Relativistic corrections to transition frequencies of Fe I and search for variation of the fine structure constant

V. A. Dzuba and V. V. Flambaum
School of Physics, University of New South Wales, Sydney 2052, Australia
(Dated: February 2, 2008)

Relativistic energy shifts of the low energy levels of Fe have been calculated using the Dirac-Hartree-Fock and configuration interaction techniques. The results are to be used in the search for the space-time variation of the fine structure constant in quasar absorption spectra. The values of the shifts are the largest among those used in the analysis so far. This makes Fe a good candidate for the inclusion into the analysis.

PACS numbers: PACS: 31.30.Jv, 06.20.Kr, 95.30.Dr

I. INTRODUCTION

Theories unifying gravity with other interactions suggest a possibility of temporal and spatial variations of the fundamental constants of nature; reviews of these theories and results of measurement can be found in Refs. [1, 2]. Strong evidence that the fine-structure constant might be smaller about ten billion years ago was found in the analysis of quasar absorption spectra [3, 4, 5, 6, 7]. This result was obtained using the data from the Keck telescope in Hawaii. However, an analysis of the data from the VLT telescope in Chile, performed by different groups [8, 9] gave a null result. There is an ongoing debate in the literature about possible reasons for the disagreement (see, e.g. [10, 11]).

All these results were obtained with the use of the so called many-multiplet method suggested in Ref. [12]. This method requires calculation of relativistic corrections to frequencies of atomic transitions to reveal their dependence on the fine-structure constant. Atomic calculations for a large number of transitions in many atoms and ions of astrophysical interest were reported in Refs. [13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23]. In present paper we perform similar calculations for neutral iron which was never considered before. Until very recent we were unaware about any lines of neutral iron observed in the quasar absorption spectra. It was Prof. P. Molnar [24] who brought to our attention the existence of such data and the intention of his group to use them in the analysis.

Using Fe I in the search for variation of the fine structure constant has several advantages. First, the values of the relativistic energy shifts are large due to relatively larger nuclear charge (Z=26) and strong configuration mixing. Second, these values vary strongly from state to state which makes it hard to mimic the effect of varying fine structure constant by any systematics. Finally, iron is very abundant element in the universe. Great part of the previous analysis was performed using the data from Fe II.

Calculations for Fe I are difficult due to large number of valence electrons and strong configuration mixing. Its ground state configuration for outermost electrons is 3d^6 4s^2 which is strongly mixed with the 3d^7 4s configuration. There is strong configuration mixing for the 3d^6 4s4p and 3d^7 4p odd-parity configurations for the excited states. With eight valence electrons and strong configuration mixing full-scale accurate ab initio calculations for Fe I would require enormous computer power. We have chosen a different approach. Below we report a simple method which is specially designed for systems with strong mixing of several distinct configurations. It combines ab initio Hartree-Fock and configuration interaction (CI) techniques with some semi-empirical fitting and gives very reasonable results at very low cost in terms of computer power. The approach is similar to the well-known multi-configuration relativistic Hartree-Fock method (see, e.g. [25]) and can probably be considered as a simple version of it. The accuracy for the energy levels of Fe I is within few per cent of experimental values while estimated accuracy for the relativistic energy shifts is on the level of 20 to 30%. Due to strong configuration mixing the results are sensitive to the distances between energy levels. Therefore, special care has been taken to reproduce experimental positions of the energy levels.

II. METHOD

It is convenient to present the dependence of atomic frequencies on the fine-structure constant \( \alpha \) in the vicinity of its physical value \( \alpha_0 \) in the form

\[
\omega(x) = \omega_0 + qx,
\]

where \( \omega_0 \) is the laboratory value of the frequency and \( x = (\alpha/\alpha_0)^2 - 1 \), \( q \) 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

\[
q \approx \frac{\omega(+\delta) - \omega(-\delta)}{2\delta}.
\]

Here \( \delta \) must be small to exclude non-linear in \( \alpha^2 \) terms. In the present calculations we use \( \delta = 0.05 \), which leads...
TABLE I: Even and odd configurations of Fe and effective core polarizability $\alpha_p$ (a.u.) used in the calculations.

| Set | Parity | Configuration | $\alpha_p$ |
|-----|--------|---------------|-----------|
| 1   | Even   | $3d^74s^2$   | 0.4       |
| 2   | Even   | $3d^74s$     | 0.4192    |
| 3   | Even   | $3d^64p^2$   | 0.4       |
| 4   | Even   | $3d^5$       | 0.465     |
| 5   | Odd    | $3d^74s^4p$  | 0.39      |
| 6   | Odd    | $3d^74p$     | 0.412     |
| 7   | Odd    | $3d^64s^24p$ | 0.409     |

To calculate the coefficients $q$ using Eq. (4), $\alpha$ must be varied in the computer code. Therefore, it is convenient to use a form of the single electron wave function in which the dependence on $\alpha$ is explicitly shown (we use atomic units in which $\hbar = 1, \alpha = 1/c$)

$$
\psi(r)_{njl} = \frac{1}{r} \left( \frac{f_v(r)\Omega(n)_{jlm}}{g_v(r)\Omega(n)_{jlm}} \right),
$$

where $n$ is the principal quantum number and an index $v$ replaces the three-number set $n, j, l$. This leads to a form of radial equation for single-electron orbitals which also explicitly depends on $\alpha$:

$$
\frac{df_v}{dr} + \frac{\beta}{r} f_v(r) - \left[ 2 + \alpha^2 (\epsilon_v - \hat{V}_{HF}) \right] g_v(r) = 0,
$$
\[ 6 \]

$$
\frac{dg_v}{dr} - \frac{\beta}{r} f_v(r) + (\epsilon_v - \hat{V}_{HF}) f_v(r) = 0,
$$

here $\beta = (-1)^{j+1/2}(j + 1/2)$, and $\hat{V}_{HF}$ is the Hartree-Fock potential. Equation (6) with $\alpha = \alpha_0\sqrt{3} + 1$ and different Hartree-Fock potential $\hat{V}_{HF}$ for different configurations is used to construct single-electron orbitals.

Table I lists configurations considered in present work. First four are even configurations and other three are odd configurations. We perform self-consistent Hartree-Fock calculations for each configuration separately. This allows to account for the fact that single-electron states depend on the configurations. For example, the $3d$ state in the $3d^74s^2$ configuration is not the same as the $3d$ state in the $3d^74s$ configuration. In principle, it is possible to account for these differences in the CI calculations. One would need to have a complete set of single-electron states and construct many-electron basis states by redistributing valence electrons over these single-electron basis states. Then actual many-electron states are found by diagonalization of matrix of the effective CI Hamiltonian. This approach works very well for the case of two or three valence electrons (see, e.g. [26, 27, 28]). However, for eight valence electrons it would lead to a matrix of enormous size making it practically impossible to saturate the basis while using limited computer power.

The results with unsaturated basis are very unstable and strongly depend on where the basis is truncated. Therefore, we prefer to account for the differences in the configurations on the Hartree-Fock rather than CI stage of the calculations.

The self-consistent Hartree-Fock procedure is done for every configuration listed in Table I separately. Then valence states found in the Hartree-Fock calculations are used as basis states for the CI calculations. It is important for the CI method that atomic core (1s$^2$ ... 3p$^6$) remains the same for all configurations. We use the core which corresponds to the ground state configuration. Change in the core due to change of the valence state is small and can be neglected. This is because core states are not sensitive to the potential from the electrons which are on large distances (like 4s and 4p electrons). The 3d electrons are on smaller distances and have larger effect on atomic core. However, in most of the cases (see Table I) only one among six 3d electrons changes its state. Therefore their effect on atomic core is also small. More detailed discussion on the effect of valence electrons on atomic core can be found in Refs. [29, 30].

All configurations in Table I correspond to an open-shell system. We perform the calculations staying within central-field approximation but using fractional occupation numbers. As a result we have 23 single-electron basis states for valence electrons: $3d_3/2, 3d_5/2, 3s_1, 4s_1, 4p_1, 4p_3, 4p_5$. Here index $i$ is the set number (as in Table I). Note that total number of basis states is less than 5 times number of sets because many configurations don’t include particular single-electron states. Note also that our basis set is non-orthogonal, e.g. $0 < \langle 3d_3/2 | 3d_5/2 \rangle < 1$. The implications of this fact will be discussed below.

The effective Hamiltonian for valence electrons has the form

$$
\hat{H}^{eff} = \sum_{i=1}^{8} \hat{h}_i + \sum_{i<j}^{8} e^2/r_{ij},
$$

where $\hat{h}_i(r_i)$ is the one-electron part of the Hamiltonian

$$
\hat{h}_i = \alpha \cdot \mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + V_{core} + \delta V.
$$

Here $\alpha$ and $\beta$ are Dirac matrices, $V_{core}$ is Hartree-Fock potential due to 18 core electrons (1s$^2$ ... 3p$^6$) and $\delta V$ is the term which simulates the effect of the correlations between core and valence electrons. It is often called polarization potential and has the form

$$
\delta V = -\frac{\alpha_p}{2(r^4 + a^4)}.
$$

Here $\alpha_p$ is polarization of the core and $a$ is a cut-off parameter (we use $a = a_p$). The form of the $\delta V$ is chosen to coincide with the standard polarization potential on large distances ($-\alpha_p/2r^4$). However we use it on distances
where valence electrons are localized. This distances are not large, especially for the 3d electrons. Therefore we consider $\delta V$ as only rough approximation to real correlation interaction between core and valence electrons and treat $\alpha_p$ as fitting parameters. The values of $\alpha_p$ for each configuration of interest are presented in Table I. They are chosen to fit the experimental position of the configurations relative to each other. The value of $\alpha_p$ for the $3d^64p^2$ configuration is taken to be the same as for the ground state configuration because actual position of this configuration in the energy spectrum is not known. For all configurations the values of $\alpha_p$ are very close. This is not a surprise since the core is always the same. One can probably say that small difference in $\alpha_p$ for different configurations simulates the effect of incompleteness of the basis and other imperfections in the calculations.

A. CI calculations with a non-orthogonal basis.

As it was mentioned above we have a set of single-electron states which is not orthogonal. The 3d, 4s and 4p states in the configurations listed in Table II are similar but not the same. In principle, it may lead to complications in the CI procedure, starting from non-orthogonality of many-electron basis states which would lead in turn to complications in calculation of matrix elements and matrix diagonalization. However, most of these complications can be avoided by appropriate selection of the configurations included in the calculations. It is sufficient to obey the two rules:

- Forbidden configurations which have single-electron states taken from different sets, e.g. $3d_{i}^m3d_{j}^n4s_{k}4s_{l}$. Here $i, j, k$ and $l$ are set numbers as in Table II ($i \neq j$ or/and $k \neq l$) and $m$ and $n$ are number of electrons in each of the 3d state ($m + n = 6$).
- Don’t generate additional configurations by exciting electrons to the orbitals of the same symmetry, e.g. $3d^64s^2 \rightarrow 3d^64s^5s$.

In present calculations we use only those configurations which are listed in Table II.

If all single-electron states for every many-electron basis state are taken from the same set then the many-electron basis states remain orthogonal to each other. Indeed, states of the same configuration are orthogonal to each other as in the standard CI technique. States of different configurations are orthogonal because at least one electron changes its angular symmetry in the transition between the configurations. For example all states of the $3d^64s^2$ configuration are orthogonal to all states of the $3d^74s$ configuration because of the $s - d$ transition involved.

Since many-electron basis functions remain orthogonal matrix diagonalization is not affected. Calculation of the matrix elements between states of the same configuration is not affected as well. The only part of the CI procedure which is affected is calculation of matrix elements between basis states of different configurations. Here single electron part $\hat{h}_1$ of the Hamiltonian does not contribute because this is a scalar operator which cannot change angular symmetry of a single-electron state. Only Coulomb integrals contribute to the matrix elements and their calculation must be accomplished by the product of overlaps between similar states from different sets. For example, Coulomb interaction between the $3d^64s^2$ and $3d^64p^2$ configurations has the form (in non-relativistic notations):

$$F_1(4s_1, 4p_3, 4s_1, 4p_3)(3d_1|3d_3)^6.$$ 

Here $F_1$ is dipole Coulomb integral, indexes 1 and 3 numerate basis sets as in Table II $\langle 3d_1|3d_3 \rangle$ is the overlap between different 3d functions.

III. RESULTS AND DISCUSSION

Neutral iron is an interesting system as a challenge for the calculations and as a candidate for the search of the variation of the fine structure constant. There is strong configuration mixing between the $3d^64s^2$ and the $3d^74s$ even configurations in the ground state and the $3d^64sp$ and the $3d^74p$ configurations for the odd excited states. The latter mixing is a fortunate feature which makes Fe I a convenient object for the analysis. Let us elaborate. It is important to have relativistic frequency shifts of the atomic transitions used in the analysis to be as large as possible. The value of the shift depends on how many electrons change their states in the transitions and how large is the change of electron momentum in each single-electron transition (see, e.g. [4]). The transition between $3d^64s^2$ and $3d^64sp$ configurations is basically a $4s - 4p$ transition. However, mixing with the $3d^74s$ configuration in the upper state adds one more single-electron transition ($4s - 3d$) and makes the frequency shift larger. Note that the presence of both the $3d^64sp$ and the $3d^74p$ configurations is important. The first configuration is needed for the transition to the ground state to be strong and electric dipole transition, otherwise it will not be observed. The second configuration is needed for the relativistic frequency shift to be large. It is fortunate that strong configuration mixing between these two configurations takes place just for most of the low odd states of Fe I.

On the other hand this strong configuration mixing is a big challenge for the calculations. It makes the results for the relativistic energy shifts (the $q$-coefficients) to be unstable since they are very sensitive to the value of the mixing. Note that the configuration mixing in the ground state is also important. The admixture of the $3d^74s$ configuration adds the contribution of the $3d - 4p$ transition to the relativistic frequency shift. This contribution has an opposite sign as compared to the $4s - 4p$ transition which adds to the instability of the results.

Since configuration mixing is very sensitive to the energy intervals between the states the most reliable re-
results can be obtained in the calculations which reproduce correctly experimental spectrum. In present calculations this is achieved with the use of the core polarization term $\alpha_p$ in the Hamiltonian and fitting the data by changing the core polarizability parameter $\alpha_p$. Note however that only fine tuning was needed since in the end the values of the $\alpha_p$ for different configurations turned to be very close to each other (see Table I).

Another source of possible numerical instability of the results for particular states is level pseudo-crossing (see, e.g., [15, 16]). Energies of the states when considered as function of $\alpha^2$ may come close to each other in the vicinity of the physical value of $\alpha$. Then small error in the position of level crossing may lead to large error in the $q$-coefficient which is actually the slope of the curve $E(\alpha^2)$ (see, formula (2)). To investigate whether this is the case for Fe I we plot the energies of few low odd states of Fe I with total momentum $J = 3, 4$ and 5 as function of $\alpha^2$ from non-relativistic limit $\alpha = 0$ to the physical value of $\alpha$. The results are presented on Figs 1, 2 and 3. As can be seen from the pictures, there are multiple level crossing for states with $J = 3$ and $J = 4$. However, all these crossings take place on safe distance from the physical value of $\alpha$ and are very unlikely to cause the instability of the results. Another interesting thing to note is that the energies are practically linear functions of $\alpha^2$ in all cases.

Table II presents experimental and theoretical energies and $g$-factors of the lowest even states of Fe I. The $g$-factors are useful for the identification of the states and for control of configuration mixing [16]. As can be seen the experimental data are reproduced in the calculations with very good accuracy for both the $3d^64s^2$ and $3d^74s$ configurations.

Table III presents experimental and theoretical energies and $g$-factors of the lowest odd states of Fe I in which the $3d^64s^4p$ configuration dominates. Theoretical relativistic frequency shifts ($q$-coefficients) are also presented. The $q$-coefficients were obtained by numerical differentiation using formula (4). Note that only states with $J=3,4$ and 5, for which electric dipole transition to the ground state is possible are needed for the analysis. However, we
TABLE II: Energy levels (cm$^{-1}$) and $g$-factors of the lowest even states of Fe

| Conf. | Term | $J$ | Experiment* | Calculations |
|-------|------|-----|-------------|--------------|
|       |      |     | Energy      | $g$ Energy   | $g$          |
| $3d^74s$ | a $^2D$ | 4   | 0.000       | 1.500       | 0.000        |
|        |      | 3   | 415.932     | 1.500       | 464.1.4997   |
|        |      | 2   | 704.004     | 1.500       | 790.1.4998   |
|        |      | 1   | 888.129     | 1.500       | 1000.1.4998  |
|        |      | 0   | 978.072     |             | 1103.0.0000 |
| $3d^74s$ | a $^3F$ | 5   | 6928.266    | 1.400       | 6862.1.3996  |
|        |      | 4   | 7376.760    | 1.350       | 7374.1.3496  |
|        |      | 3   | 7728.056    | 1.249       | 7779.1.2497  |
|        |      | 2   | 7985.780    | 0.999       | 8078.1.0000  |
|        |      | 1   | 8154.710    | -0.014      | 8275.0.0000  |
| $3d^74s$ | a $^1F$ | 3   | 11976.234   | 1.254       | 13040.1.2496 |
|        |      | 2   | 12560.930   | 1.086       | 13702.1.0835 |
|        |      | 1   | 12968.549   | 0.670       | 14171.0.6676 |

*Ref. [31]

present $q$-coefficients for all states for better illustration of the accuracy of the calculations. In the linear in $\alpha^2$ approximation the difference in $q$-coefficients for states of the same fine-structure multiplet is equal to the fine structure interval between this states. As can be seen from Figs. 12 and 13 the dependence of the energies on $\alpha^2$ is very close to linear indeed. Therefore, comparing the data for the fine structure and $q$ is another test of the calculations.

Table IV presents the data similar to those of Table III but for the states where the $3d^74p$ and $3d^74s^24p$ configurations dominate. The values of the $q$-coefficients for the states of the $3d^74p$ configuration are larger than those of the $3d^74s4p$ configuration. This is due to additional contribution from the $4s - 3d$ single-electron transition as it was explained above.

It is interesting that similar to the case of the ion Fe II [16] neutral iron also has some negative shifters ($q < 0$). Corresponding states belong to the $3d^74s^24p$ configuration. Negative sign of $q$ is due to the dominant contribution from the $4p - 3d$ single-electron transition. The data are presented in Table IV. Note however that the spin of these states is different from the spin in the ground state. This means that the electric dipole transition is suppressed by conservation of spin and goes only due to relativistic effects. This in turn probably means that the transitions may be too weak to be observed.

We estimate the accuracy of present calculations of the $q$-coefficients to be on the level of 20 to 30%. The results were obtained with a very simple method which uses small number of basis functions and some semi-empirical fitting. The main challenges for more accurate calculations are strong configuration mixing and large number of valence electrons. Further development of the methods or the use of supercomputers might be needed for better accuracy of the calculations.

Table III: Energy levels (cm$^{-1}$), $g$-factors and relativistic energy shifts ($q$-factors, cm$^{-1}$) for the states of of the $3d^74s4p$ configuration of Fe.

| Term | $J$ | Experiment* | Calculations |
|------|-----|-------------|--------------|
|      |     | Energy      | $g$ Energy   | $g$          |
| $3^2D$ | 5   | 19850.892   | 1.597       | 19166.1.587  |
|       | 4   | 19562.440   | 1.642       | 19390.1.6490 |
|       | 3   | 19757.033   | 1.746       | 19611.1.7485 |
|       | 2   | 19912.494   | 2.008       | 19793.1.9776 |
|       | 1   | 20019.635   | 2.999       | 19921.2.9950 |
| $3^7F$ | 6   | 22650.421   | 1.498       | 21663.1.4997 |
|       | 5   | 22845.868   | 1.498       | 21891.1.5005 |
|       | 4   | 22996.676   | 1.493       | 22062.1.5026 |
|       | 3   | 23110.937   | 1.513       | 22189.1.5029 |
|       | 2   | 23192.497   | 1.504       | 22282.1.5026 |
|       | 1   | 23244.834   | 1.549       | 22335.1.5029 |
|       | 0   | 23270.374   | 2.236       | 23266.0.0000 |
| $3^7P$ | 4   | 23711.457   | 1.747       | 22543.1.7470 |
|       | 3   | 24180.864   | 1.908       | 23034.1.9136 |
|       | 2   | 24506.919   | 2.333       | 23440.2.3309 |
| $3^3D$ | 4   | 25899.987   | 1.502       | 26428.1.4979 |
|       | 3   | 26140.177   | 1.500       | 26679.1.4984 |
|       | 2   | 26339.691   | 1.503       | 26924.1.4976 |
|       | 1   | 26547.376   | 1.495       | 27094.1.4971 |
|       | 0   | 26550.476   | 2.714       | 27174.0.0000 |
| $3^5F$ | 5   | 26874.549   | 1.399       | 27432.1.3999 |
|       | 4   | 27166.819   | 1.355       | 27702.1.3517 |
|       | 3   | 27394.688   | 1.250       | 27947.1.2530 |
|       | 2   | 27559.581   | 1.004       | 28119.1.0041 |
|       | 1   | 27666.346   | -0.012      | 28213.0.0062 |
| $3^7P$ | 3   | 29056.321   | 1.657       | 29340.1.6643 |
|       | 2   | 29469.020   | 1.835       | 29795.1.8307 |
|       | 1   | 29732.733   | 2.487       | 30118.2.4966 |
| $3^3F$ | 4   | 31307.243   | 1.250       | 32356.1.2504 |
|       | 3   | 31805.067   | 1.086       | 32883.1.0885 |
|       | 2   | 32133.986   | 0.682       | 33263.0.6767 |
| $3^3D$ | 3   | 31322.611   | 1.321       | 32032.1.3314 |
|       | 2   | 31686.346   | 1.168       | 32464.1.1662 |
|       | 1   | 31937.316   | 0.513       | 32750.0.5035 |

*NIST, Ref. [31]

*States observed in quasar absorption spectra

IV. CONCLUSION

We have calculated relativistic frequency shifts for a number of the lower odd states of Fe I. Some of these states were observed in the quasar absorption spectra. Calculations show that due to strong configuration mixing the values of the shifts are large and vary significantly between the states. This makes Fe I to be a good candidate for the search of variation of the fine structure constant in quasar absorption spectra.
TABLE IV: Energy levels (cm$^{-1}$), $g$-factors and relativistic energy shifts ($q$-factors, cm$^{-1}$) for the states of the 3$d^74p$ and 3$d^5s^24p$ configurations of Fe

| Conf. | Term | $J$ | Experiment$^a$ | Calculations |
|-------|------|-----|----------------|--------------|
|       |      |     | Energy         | $g$ | Energy | $g$ | $g$ |
| 3$d^74p$ | $y^2D^o$ | 4 | 33995.937$^a$ | 1.496 | 32680 | 1.451 | 2494 |
|         |       | 3 | 33507.120$^b$ | 1.492 | 33134 | 1.349 | 3019 |
|         |       | 2 | 33801.567 | 1.495 | 33466 | 1.105 | 3423 |
|         |       | 1 | 34017.098 | 1.492 | 33705 | 0.168 | 3754 |
|         |       | 0 | 34121.58  | 1.492 | 34007 | 0.000 | 3723 |
| 3$d^74p$ | $y^5F^o$ | 5 | 33695.394 | 1.417 | 32522 | 1.396 | 2672 |
|         |       | 4 | 34039.513 | 1.344 | 33029 | 1.388 | 3317 |
|         |       | 3 | 34328.749 | 1.244 | 33461 | 1.377 | 3536 |
|         |       | 2 | 34547.206 | 0.998 | 33705 | 0.168 | 3754 |
|         |       | 1 | 34692.144 | -0.016 | 33909 | 0.000 | 3723 |
| 3$d^74p$ | $z^5G^o$ | 5 | 34782.416 | 1.218 | 33971 | 1.248 | 3678 |
|         |       | 6 | 34843.94  | 1.332 | 33687 | 1.333 | 3678 |
|         |       | 4 | 35257.319 | 1.103 | 34361 | 1.140 | 3520 |
|         |       | 3 | 35611.619 | 0.887 | 34661 | 0.915 | 3864 |
|         |       | 2 | 35856.400 | 0.335 | 34883 | 0.350 | 3464 |
| 3$d^74p$ | $y^3G^o$ | 5 | 35379.206 | 1.248 | 34506 | 1.220 | 3340 |
|         |       | 4 | 35767.561 | 1.100 | 35042 | 1.073 | 3697 |
|         |       | 3 | 36079.366 | 0.791 | 35474 | 0.767 | 4096 |
| 3$d^74p$ | $y^3F^o$ | 4 | 36686.164 | 1.246 | 35697 | 1.242 | 3085 |
|         |       | 3 | 37162.740 | 1.086 | 36227 | 1.086 | 3487 |
|         |       | 2 | 37521.157 | 0.688 | 35042 | 0.688 | 3697 |
| 3$d^5s^24p$ | $y^7P^o$ | 2 | 40052.030 | 2.340 | 40529 | 2.327 | 3085 |
|         |       | 3 | 40207.086 | 1.908 | 40677 | 1.888 | -2472 |
|         |       | 4 | 40421.85 | 1.75  | 40926 | 1.749 | -2287 |

$^a$NIST, Ref. [31]
$^b$States observed in quasar absorption spectra

Acknowledgments

We are grateful to Prof. P. Molaro for bringing to our attention lines of Fe observed in quasar absorption spectra. The work was funded in part by the Australian Research Council.

[1] J-P. Uzan, Rev. Mod. Phys. 75, 403 (2003).
[2] V. V. Flambaum, Int. J. Mod. Phys. A 22, 4937 (2007).
[3] J. K. Webb, V. V. Flambaum, C. W. Churchill, M. J. Drinkwater, and J. D. Barrow, Phys. Rev. Lett. 82, 884 (1999).
[4] 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).
[5] 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).
[6] M. T. Murphy, J. K. Webb, V. V. Flambaum, C. W. Churchill, and J. X. Prochaska, Not. R. Astron. Soc. 327, 1223 (2001).
[7] M. T. Murphy, J. K. Webb, V. V. Flambaum, C. W. Churchill, and J. X. Prochaska, Not. R. Astron. Soc. 327, 1237 (2001).
[8] M. T. Murphy, J. K. Webb, V. V. Flambaum, M. J. Drinkwater, F. Combes, and T. Wilmink, Not. R. Astron. Soc. 327, 1244 (2001).
[9] R. Quast, D. Reimers, and S. A. Levshakov, Astron. Astrophys. 417, L7 (2004).
[10] R. Srianand, H. Chand, P. Petitjean, and B. Aracil, Astron. Astrophys. 417, 853 (2004); Phys. Rev. Lett. 92, 121302 (2004).
[11] M. T. Murphy, J. K. Webb, and V. V. Flambaum, arXiv:astro-ph/0612407 (2006); arXiv:astro-ph/0611080 (2006); arXiv:0708.3677 (2007).
[12] R. Srianand, H. Chand, P. Petitjean, and B. Aracil, arXiv:0711.1742 (2007).
[13] V. A. Dzuba, V. V. Flambaum, and J.K. Webb, Phys. Rev. Lett., 82, 888 (1999).
[14] V. A. Dzuba, V. V. Flambaum, J.K. Webb, Phys. Rev. A59, 230 (1999).
[15] V. A. Dzuba, V. V. Flambaum, M. T. Murphy and J. K. Webb, Phys. Rev. A63, 042509 (2001).
[16] V. A. Dzuba, V. V. Flambaum, M. G. Kozlov, and M. Marchenko, Phys. Rev. A66, 022501 (2002).
[17] J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and M. V. Marchenko, Phys. Rev. A70, 064101 (2004).
[18] J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A72 044501, (2005).
[19] J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A\textbf{73} 012504, (2006).
[20] J. C. Berengut, V. A. Dzuba, V. V. Flambaum, M. V. Marchenko, J.K. Webb, M. G. Kozlov, and M. T. Murphy, arXiv:physics/0408017 (2006).
[21] S.G. Porsev, K.V. Koshelev, I.I. Tupitsyn, M.G. Kozlov, D. Reimers, and S.A. Levshakov, preprint: arXiv:0708.1662 (2007).
[22] V. A. Dzuba, and W. R. Johnson, arXiv:physics/0710.3417 (2007).
[23] I. Savukov, and V.A. Dzuba, arXiv:physics/0710.4878 (2007).
[24] P. Molaro, private communication, (2007).
[25] I. P. Grant, Comput. Phys. Commun. \textbf{84}, 59 (1994).
[26] V. A. Dzuba, V. V. Flambaum, and M.G. Kozlov, JETP Lett. \textbf{63} 882, (1996).
[27] V. A. Dzuba, V. V. Flambaum, and M.G. Kozlov, Phys. Rev. A\textbf{54} 3948, (1996).
[28] V.A. Dzuba, and W.R. Johnson, Phys. Rev. A\textbf{57} 2459, (1998).
[29] V. A. Dzuba, Phys. Rev. A, \textbf{71}, 032512 (2005).
[30] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A. \textbf{75}, 052504 (2007).
[31] Yu. Ralchenko, F.-C. Jou, D.E. Kelleher, A. E. Kramida, A. Musgrove, J. Reader, W.L. Wiese, and K. Olsen (2007). NIST Atomic Spectra Database (version 3.1.3), [Online]. Available: http://physics.nist.gov/asd3 [2007, September 18]. National Institute of Standards and Technology, Gaithersburg, MD.