

Coupled-cluster single-double calculations of the relativistic energy shifts in C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II

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The relativistic coupled-cluster single-double method is used to calculate the dependence of frequencies of strong $E1$ -transitions in many monovalent atoms and ions on the fine-structure constant α . These transitions are used in the search for manifestations of the variation of the fine-structure constant in quasar absorption spectra. Results of the present calculations are in good agreement with previous calculations but are more accurate.

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I. INTRODUCTION

Theories unifying gravity with other interactions suggest a possibility of temporal and spatial variations of the fundamental constants of nature; a review of these theories and results of measurement can be found in Ref. [1]. A very sensitive many-multiplet (MM) method to search for the variation of the fine-structure constant $\alpha = e^2/\hbar c$ by comparison of quasar absorption spectra with laboratory spectra has been suggested in Refs. [2, 3].

Using this method, strong evidence that the fine-structure constant might be smaller about ten billion years ago was found [2, 4–8]. This result was obtained from an analysis of data from the Keck telescope in Hawaii by the group based at the University of New South Wales in Australia. However, an analysis of data from the VLT telescope in Chile, performed by different groups [9, 10] using the same MM method, gave a null result. There is an outgoing debate in the literature about possible reasons for the disagreement.

The MM method requires calculation of relativistic corrections to frequencies of atomic transitions to reveal their dependence on the fine-structure constant. All calculations used in the analysis so far were performed by a single research group based at the University of New South Wales [14–20]. Owing to the importance of detecting variations of fundamental constants and the disagreement mentioned above, it is important that the related atomic calculations be verified independently.

A positive development in this direction is a recent independent calculation of the relativistic energy shifts in the ion Fe II [21]. Fe II is the single most important element in the analysis of quasar absorption spectra. It has lines which move in opposite directions when α varies; moreover, the shifts in Fe II are relatively large. In prin-

ciple, subject to sufficient statistics, Fe II alone could serve as a probe of variation of the fine-structure constant in quasar absorption spectra [21]. However, calculations for Fe II are difficult due to the large number of valence electrons.

In a recent work [22] independent calculations of the relativistic energy shifts for monovalent and divalent atoms of astrophysical interest were reported. This work also presented a detailed analysis of Breit contributions to the relativistic energy shift. Note that, despite some overlap of authors of early [14–20] and recent [21, 22] works, the later can be regarded as independent since they use completely independent sets of computer codes and different methods of calculation.

The only fully independent calculation of relativistic energy shifts was recently reported in Ref. [23]. The calculations in that work were done for heavy monovalent and divalent atoms which are mostly of interest for atomic clock experiments.

In present work, we study the role of higher-order correlations in relativistic energy shifts of monovalent atoms and ions of astrophysical interest. We use a linearized coupled-cluster method in the single-double approximation and third-order many-body perturbation theory to perform the calculations. We demonstrate that including higher-order correlations significantly improves the accuracy of the transition energies. The values of relativistic energy shifts found in the present work are in good agreement with previous calculations but are more accurate. Note also that the present work can be considered as an independent verification of earlier calculations. This is because the calculations are performed using a method that has never before been used for this purpose.

Apart from the important task of calculating relativistic energy shifts of atomic frequencies of astrophysical interest, this work can be considered as another demonstration of the power of the single-double method. It applies the method for the first time to the ions C IV and Zn II.

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II. METHOD

It is convenient to present the dependence of atomic frequencies on the fine-structure constant α in the vicinity of its physical value α_0 in the form

$$\omega(x) = \omega_0 + qx, \quad (1)$$

where ω_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

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

To calculate this derivative numerically we use

$$q \approx \frac{\omega(+\delta) - \omega(-\delta)}{2\delta}. \quad (2)$$

Here δ must be small to exclude non-linear in α^2 terms. In the present calculations we use $\delta = 0.05$, which leads to

$$q \approx 10(\omega(+0.05) - \omega(-0.05)). \quad (3)$$

To calculate the coefficients q using (3), α must be varied in our computer codes. Therefore, it is convenient to use a form of the single electron wave function in which the dependence on α is explicitly shown (we use atomic units in which $e = \hbar = 1, \alpha = 1/c$)

$$\psi(r)_{njl} = \frac{1}{r} \begin{pmatrix} f_v(r)\Omega(\mathbf{n})_{jlm} \\ i\alpha g_v(r)\tilde{\Omega}(\mathbf{n})_{jlm} \end{pmatrix}, \quad (4)$$

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 α :

$$\begin{aligned} \frac{df_v}{dr} + \frac{\kappa_v}{r} f_v(r) - [2 + \alpha^2(\epsilon_v - \hat{V}_{HF})] g_v(r) &= 0, \\ \frac{dg_v}{dr} - \frac{\kappa_v}{r} f_v(r) + (\epsilon_v - \hat{V}_{HF}) f_v(r) &= 0, \end{aligned} \quad (5)$$

here $\kappa = (-1)^{l+j+1/2}(j + 1/2)$, and \hat{V}_{HF} is the Hartree-Fock potential. Equation (5) with $\alpha = \alpha_0\sqrt{\delta + 1}$ is used to construct a full set of single-electron orbitals.

In atomic units $\alpha = 1/c$, therefore $\alpha = 0$ corresponds to the non-relativistic limit. To make sure that varying α in computer codes gives correct behavior of atomic frequencies it is important to check this non-relativistic limit. It is known, for example, that the multi-configuration Dirac-Fock (MCDF) method may fail to converge to the eigenstates of total angular momentum \hat{L} and total spin \hat{S} operators in the non-relativistic limit [24]. For atoms with one external electron, which are considered in present work, it is sufficient to demonstrate that when $\alpha = 0$ the states with the same l and n but different j ($j = l \pm 1/2$) have the same energies. We've done such a test for the heaviest element Zn II. It

turns out that for α close to zero the energies of the $4p_{1/2}$ and $4p_{3/2}$ states are the same. In our early works [14–20], the non-relativistic limit was checked for many-body perturbation theory (MBPT) and for configuration interaction (CI) calculations.

For an arbitrary value of α the calculations go through the following stages. As a first step, equation (5) is used to calculate self-consistently single-electron states of the closed-shell core. Then, this equation is used to calculate a complete set of B-spline single-electron basis orbitals. We use 40 B-splines of order $k = 9$ in a cavity of radius $40a_B$ with angular momentum l up to $l_{max} = 5$. More details on the use of B-splines in atomic calculations can be found in Ref. [25].

This basis set is used to perform calculations with the linearized couple-cluster single-double method supplemented by third-order many-body perturbation theory. The all-order single-double (SD) method was discussed before in Refs. [26–30] and third-order many-body perturbation theory was discussed in Refs. [28, 31]. We also include results from second-order MBPT to uncover the role of higher-order correlations and to estimate the numerical uncertainty due to correlations.

The SD equations are written for the coefficients of the expansion of the many-electron wave function in terms of single and double excitations from the reference Hartree-Fock wave function. They contain Coulomb integrals between single-electron basis orbitals as parameters. The equations are first solved iteratively for the atomic core. When convergence is achieved, a similar procedure for valence states of interest is performed.

Many-body perturbation theory is used to calculate the third-order diagrams missed in the SD method (E3_{extra}). Therefore, the present calculations are complete through third order, while selected classes of higher-order diagrams are included in all orders. A number of earlier calculations (see, e.g. [26–31]) prove that this approach gives very good accuracy for a wide range of monovalent atoms and ions.

The SD equations depend on the fine-structure constant only implicitly, via the values of the Coulomb integrals, which are affected by the change of the single-electron basis states (4) due to change of α in the Hamiltonian (5). In other words, changes in α lead to changes in the basis orbitals, while the SD equations remain unchanged. The same is true for terms in the MBPT expansion. However, the change of basis means that all SD and E3 calculations must be redone. The E3 calculations must be repeated from scratch, but the SD iterations can be restarted from previous calculations for a different value of α . Since the change of α is small, [see Eq. (2)] only a few iterations are needed to solve the SD equations for new value of α . This significantly speeds up the calculations.

Although the method used in present work has been used many times before, the set of computer codes used in present work is new and independent of previous versions. The main reason for developing new codes was the

need to have them in a form that allows easy modifications, as e.g. the change of the fine-structure constant in this calculations, or inserting extra operators (Breit interaction, specific mass shift operator, etc.) for future projects. Some features of the present realization of the methods are presented in the appendix. For third-order MBPT calculations, we apply a universal algorithm that uses a numerical description of the E3 MBPT diagrams and the same piece of computer code to calculate all of them. This algorithm will be described in detail elsewhere [32].

III. RESULTS

Results of calculations of energy levels of C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II are presented in Table I. Removal energies of the lowest s and p -states, which are important for the analysis of quasar absorption data, are presented in different approximations. These include the relativistic Hartree-Fock approximation (RHF), second-order many body perturbation theory (E2), single-double (SD) approximation, and SD supplemented by third-order many-body perturbation theory (SD+E3). For each approximation the difference between theoretical and experimental energies is presented in the columns headed Δ .

The Mg II, Al III, and Si IV ions represent an isoelectronic sequence of sodium. This sequence was considered in detail in Ref. [28]. The results of present work are in good agreement with previous calculations. Some small difference can be attributed to the difference in numerical procedures and numerical parameters (such as the number of splines, the cavity radius, maximum angular momentum, etc.)

The results in Table I show that correlations are large and are strongly dominated by second-order MBPT. However, inclusion of higher-order correlations is important and leads to a significant reduction in the differences between theoretical and experimental energies. The inclusion of the E3_{extra} terms lead to some further improvement of accuracy for all systems except Zn II. Here these contributions are extremely large and lead to a change in sign of the difference between theory and experiment, while its value remains close to those in the SD approximation. This indicates poor convergence of MBPT as well as the importance of the higher-order terms not included in the SD approximation. However, as will be shown below, the q -coefficients are much less sensitive to higher-order correlations and comparison of the results in the SD and SD+E3 approximations gives an estimate of the numerical error.

Table II presents relativistic energy shifts (q coefficients) in the same approximations as the energies in Table I. One can see that the role of correlations is much less important for the q -coefficients than for energies. While second-order correlations give some rather small contribution to q , contributions from higher-order

correlations are practically negligible in most cases. Only for Zn II the higher-order contributions are significantly larger than the uncertainty of the calculations. Thus, calculations of the q -coefficients are more stable than the calculations of energies and, consequently, more accurate.

Breit corrections to the frequencies of the transitions considered in present paper were calculated in Ref. [22]. These corrections are larger than the uncertainty of the q -coefficients from omitted higher-order correlations. Therefore, they must be included for accurate results. Table III summarizes all significant contributions. The Dirac contributions in this Table are based on averaging the SD and SD+E3 approximations from Table II. Breit corrections are taken from Ref. [22].

Our final results are presented in Table IV. An estimate of the numerical uncertainty is also given and results are compared with previous calculations. There are two sources of numerical uncertainty. One is omission of certain higher-order correlations and numerical accuracy of the SD and SD+E3 calculations. This uncertainty was estimated by comparing the results in the SD and SD+E3 approximations. Another source of uncertainty is the accuracy of calculation of Breit contribution. Breit contributions are calculated very accurately within the relativistic Hartree-Fock approximation (see Ref. [22] for details). The only uncertainty which may come from the Breit interaction is due to the fact that correlation corrections to the Breit interaction are ignored. However, these contributions are small for the relatively light atoms considered in present paper. A strong argument that the Breit contribution is calculated sufficiently accurately was presented in Ref. [22], where it was demonstrated that the inclusion of the Breit interaction brings the theoretical fine-structure intervals into perfect agreement with experiment. We use a rather conservative estimate of 20% for the accuracy of the calculations of Breit contributions.

Table IV also presents results from previous calculations. All previous calculations were done in second-order of MBPT. The work of Ref. [22] also included Breit corrections. Results of the present paper are in excellent agreement with this work. Some difference for Zn II is due to higher-order correlations. The results are also in good agreement with early calculations compiled together in Ref. [20]. The principal sources of the small differences between the present results and those of Ref. [20] are Breit and higher-order correlation corrections.

IV. CONCLUSIONS

In the present work, we studied the role of higher-order correlations on relativistic energy shifts of atomic frequencies used in the search for variations of the fine-structure constant in quasar absorption spectra. We have demonstrated that the higher-order correlations are important for energies, bringing theoretical values into better agreement with experiment. However, higher-order

TABLE I: Removal energies of the lowest s and p states of C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II in different approximations, comparison with experiment (cm^{-1}).

Atom	Z	State	RHF	E2	Δ^a	SD	Δ^a	SD+E3	Δ^a	Expt ^b
C IV	6	$2s$	519255	520189	11	520233	55	520231	53	520178
		$2p_{1/2}$	454054	455640	-54	455732	38	455727	33	455694
		$2p_{3/2}$	453927	455509	-78	455600	13	455595	8	455587
Na I	11	$3s$	39952	41229	-220	41437	-12	41450	1	41449
		$3p_{1/2}$	24030	24412	-81	24486	-7	24489	-4	24493
		$3p_{3/2}$	24014	24394	-82	24468	-8	24471	-5	24476
Mg II	12	$3s$	118824	121076	-192	121278	10	121273	5	121268
		$3p_{1/2}$	84294	85453	-145	85585	-13	85586	-12	85598
		$3p_{3/2}$	84204	85357	-150	85488	-19	85489	-18	85507
Al III	13	$3s$	226396	229319	-127	229489	43	229464	18	229446
		$3p_{1/2}$	173687	175608	-155	175751	-12	175741	-22	175763
		$3p_{3/2}$	173452	175361	-168	175504	-25	175494	-35	175529
Si IV	14	$3s$	360614	364033	-60	364172	79	364132	39	364093
		$3p_{1/2}$	290074	292667	-139	292802	-4	292780	-26	292806
		$3p_{3/2}$	289606	292183	-161	292317	-27	292296	-48	292344
Ca II	20	$4s$	91440	96173	425	96097	349	95577	-171	95748
		$4p_{1/2}$	68037	70680	123	70761	204	70491	-66	70557
		$4p_{3/2}$	67837	70449	115	70529	195	70262	-72	70334
Zn II	30	$4s$	135134	143835	-1055	144618	-272	145334	444	144890
		$4p_{1/2}$	90524	95249	-1161	96184	-226	96613	203	96410
		$4p_{3/2}$	89787	94372	-1164	95311	-225	95728	192	95536

^a $\Delta = E_{\text{calc}} - E_{\text{expt}}$

^bNIST, Ref. [33]

TABLE II: Relativistic energy shifts (q -coefficients, see Eq. (1) for the lowest s and p states of C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II in different approximations (cm^{-1})).

Atom	Z	State	RHF	E2	SD	SD+E3
C IV	6	$2s$	243	244	244	244
		$2p_{1/2}$	139	141	142	142
		$2p_{3/2}$	11	10	10	10
Na I	11	$3s$	51	57	59	59
		$3p_{1/2}$	12	13	13	13
		$3p_{3/2}$	-5	-5	-6	-5
Mg II	12	$3s$	181	193	194	194
		$3p_{1/2}$	70	74	74	74
		$3p_{3/2}$	-20	-23	-23	-23
Al III	13	$3s$	405	421	422	422
		$3p_{1/2}$	197	203	203	203
		$3p_{3/2}$	-39	-45	-45	-44
Si IV	14	$3s$	753	773	774	774
		$3p_{1/2}$	416	425	425	425
		$3p_{3/2}$	-54	-62	-62	-61
Ca II	20	$4s$	354	396	394	392
		$4p_{1/2}$	161	176	176	175
		$4p_{3/2}$	-41	-58	-59	-56
Zn II	30	$4s$	2352	2863	2873	2910
		$4p_{1/2}$	990	1271	1333	1359
		$4p_{3/2}$	224	354	412	427

TABLE III: Contributions to the relativistic energy shifts (q -coefficients, see Eq. (1) for the s - p transitions in C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II (cm^{-1}))

Atom	Z	Transition	Dirac ^a	Breit ^b	Total
C IV	6	$2s - 2p_{1/2}$	102	13	115
		$2s - 2p_{3/2}$	234	-12	222
Na I	11	$3s - 3p_{1/2}$	46	-1	45
		$3s - 3p_{3/2}$	64	-2	62
Mg II	12	$3s - 3p_{1/2}$	120	1	121
		$3s - 3p_{3/2}$	217	-5	212
Al III	13	$3s - 3p_{1/2}$	219	5	224
		$3s - 3p_{3/2}$	467	-9	458
Si IV	14	$3s - 3p_{1/2}$	348	13	361
		$3s - 3p_{3/2}$	835	-12	823
Ca II	20	$4s - 4p_{1/2}$	218	3	222
		$4s - 4p_{3/2}$	450	-4	446
Zn II	30	$4s - 4p_{1/2}$	1546	-5	1541
		$4s - 4p_{3/2}$	2472	-20	2452

^aThis work, see Table II

^bSavukov and Dzuba, Ref. [22]

previous calculations but are more accurate.

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correlations give very small contributions to the relativistic energy shifts (q -coefficients) in all cases except Zn II. Results of the present work are in good agreement with

TABLE IV: Relativistic energy shifts (q -coefficients, see Eq. (1) for the $s - p$ transitions in C IV, Na I, Mg II, Al III, Si IV, Ca II and Zn II (cm^{-1}); comparison with other calculations.

Atom	Z	Transition	This work	Other
			Savukov ^a	Berengut ^b
C IV	6	$2s - 2p_{1/2}$	115(2)	115
		$2s - 2p_{3/2}$	222(2)	232(20)
Na I	11	$3s - 3p_{1/2}$	45(0)	44
		$3s - 3p_{3/2}$	62(0)	63(4)
Mg II	12	$3s - 3p_{1/2}$	121(1)	120
		$3s - 3p_{3/2}$	212(1)	211
Al III	13	$3s - 3p_{1/2}$	224(1)	223
		$3s - 3p_{3/2}$	458(2)	464(30)
Si IV	14	$3s - 3p_{1/2}$	361(2)	360
		$3s - 3p_{3/2}$	823(2)	862
Ca II	20	$4s - 4p_{1/2}$	222(1)	222
		$4s - 4p_{3/2}$	446(3)	450
Zn II	30	$4s - 4p_{1/2}$	1541(7)	1584(25)
		$4s - 4p_{3/2}$	2452(13)	2488
				2479(25)

^aSecond-order+Breit, Ref. [22]

^aSecond-order, compilation of previous results presented in Ref. [20]

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APPENDIX A: EFFICIENT WAY OF CALCULATING THE SD AND MBPT TERMS

The coupled-cluster SD method combined with MBPT has led to an accurate description of many properties of monovalent atoms; however, it is very demanding computationally. For example, for Zn II the total number of single-electron basis states used in present calculations is 319. The total number of non-zero distinctive Coulomb integrals is about 1.7×10^8 . All of them are used in both, the SD equations and the MBPT expansion. Calculating all Coulomb integrals in advance and keeping them in computer memory is practically impossible due to huge demand for computer memory. On the other hand, calculation of Coulomb integrals from single-electron basis

functions every time they are needed makes the calculations unacceptably slow. This is even more so in the case of the relativistic energy shifts considered in present paper, since we need to run all relevant codes several times for several different values of the fine-structure constant α .

To improve the efficiency of the codes, we use an approach in which Hartree screening functions Y rather than Coulomb integrals are calculated in advance and kept in memory for efficient calculation of Coulomb integrals (a similar approach was used in Ref. [34]). The Hartree screening function Y is defined as

$$Y_{knm}(r) = \int \frac{r_<^k}{r_>^{k+1}} (f_n(r') f_m(r') + \alpha^2 g_n(r') g_m(r')) dr', \quad (\text{A1})$$

where $r_< = \min(r, r')$ and $r_> = \max(r, r')$. We also need the ρ functions:

$$\rho_{jl}(r) = f_j(r) f_l(r) + \alpha^2 g_j(r) g_l(r). \quad (\text{A2})$$

Our typical coordinate grid consists of about 1000 points. Usually all points are used to calculate $Y_{knm}(r)$. However, there is no need to keep all points for successive calculations of the Coulomb integrals. It turns out that very little loss of accuracy is caused by using a subset of points defined as every 4th point in the interval $1/Z \leq r \leq R_{\text{cavity}}$, where R_{cavity} is the radius of the cavity in which the B -splines basis orbitals are defined. By cutting off points at short distances and using only every 4th point in between we reduce the number of points by an order of magnitude. Then, the Coulomb integrals are calculated in an extremely efficient way as

$$q_k(jlmn) = \sum_{i=1}^{\mu} \rho_{jl}(r_i) Y_{kmn}(r_i) w_i. \quad (\text{A3})$$

Here $\mu \approx 100$ is number of points on the sub-grid and w_i are weight coefficients corresponding to a particular method of numerical integration. Note that only one of two integrations for Coulomb integrals is done on a reduced sub-grid. The initial integration (A1) is done using all grid points.

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