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Space-Time Variation of Physical Constants and Relativistic Corrections in Atoms

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Abstract

Detection of high-redshift absorption in the optical spectra of quasars have provided a powerful tool to measure spatial and temporal variations of physical "constants" in the Universe. It is demonstrated that high sensitivity to the variation of the fine structure constant α can be obtained from a comparison of the spectra of heavy and light atoms (or molecules). We have performed calculations for the pair FeII and MgII for which accurate quasar and laboratory spectra are available. A possibility of 10^5 times enhanced effects of the fundamental constants variation suitable for laboratory measurements is also discussed.

31.30.Jv , 95.30.Dr , 95.30.-k

The first ideas about possible variation of the fundamental physical constants in the expanding Universe were suggested by Dirac [1]. Now this subject is of particular current interest because of the new possibilities opened up by the structure of unified theories, like the string theory and M-theory, which lead us to expect that additional compact dimensions of space may exist. The "constants" seen in the three-dimensional subspace of the theory will vary at the same rate as any change occurring in the extra compact dimensions (see, e.g. [2–4]).

Quasar absorption systems present ideal laboratories where to search for any temporal or spatial variation of fundamental constants by comparing atomic spectra from the distant objects with the laboratory spectra (see, e.g. [5] and references therein).

The energy scale of the atomic spectra is given by the atomic unit $\frac{me^4}{\hbar^2}$. In the absence of any corrections, all atomic spectra are proportional to this constant and no change of the fundamental constants can be detected. Indeed, any change in the atomic unit will be absorbed in the determination of the red shift parameter $1 + z = \frac{\omega}{\omega'}$ which is also found from the comparison between the cosmic and laboratory atomic spectra (ω' is the red-shifted frequency of the atomic transition and ω is this frequency in the laboratory). However, any change of the fundamental constants can be found by measuring the relative size of relativistic corrections, which are proportional to α^2, where $\alpha = e^2/\hbar c$ is the fine structure constant [6].

It would seem natural to find this change from measurements of the spin-orbit splitting within a fine-structure multiplet. However, this way is not the most efficient, and it may even give incorrect results, since other relativistic effects are ignored. The aim of this letter is to demonstrate that the change in α produces an order of magnitude larger effect in the difference between transition frequencies in heavy and light atoms (or molecules). We have calculated the dependence of the transition frequencies on α for FeII (see eq.(8)) and MgII (see eq.(6)) where accurate data exist both for laboratory and quasar spectra. Other possibilities include comparisons of different optical transitions, for example $s - p$ and $p - d$, in the same atom or molecule, or comparisons of microwave transitions in molecules which contain rotational and hyperfine intervals.

We also propose another interesting possibility: to use transitions between "accidentally" degenerate levels in the same atom or molecule. This degeneracy would disappear after a minor change in α. For example, in the Dy atom there are two degenerate opposite-parity levels [7,8]. The frequency of the $E1$-transition between them is smaller then the hyperfine splitting of each level. As a result, the relative effect of the change in α is enhanced by five orders of magnitude (the ratio of the size of the relativistic effect to the transition frequency). This case seems to be more suitable for laboratory experiments. Similar experiments with "accidentally" degenerate molecular levels belonging to different electron terms are also sensitive to the smallest changes in the ratio of the nucleon to electron masses since in this case the difference in electron energies is compensated by the difference in the vibrational and rotational energies of the nuclei. As is known, the nuclear mass is a function of the strong interaction constants and vacuum condensates.

A competitive possibility is an accurate measurement of a very small difference between the frequencies of two transitions in different atoms or molecules (like in the comparison with the frequency standard). This small difference can be measured with a very high absolute accuracy, up to few Hz, and one can have the same enhanced effects of the change in α or

the nucleon mass.

Let us start our calculations from simple analytical estimates of the relativistic effects in transition frequencies. Consider first the relativistic corrections to the frequency of an atomic transition in a hydrogen-like atom. The relativistic correction to the energy level is given by (see, e.g. [9])

$$\Delta_n = -\frac{me^4 Z^2}{2\hbar^2} \frac{(Z\alpha)^2}{n^3} \left(\frac{1}{j+1/2} - \frac{3}{4n}\right), \tag{1}$$

where Z is the nuclear charge, n is the principal quantum number and j is the total electron angular momentum. This value of the relativistic correction can be obtained as an expectation value $\langle V \rangle$ of the relativistic perturbation V, which is large in the vicinity of the nucleus only. Therefore, the relativistic correction Δ is proportional to the electron density near the nucleus $|\Psi(r < \frac{a}{Z})|^2 \propto \frac{Z^3}{n^3 a^3}$ (a is the Bohr radius, $\frac{a}{Z}$ is the size of the hydrogen-like ion). For an external electron in a many-electron atom or ion the electron density near the nucleus is given by the formula (see, e.g. [10]) obtained in the semiclassical approximation ($n \gg 1$)

$$|\Psi(r < \frac{a}{Z})|^2 \propto \frac{Z_a^2 Z}{\nu^3 a^3},$$

where Z_a is the charge "seen" by the external electron outside the atom, i.e. $Z_a = 1$ for neutral atoms, $Z_a = 2$ for singly charged ions, etc.; ν is the effective principal quantum number, defined by $E_n = -\frac{me^4}{2\hbar^2} \frac{Z_a^2}{\nu^2}$, where E_n is the energy of the electron. For hydrogen-like ions $\nu = n, Z_a = Z$. Thus, to find the single-particle relativistic correction, we should multiply Δ in Eq. (1) by the ratio of $|\Psi(r < \frac{a}{Z})|^2$ in the multi-electron ion and hydrogen-like ion. The result is

$$\Delta_n = -\frac{me^4 Z_a^2}{2\hbar^2} \frac{(Z\alpha)^2}{\nu^3} \left[\frac{1}{j+1/2} - \frac{Z_a}{Z\nu}(1 - \frac{Z_a}{4Z})\right] \simeq E_n \frac{(Z\alpha)^2}{\nu(j+1/2)}. \tag{2}$$

The second term in the square brackets is presented to provide a continuous transition from the hydrogen-like ion Eq. (1) to the multi-electron ion Eq. (2). In multi-electron ions ($Z \gg Z_a$) this term is, in fact, a rough estimate based on the direct calculation of $\langle V \rangle$. We should neglect this small term since there are more important many-body corrections (the accurate many-body calculations discussed below give approximately constant correction term in square brackets with the value about -0.6).

We see that the relativistic correction is largest for the $s_{1/2}$ and $p_{1/2}$ states, where $j = 1/2$. The fine structure splitting is given by

$$\Delta_{ls} = E(p_{3/2}) - E(p_{1/2}) \simeq -\Delta(p_{1/2})/2 \simeq -\Delta(p_{3/2}). \tag{3}$$

In the quasar absorption spectra transitions from the ground state have been observed. Therefore, it is important to understand how the frequencies of these transitions are affected by the relativistic effects. The fine splitting in excited states is smaller then the relativistic correction in the ground state, since the density of the excited electron near the nucleus is smaller. As a result, the fine splitting of the $E1$-transition from the ground state (e.g., $s - p$) is substantially smaller than the absolute shift of the frequency of the $s - p$ transition. The mean energy of the p-electron is defined as

$$E(p) = \frac{2}{3}E(p_{3/2}) + \frac{1}{3}E(p_{1/2}) \simeq E_n(p) - \frac{4}{3}\Delta_{ls},$$

where E_n is the non-relativistic energy. Therefore, the relativistic shift of the mean $s - p$ transition frequency is given by

$$\Delta(p - s) \simeq -\frac{4}{3}\Delta_{ls} - \Delta(s_{1/2}).$$

The relative size of the relativistic corrections is proportional to Z^2, so they are small in light atoms. Therefore, we can find the change of α by comparing transition frequencies in heavy and light atoms. We stress that the most accurate and effective procedure to search for the change of α must include all relativistic corrections and the analysis of all available lines (rather then the fine splitting within one multiplet only).

Let us consider an example of the $s-p$ transitions from the ground state in MgII (Z=12) and FeII (Z=26) ions where accurate data exist for both laboratory and quasar spectra (see detailed analysis in [11–13]). MgII is a simple system with one external electron above closed shells. The frequency of the transition can be presented in the following form

$$
\begin{aligned}
E(3p_{1/2}) - E(3s_{1/2}) &= E_l(3p_{1/2}) - E_l(3s_{1/2}) + K_1[(\tfrac{\alpha}{\alpha_l})^2 - 1] \\
E(3p_{3/2}) - E(3s_{1/2}) &= E_l(3p_{3/2}) - E_l(3s_{1/2}) + K_2[(\tfrac{\alpha}{\alpha_l})^2 - 1]
\end{aligned}
\tag{4}
$$

$$
\begin{aligned}
K_1 &\simeq -2\Delta_{ls} - \Delta(3s_{1/2}), \\
K_2 &\simeq -\Delta_{ls} - \Delta(3s_{1/2}).
\end{aligned}
\tag{5}
$$

Here α_l and E_l are the laboratory values of fine structure constant and energy, α and E are the values at the distant object. The formulae (2)-(3) for the spin-orbit splitting Δ_{ls} and relativistic shift $\Delta(3s_{1/2})$ have been obtained in the single-particle approximation. There are large corrections to these formulae due to partial electron screening of the nuclear potential, which appears in the equation for the relativistic correction $\langle V \rangle$, and due to a change of the total atomic potential acting on external electron when we change α. Indeed, the wave functions of all inner electrons change due to the relativistic corrections ($\Psi \to \Psi + \delta\Psi$), which in turn produces a change in the mean-field atomic potential ($V \to V + \delta V$). In part these effects can be taken into account by using the experimental value of $\Delta_{ls} = 91.6$ cm^{-1} and the semiempirical formula for $\Delta(3s) = -2\Delta_{ls}(\frac{\nu_{3p}}{\nu_{3s}})^3 = -3.37\Delta_{ls} = -309$ cm^{-1} obtained from Eqs. (2)-(3). This yields $K_1 = 126$ cm^{-1} and $K_2 = 217.6$ cm^{-1}. To obtain more accurate values of K_1 and K_2 we performed calculations of the MgII spectra using many-body perturbation theory. We have used the complete set of the relativistic Hartree-Fock energies and wave functions as a zero approximation and then calculated all second-order correlation corrections in the residual electron-electron interaction (this technique is described in [14]). This *ab initio* calculation reproduces the experimental energy levels of the external electron with 0.2% accuracy (the single-electron energy levels in the many-body problem are defined as the ionization energies with a minus sign). To find the value of relativistic corrections we performed calculations for the two values of α : $\alpha = \alpha_l$ and $\alpha = \alpha_l/2$. The calculated relativistic corrections to the energy levels of the external electron are : $\Delta(3s) = -189.4$, $\Delta(3p_{1/2}) = -72.1$, $\Delta(3p_{3/2}) = 24.4$, $\Delta_{ls} = 96.5$cm^{-1}. Note that the many-body corrections change the sign of $\Delta(3p_{3/2})$. The final results are the following:

$$3s_{1/2} - 3p_{1/2} : \omega_1 = 35669.26 + 119.6[(\tfrac{\alpha}{\alpha_l})^2 - 1] \text{ cm}^{-1}$$
$$3s_{1/2} - 3p_{3/2} : \omega_2 = 35760.834(4) + 211.2[(\tfrac{\alpha}{\alpha_l})^2 - 1] \text{ cm}^{-1} \tag{6}$$

We changed slightly the values of the calculated coefficients K_1 and K_2 to reproduce exactly the experimental value of the fine splitting $\Delta_{ls} = 91.6 \text{cm}^{-1}$. The laboratory frequency of the $3s_{1/2} - 3p_{3/2}$ transition in the main isotope ^{24}Mg (abundance 79 %) has been taken from [12]. The increase of the frequencies (isotope shifts) for the transition in ^{25}Mg (abundance 10 %) and ^{26}Mg (abundance 11 %) are equal to 0.053 and 0.102 cm^{-1}, respectively [12]. The laboratory frequency of the $3s_{1/2} - 3p_{1/2}$ transition has been taken from [11].

Now consider FeII. We are interested in the $E1$-transition from the ground state $3d^64s \ \ ^6D_{9/2}$ to the members of the multiplets $3d^64p \ \ ^6D$, $\ ^6F$ and $\ ^6P$. Due to the selection rule $\Delta J \le 1$ the transitions from the ground state $J = 9/2$ can involve only few components of the excited multiplets. The splitting between the nearby components of the same multiplet (e.g. $J = 9/2$ and $J = 7/2$) are about 100 - 200 cm^{-1}. On the other hand, the total relativistic correction to the mean frequency of the $4s - 4p$ transition is about 1800 cm^{-1}, i.e. ~ 10 times larger! Unfortunately, we can not measure the effect of this large correction by measuring the frequency of $4s - 4p$ transitions in one element (FeII) since it will be hidden in the definition of the red shift parameter $1 + z$. Therefore, to make use of this large effect we need to consider two elements with different relativistic shifts, e.g. MgII and FeII, or different transitions in the same element, e.g. $s - p$ and $d - p$.

We can also consider $s - p$ transitions to the different multiplets. However, the relativistic effects in the differences between the central energy points E_0 of different multiplets (D, F and P) are substantially smaller ($\sim$ 100 - 200 cm^{-1}) than the relativistic shift of the $s - p$ transition frequency, since these differences are due to the dependence of the Coulomb interaction Q between external electrons on the relativistic correction to their wave functions ($\Delta\omega \sim QZ^2\alpha^2$ where Q is the non-diagonal matrix element of the Coulomb interaction producing configuration mixing). There are also small relativistic corrections to the interval between the different multiplets due to the second order in the spin-orbit interaction. However, the relativistic effect in the difference of the frequencies of particular components of different multiplets can be larger. The maximal relativistic shift in the differences of the FeII frequencies (for the transitions which have been observed in the quasar spectra) is 387 cm^{-1} in the difference between $^6F_{9/2}$ and $^6P_{7/2}$ (see below).

In principle, approximate calculations of the average relativistic frequency shift of the $4s - 4p$ transition and the dependence of the fine structure intervals on α could be done using semiempirical formulae (2) - (5) which give average the shift 1550 cm^{-1}, and laboratory experimental data. However, to calculate accurately the relativistic shift for each transition we performed relativistic many-body calculations for energy levels of FeII.

1. We used averaged relativistic Hartree-Fock potential of the FeIII d^6 state to generate a complete set of the zeroth approximation wave functions and energies.

2. Correlations of the second-order in the residual Coulomb interaction between the valence and core electrons were included by means of the correlation potential (self - energy operator) method [14].

3. Most of the valence correlations were included by means of a configuration interaction method. Excited configurations were constructed from the s, p and d single-electron

Hartree-Fock states with $n \leq 6$ (17 single-electron orbitals). Only those configurations were included that can be obtained by a single or double-electron excitation from the main configuration. Thus, the total number of configurations was few hundred. This is a rather small-scale configuration interaction and full convergence was not achieved. However, good agreement with experimental data for the energy levels shows that a greater part of the valence correlations were included.

4. To imitate the effect of higher-order many-body corrections we introduced two fitting parameters. The *ab initio* correlation potentials for the s and p electrons were multiplied by the factors $f_s = 0.94$ and $f_p = 0.9$, respectively. These factors imitated the effect of screening of the Coulomb interaction between the core and valence electrons which reduces the correlations between these electrons (accurate calculation of this screening has been done in [14]). The values of f_s and f_p were chosen to fit the ionization energies of the $3d^64s$ and $3d^64p$ states.

To find the dependence of frequencies on α we use the following formula for the energy levels within one fine-structure multiplet:

$$E = E_0 + Q_1((\frac{\alpha}{\alpha_l})^2 - 1) + K_1(\mathbf{LS})(\frac{\alpha}{\alpha_l})^2 + K_2(\mathbf{LS})^2(\frac{\alpha}{\alpha_l})^4. \tag{7}$$

Here L is the total orbital angular momentum and S is the total electron spin. We introduce an $(\mathbf{LS})^2$ term to describe deviations from the Lande interval rule. There are two sources of the $(\mathbf{LS})^2$ term: the second order in the spin-orbit interaction ($\sim (Z\alpha)^4 = 1.3 \times 10^{-3}$) and the first order in the spin-spin interaction ($\sim \alpha^2 = 5.3 \times 10^{-5}$). In FeII the second-order spin-orbit interaction is larger. Therefore, we first fitted the experimental fine structure intervals to find K_1 and K_2 (numerical calculations give close values of K_1 and K_2). Then we used numerical calculations for $\alpha = \alpha_l$ and $\alpha = \alpha_l/2$ to find the dependence of the configuration centers E_0 on α (coefficient Q_1). The coefficients Q_1, K_1 and K_2 are presented in table I. Very accurate values of the laboratory frequencies ($\alpha = \alpha_l$) can be found in [13]. The errors are about 0.003 cm^{-1}. The Fe atom has one dominating isotope ^{56}Fe (92 %) and small isotope shifts. Now we can use Eq. (7) and table I to calculate the frequencies of the $E1$ transitions from the ground state (in cm^{-1}) as functions of α:

$$
\begin{aligned}
^6D \quad & J = 9/2 \quad \omega = 38458.9871 + 1394x + 38y, \\
& J = 7/2 \quad \omega = 38660.0494 + 1632x + 0y, \\
^6F \quad & J = 11/2 \quad \omega = 41968.0642 + 1622x + 3y, \\
& J = 9/2 \quad \omega = 42114.8329 + 1772x + 0y, \\
& J = 7/2 \quad \omega = 42237.0500 + 1894x + 0y, \\
^6P \quad & J = 7/2 \quad \omega = 42658.2404 + 1398x - 13y,
\end{aligned}
\tag{8}
$$

where $x = (\frac{\alpha}{\alpha_l})^2 - 1, y = (\frac{\alpha}{\alpha_l})^4 - 1$. One can use Eqs. (6) and (8) to fit FeII and MgII lines in the quasar spectra and find the variation of α. Note that besides FeII one can use $s - p$ transitions from the ground state of GeII, ZnII, NiI, FeI, MnII, CaI and CaII, where the relativistic corrections have the same order of magnitude, and any light atom besides MgII.

One more interesting possibility more suitable for a laboratory experiment is to use transitions between "accidentally" degenerate levels in the same atom. Such meta-stable levels exist, for example, in the Dy atom: two $J = 10$ opposite parity levels $4f^{10}5d6s$ and $4f^95d^26s$

lying 19797.96 cm^{-1} above ground state.(This pair of levels was used to study parity non-conservation in Refs. [7,8]). There are other examples of "accidentally" degenerate levels in the rare-earth and actinide atoms and many close levels in other heavy atoms and ions (in the absence of degeneracy one should look for $s - d$ or $s - p$ transitions where the relativistic effects are larger). In the case of "accidental" degeneracy the contributions of the relativistic corrections to the frequency of the $E1$ transition in a heavy atom $(\sim 1000 cm^{-1})$ is compensated by the difference in the Coulomb interaction energies of the two configurations. However, if α varies with time, this compensation will eventually disappear. Thus, we have a correction ~ 1000 cm$^{-1}((\frac{\alpha}{\alpha_l})^2 - 1)$ to the very small (¡ 0.01 cm^{-1}) frequency of the transition. One can measure, for example, the time dependence of the ratio of frequencies for transitions between the hyperfine components of these two states. In the case of "accidentally" degenerate levels belonging to different electron terms in a molecule one can have enhanced effects of the change of both α and the nucleon mass. In the latter case the enhancement factor is the ratio of the vibration energy to the small frequency of the transition.

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TABLES

TABLE I. Relativistic energy parameters of some FeII multiplets (cm^{-1}) (Eq. (7))

Multiplets	E_0	K_1	K_2	Q_1
^6D	38686.19	-53.034	1.5189	1659
^6F	42168.91	-27.136	0.04741	1826
^6P	43078.15	-162.602	-2.145	1805