Q}$ are usually quite large even for atoms with $Z\sim 10$. The sign of $\Delta\mathcal{Q}$ is negative for atoms with configuration ns^2np^2 and positive for atoms with configuration ns^2np^4. These features are not surprising if we consider the level structure of the respective configurations [63]. Both of them have three terms $^3P_{0,1,2}$, $^1D_2$, and $^1S_0$, but for the configuration ns^2np^4, the multiplet ^3P_J is "inverted." The splitting between these terms is caused by the residual Coulomb interaction of p electrons and is rather small compared to the atomic energy unit $2\mathcal{R}$.

For example, the level $^1D_2$ for Si I lies only 6299 cm^{-1} above the ground state, which corresponds to $E_D-E_P=0.029$ a.u. Relativistic corrections to the energy are dominated by the spin-orbit interaction, which for p electrons has the order of $0.1(\alpha Z)^2$ a.u. The diagonal part of this interaction leads to the second term in Eq. (8), i.e., $A(\alpha Z)^2\sim 200$ cm^{-1}. In the second order the nondiagonal spin-orbit interaction causes repulsion between the levels $^3P_2$ and $^1D_2$ and results in nonzero parameter B_2. We can estimate this correction as $B_2(\alpha Z)^4\sim A^2(\alpha Z)^4/(E_P-E_D)\sim -10$ cm^{-1}. This estimate has an expected order of magnitude. Note that B_2 is negative. For normal multiplets it reduces the ratio $\omega_{2,1}/\omega_{1,0}$, whereas for the inverted multiplet the ratio increases. We see that this is in a qualitative agreement with Table I. Iron and titanium ions have configurations $3d^k2s^l$, with $k=6,l=2$ for Fe I and $k=2,l=0,2$ for Fe VII and Ti I, respectively. As we can see from Table I, here also all normal multiplets (for Ti I, Fe VI, and Fe VII) have negative values of $\Delta\mathcal{Q}$, while inverted multiplets for all other ions have positive values of $\Delta\mathcal{Q}$.

Equation (11) shows that sensitivity to α variation grows with Z. For heavy atoms, $\alpha Z\sim 1$, neglected terms in expansion (8) become important. That breaks relation (14) between $\Delta\mathcal{Q}$ and FS intervals and sensitivity coefficients $\mathcal{Q}$ have to be calculated numerically. According to Table I, the largest coefficients B_J appear for Ca V and Si VII. The neglected corrections to $\Delta\mathcal{Q}$ can be estimated as $\sim[A(\alpha Z)^2/(E_P-E_D)]^2$, i.e., the uncertainty in $\Delta\mathcal{Q}$ for Ca V and Si VII is less than 20%. For other elements listed in Table I this correction should be smaller. Note that for iron ions, which have the largest Z, the relativistic effects are suppressed, because for d electrons they are typically an order of magnitude smaller, than for p electrons.

TABLE II. The differences between sensitivity coefficients of the FS transitions within ground ^6D_J multiplet of Fe II, $\Delta\mathcal{Q} \equiv \mathcal{Q}_{J,J-1} - \mathcal{Q}_{J-1,J-2}$. In the third column we use calculated q factors from Ref. [60] (see Table I from this reference, basis set [7*spdf*]). In the fourth and fifth columns we apply Eq. (14) to calculated and experimental FS intervals, respectively.

Transitions		$\Delta\mathcal{Q}$		
(5/2,7/2)	(7/2,9/2)	0.045	0.049	0.058
(3/2,5/2)	(5/2,7/2)	0.023	0.029	0.037
(1/2,3/2)	(3/2,5/2)	0.017	0.016	0.022

For light elements the accuracy of our estimate depends on the neglected terms $\sim\alpha^2$. The discussion of these terms can be found in Ref. [63] [see Eq. (5.197) and Table V.21 therein]. The corresponding correction decreases from almost 50% for Na VI to 30% for Mg VII and to 15% for Si IX.

For atoms with $Z \lesssim 10$ one can calculate $\Delta\mathcal{Q}$ using Eq. (5.197) from Ref. [63]. For example, for C I, N II, and O III, we get $\Delta\mathcal{Q}=-0.008$, -0.016, and -0.027, respectively. As expected, these values are much smaller than those for the heavier elements. On the other hand, these ions are so important for astrophysics, that we keep them in Table I.

Numerical calculations for heavy many-electron atoms are rather difficult to perform and the computed $\Delta\mathcal{Q}$ values may not be very accurate. For atoms with $\alpha Z \ll 1$ one can use Eq. (14) to check the accuracy of the numerical results.

As an example we consider the ground ^6D_J multiplet of Fe II ion (Table II). One can see that numerical results in Ref. [60] are in good agreement with the values obtained from Eq. (14) for the calculated FS intervals. However, when we apply Eq. (14) to actual experimental FS intervals, the agreement worsens noticeably. It is well known that deviations from the Landé rule for FS intervals depend on the interplay between the (nondiagonal) spin-orbit and the residual Coulomb interactions [63]. For this reason numerical results are very sensitive to the treatment of the effects of the core polarization and the valence correlations. Note also that the calculated q factors are first used to find sensitivity coefficients $\mathcal{Q}$, and then the (small) differences are taken. Obviously this makes the whole calculation rather unstable. Similarly, Eq. (14) can be used to check calculations of the q factors for other atoms considered in Refs. [61,65,66].

Numerical calculations for light atoms with $Z \lesssim 10$ are usually much simpler and more reliable. However, as we have pointed out above, the differences in the sensitivity coefficients of the light atoms depend on the relativistic corrections $\sim\alpha^2$. This means that the Breit interaction between valence electrons should be accurately included, while the majority of the published results were obtained in the Dirac-Coulomb approximation.

There is a certain similarity between the present method and the method of optical doublets, used previously to study α variation (see, e.g., Ref. [18], and references therein). In that method, however, the FS energy constitutes a small fraction of the total transition energy. Therefore, the parameter $\Delta\mathcal{Q}$ for optical transitions is much smaller. Note that for the mid- and far-infrared FS lines, the transition energy and the FS splitting coincide, which leads to a much larger parameter $\Delta\mathcal{Q}$.

IV. DISCUSSION AND CONCLUSIONS

In this paper we suggest to use two, or more FS lines of the same ion to study possible variation of α at early stages of the evolution of the Universe up to $\Delta T \sim 96\%$ of T_U. The sensitivity of the suggested method is proportional to $\Delta\mathcal{Q}$, as seen from Eq. (6). We have deduced a simple analytical expression to calculate $\Delta\mathcal{Q}$ for the FS transitions in light atoms and ions within the range of nuclear charges $11 \leq Z \leq 26$. We found that $|\Delta\mathcal{Q}|$ grows with Z and reached 0.2–0.4 for the ions of Ar and Ca. This is about one order of magnitude higher than typical sensitivities in the optical and uv range.

In addition of being more sensitive, this method provides also a considerable reduction of the Doppler noise, which limits the accuracy of the optical observations. Using the lines of the same element reduces the sources of the Doppler noise to the inhomogeneity of the excitation temperature $T_{\rm ex}$ within the cloud(s). Alternatively, when the lines of different species are used, the Doppler noise may be significantly higher because of the difference of the respective spatial distributions.

At present, the precision of the existing radio observations of the FS lines from distant objects is considerably lower than in the most accurate optical observations. For example, the error in the line center position for the C I $J=2\rightarrow1$ and $J=1\rightarrow0$ lines at $z=2.557$ was $\sigma_{v,\rm radio}=8$ and 25 km s^{-1}, respectively [25,26]. This has to be compared with the precision of the modern optical measurements of $\sigma_{v,\rm opt}=85$ m s^{-1} [12,67]. In the optical range the error $\sigma_{v,\rm opt}$ includes both random and systematic contributions. The systematic error is the wavelength calibration error which is negligible at radio frequencies.

In the forthcoming observations with ALMA, the statistical error is expected to be several times smaller than 85 m s^{-1}. Together with the higher sensitivity to α variation, this would allow us to estimate $\Delta\alpha/\alpha$ at the level of one tenth of ppm—well beyond the limits of the contemporary optical observations and comparable to the anticipated sensitivity of the next generations of spectrographs for the VLT and the EELT [68,69]. Thus, FIR lines offer a very promising strategy to probe the hypothetical variability of the fine-structure constant both locally and in distant extragalactic objects.

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