Fine-structure anomalies and search for variation of the fine-structure constant in laboratory experiments

V. A. Dzuba[1,*] and V. V. Flambaum[1,2,†]
[1]*School of Physics, University of New South Wales, Sydney 2052, Australia*
[2]*Physics Division, Argonne National Laboratory, Argonne, Illinois 60439-4843, USA*
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The configuration interaction in many-electron atoms may cause anomalies in the fine structure which make the intervals small and very sensitive to variation of the fine-structure constant. Repeated precision measurements of these intervals over a long period of time can put strong constraints on possible time variation of the fine-structure constant. We consider the $5p^4\,{}^3P_{2,1,0}$ fine-structure multiplet in the ground state of neutral tellurium as an example. Here the effect of change of the fine structure constant is enhanced about 100 times in the relative change of the small energy interval between the ${}^3P_1$ and ${}^3P_0$ states.

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I. INTRODUCTION

The possibility of fundamental constants to vary is predicted by theories unifying gravity with other interactions (see, e.g., review by Uzan [1]). There is evidence found in quasar absorption spectra that the fine-structure constant α ($\alpha=e^2/\hbar c$) might be smaller in the early cosmological epoch [2–5]. However, a similar analysis applied by other authors to different sets of data does not support this claim [6,7]. Recent progress in improving atomic clocks and developing optical frequency standards (see, e.g., [8]) made it possible to put strong constraints on the possible time variation of fundamental constants in laboratory measurements. In particular, constraints obtained for the fine-structure constant α need only about one order of magnitude improvement to see whether they are consistent with the quasar absorption spectra data if the same rate of change is assumed over cosmological time. These constraints were obtained with the full use of a technique developed for highly accurate optical standards. However, the choice of atomic transitions was not optimal for searching of variation of the fine-structure constant. Frequencies used so far change at about the same rate as α if α changes; i.e., there is no enhancement.

An alternative approach was suggested in Refs. [9,10]. It was proposed to measure the small frequency between two close states with different dependence on α. Here a small change of α may lead to an orders of magnitude larger relative change in frequency. The enhancement factor k can be expressed as $k=2q_{12}/\omega$, where q_{12} is the difference in relativistic energy shifts of two levels and ω is the transition frequency. A good candidate for such experiments is the dysprosium atom [9–11]. It has two almost degenerate states of opposite parity, and the corresponding enhancement factor is of the order of 10^8 [10]. Measurements for dysprosium are currently underway at Berkeley [11].

While it is hard to find anything better than dysprosium in terms of enhancement factor, it has its disadvantages too. The levels involved are not so narrow. While one of the states lives long enough to cause no problem, the other level does not. One has to work inside the linewidth to have the desirable accuracy. This puts certain limitations on achievable constraints on α variation. Therefore, it would be important to find something which combines the advantages of having metastable states and strong enhancement. A number of such transitions were considered in a recent work [12]. It has been suggested to look at the close metastable states of different configurations. The energies of different configurations change at different rates when α is changing. This, together with small energy intervals between the states, ensures strong enhancement [12].

In present work we consider a slightly different possibility. We suggest to study anomalously small fine-structure intervals in ground configurations of many-electron atoms. The use of the ground-state fine-structure multiplet ensures that states are metastable. They can only decay via $M1$ transitions which are very much suppressed due to small values of the transition frequency. On the other hand, the configuration interaction in many-electron atoms can reduce fine-structure intervals and lead to strong sensitivity to the change in the fine-structure constant. In the next sections we consider in detail the fine structure of the ground state of tellurium and discuss some other possibilities.

II. THEORY AND RESULTS FOR TELLURIUM

To study the sensitivity of atomic frequencies to variation of the fine-structure constant α it is convenient to present them in the vicinity of the physical value of α ($\alpha=\alpha_0=1/137.036$) in the form

$$\epsilon = \epsilon_0 + qx, \tag{1}$$

where $x=(\alpha/\alpha_0)^2-1$ and the coefficient q defines the sensitivity of the frequency to variation of α. In general, its value can be found from atomic calculations. If α changes, the relative frequency changes at the rate

$$\frac{\Delta\omega}{\omega} = \frac{2q_{12}}{\omega_0}\frac{\Delta\alpha}{\alpha_0} \equiv k\frac{\Delta\alpha}{\alpha_0}, \tag{2}$$

where $k=2q_{12}/\omega_0$ is the enhancement factor. To search for variation of the fine-structure constant one needs to compare

*Electronic address: V.Dzuba@unsw.edu.au
†Electronic address: V.Flambaum@unsw.edu.au

TABLE I. Experimental and theoretical energies and q coefficients (cm^{-1}) for the $5p^4$ ground-state configuration of Te I.

State	J	E (expt)	E (theor)	q
$5p^4\,{}^3p$	2	0	0	0
	1	4751	4770	5927
	0	4707	4713	3594
$5p^4\,{}^1D$	2	10559	10745	5207
$5p^4\,{}^1S$	0	23199	22845	8571

atomic frequencies with different enhancement factors over a long period of time. The larger this difference, the more sensitive the experiment to variation of α. Note that k can have a negative value which means that changes of α and frequency go in opposite directions: the frequency decreases when α increases and vice versa.

For "normal" fine-structure intervals which are proportional to $(Z\alpha)^2$ formula (1) is valid for all values of α, $0<\alpha<\alpha_0$. Therefore, $q_{12}=\omega_0$ and $k=2$. In other words, the factor k is the same for all "normal" fine-structure intervals and comparison between them cannot reveal any drift of α. These fine-structure intervals can still be used in searches for variation of the fundamental constants if they are compared to hyperfine structure or to frequencies of suitable optical transitions.

Situation changes dramatically if the fine-structure multiplet is strongly perturbed by a configuration interaction with neighboring states. We consider the neutral tellurium atom in its ground state as an example.

Experimental and theoretical energies of the ground-state $5p^4$ configuration of tellurium are presented in Table I. There are strong anomalies in the fine-structure multiplet $^3P_{2,1,0}$. The $^3P_2$-$^3P_1$ and $^3P_1$-$^3P_0$ intervals have opposite signs and differ in value more than 100 times. This is because of the configuration interaction between the $^3P_2$ and $^1D_2$ states and between the $^3P_0$ and $^1S_0$ states while the $^3P_1$ state has no close neighbors to mix with. The configuration interaction leads to accidental almost exact cancellation between spin-orbit and Coulomb terms in the energy interval between the $^3P_1$ and $^3P_0$ states. Since the spin-orbit interaction is much more sensitive to the change of α than the Coulomb term, it is natural to expect that the $^3P_1$-$^3P_0$ energy interval is very sensitive to the variation of α.

To check how strong is sensitivity of the fine-structure intervals of Te I we perform model configuration interaction (CI) calculations for the $5p^4$ configuration of the atom. First, we perform Hartree-Fock calculations for open shells to find the $5p_{1/2}$ and $5p_{3/2}$ states of neutral tellurium. Then we use the CI technique to construct four-electron states of the $5p^4$ configuration and to calculate their energies (in fact, in this approximation the CI technique is reduced to diagonalization of the interaction Hamiltonian describing direct mixing of different $5p^4$ states). It turns out that some extra fitting is needed to have good agreement with experiment. Namely, we reduce the value of the $F_2(5p_{3/2},5p_{3/2})$ Coulomb integral by 25%. This reduction simulates the effect of screening of the Coulomb interaction between valence electrons by core electrons. The results for energies are presented in Table I.

TABLE II. Frequencies (in cm^{-1}) and enhancement factors ($k=2\Delta q/\omega$) for transitions within the $^3P_{0,1,2}$ fine-structure multiplet of Te I

Transition	Type	ω	k
$^3P_1$-$^3P_2$	$M1$	4751	2.2
$^3P_0$-$^3P_2$	$E2$	4707	1.5
$^3P_1$-$^3P_0$	$M1$	44	106

One can see that in spite of the simple approximation used in calculations, the agreement with experiment is very good.

The coefficients q [see Eq. (1)] are found by varying α in computer codes:

$$q=\frac{\epsilon(x=+0.1)-\epsilon(x=-0.1)}{0.2}.$$

The results for q are also presented in Table I. Since we have good agreement with experiment for the energies, it is natural to assume that the accuracy for the q coefficients is also good.

Table II presents frequencies and enhancement factors for transitions between all states of the $^3P_{0,1,2}$ fine-structure multiplet. The enhancement for the $^3P_1$-$^3P_0$ is more than 100 due to the anomalously small frequency of the transition. The ratio of this small frequency to almost any other atomic frequency is extremely sensitive to variation of α. However, other transitions from Table II can also be used.

Because of the very exotic behavior of the fine-structure intervals of Te I, it is very interesting to see what happens to them when α varies from zero (nonrelativistic limit) to its physical value α_0. We have performed such calculations, and results for five low states of the $5p^4$ ground-state configura-

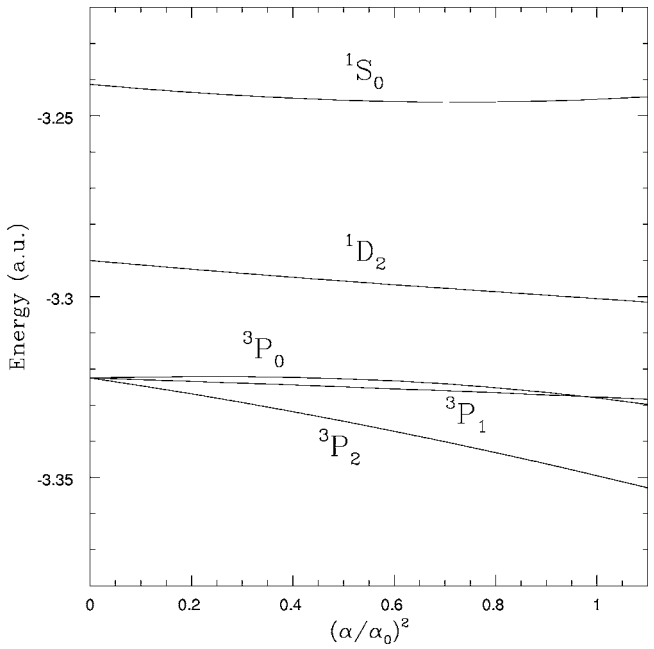

FIG. 1. Energy levels of lower states of Te I as functions of the fine-structure constant.

TABLE III. Experimental and theoretical energies and q coefficients (cm^{-1}) for the $6p^4$ ground-state configuration of Po I.

State	J	E (exp)	E (theor)	q
$6p^4\ ^3P$	2	0	0	0
	1	16831	17248	26720
	0	7514	7397	1910
$6p^4\ ^1D$	2	21679	22189	25850
$6p^4\ ^1S$	0	42718	45101	54130

tion of Te I are presented in Fig. 1. Valence energies (energy to remove all four valence electrons from atom) are shown as functions of $(\alpha/\alpha_0)^2$. All three energies of the $^3P_{0,1,2}$ multiplet have the same value at $\alpha=0$, and the fine-structure intervals are proportional to α^2 at small α. At larger values of α interaction with the $^1D_2$ and $^1S_0$ leads to a significant perturbation of the ^3P multiplet. In particular, repulsion between the $^1S_0$ and $^3P_0$ levels causes the latter to cross with the $^3P_1$ level in the vicinity of the physical value of α. This explains anomalously small energy interval between the two states.

Let us mention at the end of this section that both upper states of the ^3P multiplet are metastable. The $^3P_1$ state decays mostly by $M1$ transition to the ground state. Its lifetime is about 1 sec. The $^3P_0$ state decays via $E2$ transition to the ground state and its corresponding lifetime (if no other factors are involved) is about 4×10^3 sec.

III. POLONIUM AND CERIUM

There are many other examples of the anomalous fine structure in the ground and low excited states of many-electron atoms which involve metastable states and large enhancement and therefore are suitable for a search of variation of the fine-structure constant. The actual choice between them would involve consideration of many other factors which are important for experimentalists but not discussed in present paper. Below we discuss two more examples just to have broader picture.

TABLE IV. Frequencies (in cm^{-1}) and enhancement factors ($k=2\Delta q/\omega$) for transitions within the $^3P_{0,1,2}$ fine-structure multiplet of Po I.

Transition	Type	ω	k
$^3P_1$-$^3P_2$	$M1$	16831	3.2
$^3P_0$-$^3P_2$	$E2$	7514	0.5
$^3P_1$-$^3P_0$	$M1$	9317	5.3

A brief look at the spectra of elements presented in Moore's tables [13] reveals that practically all elements with the np^4 configuration in the ground state have anomalies in the fine structure (though none of them has so small an energy interval as Te I). The most interesting case after Te I is probably polonium (Po I). It has the largest nuclear charge Z ($Z=84$) among the np^4 elements which mean strong relativistic effects and large q and k coefficients [see formulas (1) and (2)]. Experimental and theoretical data similar to those considered for Te I are presented in Tables III and IV. We see that the enhancement factors k are large and different for different transitions. This is exactly what is needed for the search of variation of the fine-structure constant.

Another interesting example is the positive ion of cerium (Ce II). An extract from the tables [14] presenting experimental energies and Landé g factors of lower states of Ce II is presented in Table V together with nonrelativistic (NR) values of the g factors. Nonrelativistic g factors were calculated according to the formula

$$g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}. \tag{3}$$

The data presented in Table V reveal an interesting picture. Fine-structure multiplets of Ce II intersect. There are many states with the same total momentum J within an energy interval spanned by a single fine-structure multiplet. For example, there are four states of $J=4.5$ within energy interval of the lowest fine-structure multiplet $^4H^o$. It is clear that they must be strongly mixed. Fine-structure intervals do not

TABLE V. Energies (cm^{-1}) and g factors of lower states of Ce II.

Config.	Term	J	E (expt)	g (expt)	g (NR)
$4f5d^2$	$^4H^o$	3.5	0.000	0.794	0.667
		4.5	2581.257	1.023	0.970
		5.5	2879.695	1.123	1.133
		6.5	4203.934	1.189	1.231
$4f5d^2$		4.5	987.611	0.948	1.000
$4f5d^2$	$^4I^o$	4.5	1410.304	0.856	0.727
		5.5	2563.233	0.968	0.965
		6.5	3793.634	1.128	1.107
		7.5	5455.845	1.196	1.200
$4f5d^2$		3.5	1873.934	0.806	1.000
$4f5d^2$		0.5	2140.492	0.985	1.000
$4f5d6s$		4.5	2382.246	1.039	1.000

obey Landé's rule and experimental g factors deviate significantly from the nonrelativistic values. All these suggest strong configuration mixing and sensitivity of the intervals to variation of α. An interval of particular interest is the $^4H^o_{11/2}$-$^4H^o_{9/2}$ one. It is small, only 299 cm^{-1}, and states involved are strongly mixed with other close states. This ensures strong enhancement of the change of α in the relative change of frequency.

Calculations for Ce II are more difficult than for Te I and Po I because of valence states of high angular momentum ($5d$ and $4f$). Therefore we believe that it is premature to attempt them now. The presence of enhancement is obvious but its actual value would become important only on the stage of planning the measurements. We are ready to perform the calculations if there is any interest from experimentalists.

Cases of fine-structure anomalies similar to what is presented here for Ce II can be easily found in spectra of many other rare-earth elements. Which of them are suitable for the search of α variation is the question which needs further consideration.

IV. CONCLUSION

We present an alternative way to search for variation of the fine-structure constant in laboratory measurements. We propose to use fine-structure intervals in the ground or low excited states of many-electron atoms which are strongly perturbed by configuration interactions with neighboring states. This method has double advantages. On the one hand, the use of low states ensures that they are metastable. This is important for very accurate frequency measurements. On the other hand, a strong perturbation may lead to an anomalously small fine-structure interval and strong enhancement of the relative sensitivity of the frequencies to the change of the fine-structure constant. Because of the high relative sensitivity, one does not need extremely accurate absolute measurements of the frequencies (this is the difference with conventional atomic clock measurements). A large value of the effect/frequency ratio may also help to reduce the importance of some systematic effects (e.g., the Doppler shift and broadening). Note, however, that we do not consider in this paper any practical measurement scheme.

Enhanced and highly nonlinear dependence of the small fine-structure intervals on the magnitude of the relativistic corrections also presents a certain theoretical interest.

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