Sensitivity of the energy levels of singly ionized cobalt to the variation of the fine structure constant

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We use relativistic Hartree-Fock and configuration interaction methods to calculate the dependence of transition frequencies for singly ionized cobalt on the fine structure constant. The results are to be used in the search for variation of the fine structure constant in quasar absorption spectra.

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I. INTRODUCTION

Search for variation of fundamental constants is motivated by theories unifying gravity with other interactions as well as by many cosmological models. The search spans the whole lifetime of the universe from Big-Bang nuclear synthesis to the present-day very precise atomic clock experiments (see, e.g. reviews [1–4]). No unambiguous manifestation of the variation of fundamental constants have been found so far. However, there is large amount of data which is consistent with variation of the fine structure constant or the ratio of the electron to proton mass [1–4]. Most of this data comes from the analysis of the quasar absorption spectra. The analysis of the data obtained on the Keck telescope in Hawaii indicate that the fine structure constant $\alpha$ might be smaller in early universe [5–10]. However, an analysis of the data from the VLT telescope in Chile, performed by different groups [11, 12] gave a null result. There is an intensive debate in the literature about possible reasons for the disagreement (see, e.g. [13–16]).

The most probable reason for disagreement is the effect of some unknown systematics. One of the ways to deal with any unknown systematics is to include as many atomic lines into analysis as possible and compare the results for different lines for consistency. Atomic frequencies in different atoms and even frequencies of different transitions in the same atom depend on the fine structure constant very differently. It is extremely unlikely that any unknown systematics would behave exactly the same way thus mimicking the variation of the fine structure constant.

It was recently brought to our attention that some lines of single-ionized cobalt are observed in the quasar absorption spectra [17]. To include these lines into analysis one needs to know how the frequencies of the corresponding transitions depend on the fine structure constant. To reveal this dependence we perform atomic calculations following the technique developed in our previous works [18–19].

II. METHOD

The dependence of atomic frequencies on the fine-structure constant $\alpha = e^2/\hbar c$ appears due to relativistic corrections. In the vicinity of its physical value $\alpha_0 = 1/137.036$ it is presented in the form

$$\omega(x) = \omega_0 + qx,$$

where $\omega_0$ is the present laboratory value of the frequency and $x = (\alpha/\alpha_0)^2 - 1$, and $q$ is the coefficient which is to be found from atomic calculations. Note that

$$q = \frac{d\omega}{dx} \bigg|_{x=0}.$$ 

To calculate this derivative numerically we use

$$q \approx \frac{\omega(x) - \omega(-x)}{2x}.$$ 

Here $x$ must be small to exclude non-linear in $\alpha^2$ terms. In the present calculations we use $x = 0.01$.

The atomic structure calculations are performed with the use of the relativistic Hartree-Fock method (RHF) and the configuration interaction technique (CI). The RHF self-consistent procedure is done separately for two even and two odd configurations presented in Table I. The resulting 3$d$, 4$s$, and 4$p$ single-electron functions are used as a basis for the CI calculations. Note that these states are different in different configurations. For example the 3$d$ state in the 3$d^6$ configuration is not the same as the 3$d$ state in the 3$d^74$p configuration, etc. See Ref. [18] for details.

The effective Hamiltonian for $N_v$ valence electrons has the form

\begin{table}
\centering
\begin{tabular}{|c|c|}
\hline
Parity & $\alpha_c$ (a.u.) \\
\hline
Even & 3$d^6$ 0.4 \\
Even & $3d^74s$ 0.5177 \\
Odd & $3d^74p$ 0.448 \\
Odd & $3d^84s4p$ 0.75 \\
\hline
\end{tabular}
\caption{Configurations and effective core polarizabilities $[\alpha_c \text{ (a.u.)}]$ used in the calculations.}
\end{table}
FIG. 1: Energy levels of cobalt between 45000 cm$^{-1}$ and 50000 cm$^{-1}$ as functions of ($\alpha/\alpha_0$)$^2$. Dotted line: $J = 3$, short dash line: $J = 4$, long dash line: $J = 5$

\[ H_{\text{eff}} = \sum_{i=1}^{N_v} \hat{h}_1 + \sum_{i<j} e^2/r_{ij}, \]  

(4)

Here, $\hat{h}_1(r_i)$ is the one-electron part of the Hamiltonian:

\[ \hat{h}_1 = c\alpha \cdot p + (\beta - 1)mc^2 - Ze^2/r + V_{\text{core}} + \delta V. \]  

(5)

Here $\alpha$ and $\beta$ are Dirac matrices, $V_{\text{core}}$ is Hartree-Fock potential due to core electrons and $\delta V$ is the term which simulates the effect of the correlations between core and valence electrons. It is often called the polarization potential and has the form

\[ \delta V = -\frac{\alpha_c}{2(r^4 + a^4)}. \]  

(6)

Here $\alpha_c$ is the polarization of the core and $a$ is a cut-off parameter (we use $a = a_B$). We treat $\alpha_c$ as fitting parameters and choose their values to reproduce experimental position of the configurations on the energy scale. Corresponding values of $\alpha_c$ are presented in Table I.

III. RESULTS

The results of calculations are presented in Table II. We include experimental and theoretical energy levels,

FIG. 2: Energy levels of cobalt between 64500 cm$^{-1}$ and 67500 cm$^{-1}$ as functions of ($\alpha/\alpha_0$)$^2$. Dotted line: $J = 3$, short dash line: $J = 4$, long dash line: $J = 5$

FIG. 3: Energy levels of cobalt between 71000 cm$^{-1}$ and 75000 cm$^{-1}$ as functions of ($\alpha/\alpha_0$)$^2$. Dotted line: $J = 3$, short dash line: $J = 4$, long dash line: $J = 5
g-factors and q-coefficients. Non-relativistic g-factors are given by

\[ g_{NR} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}, \tag{7} \]

where \( J \) is total momentum of the atom, \( L \) is its angular momentum and \( S \) is spin. The \( g \)-factors are useful for identification of states. As can be seen from Table 1, experimental \( g \)-factor is close to the non-relativistic values given by (7). This justifies non-relativistic notations for the states and allows to group them into fine structure multplets. This is why \( g \)-factors are often more important than energies for the identification of the states. An interesting example of this kind will be discussed below.

Meanwhile we would like to stress that the accuracy for the calculated \( g \)-factors can also serve as an indicator on what kind of accuracy can be expected for the \( q \)-coefficients. This is because \( g \)-factors are sensitive to configuration mixing in a very similar way as the \( q \)-coefficients. They can even be used to tune configuration mixing to reproduce experimental \( g \)-factors and therefore improve the accuracy for the \( q \)-coefficients. Corresponding procedure can be used when the energies of two states with the same total momentum \( J \) come very close to each other in the vicinity of the physical value of \( \alpha \) indicating possible level pseudo crossing when energies are considered as functions of the ratio \((\alpha/\alpha_0)^2\). Figures 12 and 3 show energy levels of Co II as functions of the fine structure constant from its non-relativistic limit \( \alpha = 0 \) to the physical value \( \alpha = \alpha_0 = 1/137.036 \). One can see that there are many level crossings but most of them are at safe distance from the physical point \( \alpha = \alpha_0 \).

An interesting example is the mixing of three levels of total momentum \( J = 3 \): \( E = 50036.55 \text{ cm}^{-1} \), \( E = 50381.86 \text{ cm}^{-1} \) and \( E = 51512.41 \text{ cm}^{-1} \). Fig. 1 shows that these three levels cross each other at about \((\alpha/\alpha_0)^2 = 0.5 \). This probably means that mixing should have little effect on \( g \)-factors or \( q \)-coefficients at \((\alpha/\alpha_0)^2 = 1 \). However, calculations do not reproduce correct order of states on the energy scale. Here we have to use comparison between calculated, experimental and non-relativistic \( g \)-factors to decide which fine structure multiplet a calculated state should go to.

In spite of the fact that calculations does not always reproduce correct order of states the results for energies and \( g \)-coefficients are stable with respect of variation of the details of the calculation procedure. We estimate that the absolute uncertainty in values of \( q \) for all states is about the same and of the order of 200 \text{ cm}^{-1}. Therefore, relative uncertainty for smaller \( q \) is higher. This is because all states belong to the same 3d\(^7\)4p configuration and small values of \( q \) are due to repulsion from lower states of the same total momentum \( J \). Variation in the strength of this repulsion or in any other details of the calculations are likely to change the values of the \( q \)-coefficients for both interacting states by about the same amount. Note however that in cases of poor accuracy for \( g \)-factors and wrong order of states the uncertainty might be slightly higher than 200 \text{ cm}^{-1}.

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1] J-P. Uzan, Rev. Mod. Phys. 75, 403 (2003).
2] V. V. Flambaum, Int. J. Mod. Phys. A 22, 4937 (2007).
3] V. A. Dzuba and V. V. Flambaum, Can. J. Phys. 87, 15-23 (2009).
4] V. V. Flambaum and V. A. Dzuba, Can. J. Phys. 87, 25-33 (2009).
5] J. K. Webb, V. V. Flambaum, C. W. Churchill, M. J. Drinkwater, and J. D. Barrow, Phys. Rev. Lett. 82, 884 (1999).
6] J. K. Webb, M. T. Murphy, V. V. Flambaum, V. A. Dzuba, J. D. Barrow, C. W. Churchill, J. X. Prochaska, and A. M. Wolfe, Phys. Rev. Lett. 87, 091301 (2001).
7] M. T. Murphy, J. K. Webb, V. V. Flambaum, V. A. Dzuba, C. W. Churchill, J. X. Prochaska, J. D. Barrow, and A. M. Wolfe, Not. R. Astron. Soc. 327, 1208 (2001).
8] M. T. Murphy, J. K. Webb, V. V. Flambaum, C. W. Churchill, and J. X. Prochaska, Not. R. Astron. Soc. 327, 1223 (2001).
9] M. T. Murphy, J. K. Webb, V. V. Flambaum, C. W. Churchill, and J. X. Prochaska, Not. R. Astron. Soc. 327, 1237 (2001).
10] M. T. Murphy, J. K. Webb, V. V. Flambaum, M. J. Drinkwater, F. Combes, and T. Wiklind, Not. R. Astron. Soc. 327, 1244 (2001).
11] R. Quast, D. Reimers, and S. A. Levshakov, Astron. Astrophys. 417, L7 (2004).
12] R. Srianand, H. Chand, P. Petitjean, and B. Aracil, Astron. Astrophys. 417, 853 (2004); Phys. Rev. Lett. 92, 121302 (2004).
13] M. T. Murphy, J. K. Webb, and V. V. Flambaum, Phys. Rev. Lett. 99, 239001 (2007).
14] R. Srianand, H. Chand, P. Petitjean, and B. Aracil, arXiv:0711.1742 (2007).
15] M. T. Murphy, J.K. Webb, and V. V. Flambaum, MNRAS 384, 1053 (2008).
16] K. Griest, J. B. Whitmore, A. M. Wolfe, et al, Astr. J. 708, 158 (2010).
17] S. L. Ellison, S. G. Ryan, and J. X. Prochaska, MNRAS 326, 628 (2001).
18] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A, 77, 012514 (2008).
19] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A, 77, 012515 (2008).
20] V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, and M. Marchenko, Phys. Rev. A, 66, 022501 (2002).
21] J. Sugar and C. Corliss, J. Phys. Chem. Ref. Data 10, 1097 (1981).