Relativistic frequency shifts in Cr, Ti, Fe, Ni, Ca, Na, and V to search for variation in the fine structure constant

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Sensitivity of the frequencies of twenty two atomic transitions to the variation of the fine structure constant $\alpha$ is calculated. The findings are to be used in search for possible variation of $\alpha$ across our Galaxy using high quality spectroscopic data for stars similar to our Sun.

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I. INTRODUCTION

Theories unifying particle physics and cosmology predict possible variation of the fundamental constants in space and time. Values of these constants may depend on a cosmological scalar field representing dark energy or dark matter [1–5].

Many searches for variations in the low-energy value of the fine-structure constant, $\alpha \equiv e^2/\hbar c$, rely on understanding the sensitivity of atomic transition frequencies on $\alpha$ (e.g. [6, 7]). Indeed, these were recently calculated for 13 transitions seen in infrared stellar spectra and used to probe for differences between $\alpha$ in giant stars near the Galactic Centre and the laboratory value [8]. This is also required for a new probe of $\alpha$-variation across our Galaxy, using stars very similar to our Sun, called ‘solar twins’ [9–11]. This star-to-star comparison largely avoids systematic errors in the usual star-to-laboratory approach, particularly effective shifts and asymmetries in absorption lines from several physical processes as they arise in stellar atmospheres.

The solar twins approach seeks to take advantage of the richness of optical stellar spectra, with potentially hundreds of strong (but unsaturated) absorption lines available, in principle, for comparison between stars to measure any differences in $\alpha$. However, in practice, there are many reasons to carefully select only transitions which are likely to be most reliable [11]. In particular, using closely-separated pairs of transitions, which have very similar strengths in solar twin spectra, suppresses many systematic errors of instrumental and astrophysical origin. To use the thousands of high-quality archival stellar spectra available from the High-Accuracy Radial velocity Planetary Searcher (HARPS) spectrograph [12] on the European Southern Observatory’s (ESO) 3.6-m telescope at La Silla Observatory (Chile), 164 different transitions were selected, which form 229 close pairs [11]. However, the sensitivity of these transitions to variations in $\alpha$ have not been calculated before. Here we calculate sensitivities for 22 of these transitions, forming 17 pairs, which have been used to compare $\alpha$ between 18 solar twins in [9–11].

II. CALCULATIONS

The dependence of atomic transition frequencies on the fine structure constant $\alpha$ was studied before for a number of systems (see, e.g. [6, 7]). In particular, Ti and Fe where considered in Refs. [13, 14]. However, in present work we use atomic transition which were never considered before. To perform the calculations we use similar approaches as before accompanied with a new method for atoms with complicated electronic structure (many electrons in open shells). For atomic transitions it is convenient to use atomic units and transition frequencies on $\alpha$ appears due to the relativistic corrections. It is convenient to present frequencies of atomic transitions in a form

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

where $x = (\alpha/\alpha_0)^2 - 1$, $\omega_0$ and $\alpha_0$ are the present values of the transition frequency and the fine structure constant, $q$ is sensitivity coefficient which can be found by varying the value of $\alpha$ in computer codes

$$q = \frac{\omega(\Delta x) - \omega(-\Delta x)}{2\Delta x}. \quad (2)$$

We use small value of $\Delta x$ ($\Delta x = 0.01$) to avoid non-linear effects, e.g. those which are caused by level crossing [1].

To calculate transition frequencies, we use a range of methods depending on the number of electrons above closed shells. For atoms with one external electron (e.g., Na I) we use the correlation potential method [13]. In this method the calculations start from the relativistic Hartree-Fock (RHF) procedure for the closed-shell core, with one external electron removed. Then, states of external electron are calculated by solving RHF-like equations which also include core-valence correlations

$$(\hat{H}_0 + \hat{\Sigma}_1 - \epsilon_v)\psi_v = 0. \quad (3)$$

Here $\hat{H}_0$ is the RHF Hamiltonian, $\hat{\Sigma}_1$ is a single-electron non-local operator (correlation potential) which describes correlation interaction of an external electron with the...
| Z  | Atom/State | Ion | Energy Expt. [18] | Theory |
|----|------------|-----|-------------------|--------|
| 11 | Na I       | 2p^63p | 2P^1_1/2 | 16956.170 | 16862 |
|    |            | 2p^63p | 2P^1_3/2 | 16973.366 | 16881 |
|    |            | 2p^65s | 2S^1_1/2 | 30063.703 | 33057 |
| 20 | Ca I       | 3p^64s^4p | 3P^0 | 15210.063 | 15544 |
|    |            | 3p^63d^4s | 3D^1 | 20335.360 | 19568 |
|    |            | 3p^64s^5s | 3S^1 | 31395.695 | 31816 |
|    |            | 3p^65s^5p | 3P^0 | 36547.688 | 36766 |
| 22 | Ti I       | 3d^6(4S)4s | a^1H | 18141.265 | 21534 |
|    |            | 3d^6(4S)4s | a^3H | 18192.570 | 21309 |
|    |            | 3d^6(4S)4p | a^1S | 39152.103 | 41034 |
|    |            | 3d^6(4S)4p | a^3S | 39198.323 | 41050 |
| 23 | V I        | 3d^6(4S)4s | a^1D | 8710.567 | 10577 |
|    |            | 3d^6(4S)4p | a^1D | 15265.700 | 17936 |
|    |            | 3d^6(4S)4p | a^3D | 29544.454 | 29005 |
|    |            | 3d^6(4S)4p | a^5D | 34543.380 | 33930 |
| 24 | Cr I       | 3d^64s^2 | a^1S | 7927.441 | 7114 |
|    |            | 3d^64s^2 | a^3S | 8093.184 | 7161 |
| 26 | Fe I       | 3d^6(4F)4s | a^1P | 12968.554 | 11964 |
|    |            | 3d^6(4F)4s | a^3P | 17550.181 | 23061 |
|    |            | 3d^6(4F)4s | a^3P | 17927.382 | 22558 |
|    |            | 3d^64s^2 | a^1D | 19552.478 | 24345 |
|    |            | 3d^64s^2 | a^3D | 19788.251 | 22233 |
|    |            | 3d^64s^2 | a^5D | 20874.482 | 25230 |
|    |            | 3d^64s^2 | a^7D | 21083.987 | 25746 |
| 28 | Ni I       | 3d^6(4S)4s | a^1D | 13521.347 | 15768 |
|    |            | 3d^6(4S)4s | a^3D | 32982.260 | 30508 |
|    |            | 3d^6(4S)4s | a^5D | 29668.893 | 28002 |

We calculate \( \hat{\Sigma}_1 \) in the lowest, second order of the many-body perturbation theory using the B-spline technique [17]. Index \( v \) in (3) numerates states of the valence electron. Solutions of (3) are usually called Bruekner electrons. The single-electron basis states for valence electrons are calculated in the field of the ion using the B-spline technique similar to how it is done for a single-valence-electron atom. The effective CI Hamiltonian for two valence electrons has the form

\[
\hat{H}^{CI} = \hat{h}_1(r_1) + \hat{h}_1(r_2) + \hat{h}_2(r_1, r_2).
\]

Here \( \hat{h}_1 = \hat{H}_0 + \hat{\Sigma}_1 \) is a single-electron part of the Hamiltonian. It includes the RHF operator \( \hat{H}_0 \) and the correlation potential \( \hat{\Sigma}_1 \), the same as in (3). The two-electron part of the CI Hamiltonian is the sum of the Coulomb interaction and correlation operator \( \hat{\Sigma}_2 \),

\[
\hat{h}_2(r_1, r_2) = e^2/|r_1 - r_2| + \hat{\Sigma}_2(r_1, r_2).
\]

The later can be understood as screening of the Coulomb interaction between valence electrons by core electrons (see Ref. [19] for details). Calculated energies of the states of Ca I which are used in the analysis are compared with experimental data in Table I.

For atoms with more than two external electrons (Ti I, Ti II, Cr I, V I, Fe I, Ni I) we use a combination of the configuration interaction and perturbation theory (the CIPT method [21]). All electrons above the Ar-like core are considered as external electrons and treated with configuration interaction (CI) approach. The CI Hamiltonian has a form

\[
\hat{H}^{CI} = \sum_i \hat{H}_0(r_i) + \sum_{i<j} e^2/r_{ij},
\]

where \( \hat{H}_0 \) is the RHF operator, second term presents Coulomb interaction between external electrons, the summation goes over all external (valence) electrons \( N_v \). Correlation operators \( \hat{\Sigma}_1 \) and \( \hat{\Sigma}_2 \) are not included for reasons explained below. The number of valence electrons varies from \( N_v = 4 \) for Ti to \( N_v = 10 \) for Ni. With the number of external electrons being that large, the number of lines in the CI matrix may go up to \( \sim 10^8 \) in the standard CI approach. This would make the calculations impossible. Therefore, we use the CIPT approach, in which the off-diagonal matrix elements between high-energy states are neglected. Indeed, it is easy to show that these matrix elements formally appear in a higher order of the perturbation theory and are suppressed by large energy denominators. This allows to reduce the size of the effective CI matrix by many orders of magnitude. The high-energy states are still included in the correction to the CI matrix elements between low-energy states,

\[
\langle a | \hat{H}^{eff} | b \rangle = \langle a | \hat{H}^{CI} | b \rangle + \sum_n \frac{\langle a | \hat{H}^{CI} | n \rangle \langle n | \hat{H}^{CI} | b \rangle}{E_n - E_{n}}.
\]

Here \( \hat{H}^{eff} \) is the effective CI operator, \( |a\rangle \) and \( |b\rangle \) are many-electron single-determinant low-energy basis
states, \(|n\rangle\) are high-energy many-electron basis states, \(E_n\) is the energy of the high-energy state, \(\langle n|H|n\rangle\), \(E\) is the energy of the state of interest. Since the later energy is not known, the CIPT equations, \((H_{\text{eff}} - E)X = 0\), are solved iteratively, using the energy found on the previous iteration to calculate second term in Eq. (2), the number of configurations is approximated only in the \(V^{N-M}\) approximation [21], where \(M\) is the number of valence electrons. In any other starting potential one has to include subtraction diagrams [19] and even three-body diagrams [22], which is significant complication to the method. On the other hand, in the considered systems, the correlations are dominated by correlations between valence electrons which are treated pretty accurately in the CI technique. The effect of neglecting the core-valence correlations is smaller than the effect of neglecting the off-diagonal matrix elements between the high-energy states.

Calculated energies of the states of Ti I, Ti II, Cr I, V I, Fe I and Ni I, which are used in the analysis are compared with experimental data in Table II. The accuracy is lower than for systems with simple electron structure, like Na I and Ca II. However, it is sufficient for the purposes of the present work.

The pairs of transitions, which are used in the analysis, are presented in Table III together with the calculated sensitivity coefficients \(q\). Error bars for the \(q\)-coefficients are estimated by varying computational parameters, such as the value of \(\Delta x\) in Eq. (2), the number of configurations included into the low-energy basis, etc. In most cases the uncertainty is significantly smaller than the value of
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