

Relativistic calculation of the $2^1S_0-2^1,3P_1$ transitions in berylliumlike molybdenum and berylliumlike iron

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The $2^1,3P_1-2^1S_0$ transitions in berylliumlike molybdenum and berylliumlike iron have been calculated including all-order relativistic correlations due to the Coulomb as well as the Breit interaction. Important correlation corrections to the radiative contributions to the ground state were found due to the large admixture of p^2 character in the 2^1S_0 wave function. Comparison with experiment is done after the addition of the Lamb shift for the corresponding hydrogenlike systems and an estimate of the screening caused by the $1s^2$ electrons. The results of Mo^{38+} are $725\,751\pm 300$ and $2\,004\,464\pm 300\text{ cm}^{-1}$ for the $2^1S_0-2^3P_1$ and $2^1S_0-2^1P_1$ transitions, respectively, which agree well with the experimental results $725\,758\pm 158$ and $2\,003\,847\pm 1200\text{ cm}^{-1}$. The corresponding results for Fe^{22+} are $379\,118\pm 90$ and $752\,459\pm 90\text{ cm}^{-1}$, which can be compared to the experimental values $379\,140\pm 20$ and $752\,372\pm 57\text{ cm}^{-1}$. The uncertainty in the theoretical value is completely dominated by the uncertainty in the evaluation of the radiative effects in the electronic field.

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I. INTRODUCTION

Recent years have seen a development of methods to treat many-body systems completely relativistically. Among the driving forces behind this development are experiments made on highly charged ions. Calculations of an accuracy comparable to experiments are needed in order to obtain information about, e.g., QED effects in intense Coulomb fields.

Relativistic calculations have been performed for helium and heliumlike systems by several groups [1–5] and for some of the alkali-metal sequences [6–8] among them the lithiumlike sequence inspired especially by the experiments of lithiumlike uranium [9]. Berylliumlike systems constitute the simplest real many-body system, and the excited states involve two open shells, which makes the theoretical treatment rather different compared to alkali-metal-like systems. While Li-like systems are well represented using third-order Coulomb correlation and second-order Breit correlation [6] this is not expected to be enough for the Be sequence. Several experiments have been made on berylliumlike systems, Denne *et al.* [10] list results for the $2S_0-2^1,3P_1$ transitions in nine elements from titanium to molybdenum. Comparison was in Ref. [10] made with semiempirical calculations by Edlén [11].

The position as the simplest, more general, many-body system has led to a number of extensive calculations of the ground state of neutral beryllium. A classical work, using the configuration-interaction (CI) method, was done by Bunge [12] and later a number of approximation schemes have been tested on this system as reviewed in a recent publication by Mårtensson-Pendrill *et al.* [13]. Very recently relativistic calculations have also been made [14,15]. The present calculation on Fe^{22+} and Mo^{38+} is to our knowledge the only attempt on highly charged berylliumlike ions. It will be followed by calculations on other elements.

The calculation uses the relativistic coupled-cluster approach implemented by Salomonson and Oster [5,16] and includes correlation due to the Coulomb interaction iterated to all orders. By an extension of the program, the correlation due to the Breit interaction, mixed with the Coulomb interaction in all orders, is also included. Together with results presented in Refs. [15,17] the present work constitutes to our knowledge the only relativistic all-order calculation of the Breit interaction.

The two $2P_1$ states include a linear combination of the $2s2p_{1/2}$ and $2s2p_{3/2}$ configurations. Rather than approximating a certain P_1 state with only one of these, and including the admixture of the other in the perturbation expansion, the lowest-order approximation is initially described by a sum of these configurations. The perturbation expansion is then made from an “extended model space” [18]. The formalism for this treatment has been described and applied in a nonrelativistic calculation on the ground state of neutral beryllium by Lindgren *et al.* [19]. This treatment has the advantage that configurations with very close energies are removed from the perturbation expansion, thus small-energy denominators are avoided, and the expansion converges rapidly. Another advantage is that certain effects, involving the other $2s2p$ configuration, which normally would be classified as three-particle effects, in this approach is obtained already at the level of singles and doubles. The many-body calculation is described in more detail in Sec. II.

The QED effects for the corresponding hydrogenlike system is taken from the literature [20]. The evaluation of radiative effects in the electronic field is still, at least in practice, an unsolved problem. For Be-like systems there are two major many-body corrections to the Lamb shift. The first correction is the screening of the nuclear field by the presence of the $1s^2$ core electrons. The other effect is the large admixture of p^2 configurations in the ground-state wave function which has a considerably smaller

Lamb shift than the dominating $2s^2$ configuration. While the second effect is obtainable from a combination of the present calculation and Ref. [20], the first effect can only be approximated [8,21]. We add the screening obtained for the corresponding lithiumlike system in [8] before comparing with experiments and emphasize that the major uncertainty in the calculation arise from this effect. Retardation effects, beyond what is already included in the Breit interaction, are evaluated in first order using the GRASP code [22].

II. CALCULATION OF MANY-BODY EFFECTS

As described by Salomonson and Öster [5], the atom is placed in a spherical box, large enough not to influence the property studied. Inside the box a discrete radial grid is used. Diagonalization of a discretized one-particle Hamiltonian yields a discrete basis set, complete on the grid chosen, which is used to describe the physical states.

The calculation of the $2P_1$ states uses an extended model space and can be explained in the following way: The two P_1 states are dominated by antisymmetric combinations of the two $2s2p$ configurations and, in lowest order, we write the wave functions as

$$\begin{aligned}\Phi_1^0 &= \{ |2s2p_{1/2}\rangle_{J=1} \}, \\ \Phi_2^0 &= \{ |2s2p_{3/2}\rangle_{J=1} \},\end{aligned}\quad (1)$$

where the curly brackets denote antisymmetrization. The radial parts of the wave functions are antisymmetric and symmetric, respectively. The usual approach is now to let, e.g., the 3P_1 state be represented by Φ_1^0 in lowest order, i.e., the model space consists of only one configuration. An effective Hamiltonian is then constructed which works only on Φ_1^0 and the eigenvalue of the effective Hamiltonian is, in principle, the exact energy of the 3P_1 state, as described by Lindgren and Morrison [23]. The admixture of the $2s2p_{3/2}$ configuration is, in this approach, included in the effective Hamiltonian, i.e. in the perturbation expansion. Correspondingly, the 1P_1 state is in lowest order represented by Φ_2^0 . In this work we use instead a model space consisting of both Φ_1^0 and

Φ_2^0 and the effective Hamiltonian works in the space spanned by these states. The two eigenvalues of h_{eff} are the exact energies of the two P_1 states. The effective Hamiltonian is formally written as [19,23]

$$H_{\text{eff}} = PH\Omega P \equiv PH_0P + PV\Omega P, \quad (2)$$

where P is the projection operator onto the model space, in this case spanned by Φ_1^0 and Φ_2^0 , and Ω is the wave operator which transforms the model functions into the exact ones. The full Hamiltonian, H , is partitioned into a zeroth-order Hamiltonian H_0 , of which Φ_1^0 and Φ_2^0 are eigenstates, and a perturbation V . For the present problem the effective operator can be written as

$$H_{\text{eff}} = \begin{pmatrix} \langle \Phi_1^0 | H_0 + V\Omega | \Phi_1^0 \rangle & \langle \Phi_1^0 | V\Omega | \Phi_2^0 \rangle \\ \langle \Phi_2^0 | V\Omega | \Phi_1^0 \rangle & \langle \Phi_2^0 | H_0 + V\Omega | \Phi_2^0 \rangle \end{pmatrix}. \quad (3)$$

The eigenvectors of H_{eff} are projections onto the model space of certain eigenvectors of the complete Hamiltonian. Since the eigenvectors of H_{eff} are projections of orthogonal vectors onto a smaller space, they are normally not orthogonal and the effective Hamiltonian is not Hermitian, which can be seen explicitly in (4) and (5) below.

H_0 in Eqs. (2) and (3) is chosen here to be the Dirac-Fock-Breit Hamiltonian, a generalization of the Dirac-Fock Hamiltonian which includes the Breit interaction on the same footing as the Coulomb interaction [24]. The Breit interaction includes magnetic interaction as well as the retardation of the electromagnetic field in the low-energy limit. Retardation effects beyond the low-energy limit are treated in first-order only. In order to see the effect of the Breit interaction, the difference between the use of the Dirac-Fock and the Dirac-Fock-Breit Hamiltonian is given in Table I. Only the $1s$ electrons are included in the Dirac-Fock (-Breit) potential. The interaction with and among the outer $2s^2$ or $2s2p$ electrons is included by means of the perturbation expansion.

The perturbation, V , describes the correlation between the electrons due to the Coulomb as well as to the Breit interaction. Also, mass polarization and certain radiative effects are included in V as described below. The wave operator, Ω , includes all double and single excitations as

TABLE I. Binding energies of the valence $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$ electrons in lithiumlike Fe and Mo. These enter in the diagonal elements in the matrix H_{eff} in (3)–(5). The results are given in atomic units for ^{56}Fe and ^{98}Mo .

	Fe^{22+}			Mo^{38+}		
	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
Dirac-Fock orbital energy	−75.211 66	−73.419 69	−72.812 98	−210.135 96	−206.957 88	−202.235 47
Dirac Fock Breit	0.020 24	0.039 54	0.017 64	0.092 77	1.185 80	0.081 24
Retardation beyond Breit ^a	0.000 04	−0.000 05	−0.000 39	0.000 51	−0.000 51	−0.004 49
Lamb shift (hydrogenlike) ^b	0.019 91	−0.000 55	0.001 08	0.103 05	−0.00146	0.008 77
Mass polarization	0.000 00	−0.000 46	−0.000 45	−0.000 00	−0.000 81	−0.000 73
Coulomb correlation	−0.006 66	−0.013 37	−0.012 60	−0.007 15	−0.015 22	−0.012 92
Breit correlation	−0.000 59	−0.000 55	−0.000 39	−0.001 47	−0.001. 64	−0.001 03
Total	−75.178 72	−73.395 13	−72.808 07	−209.948 15	−206.791 73	−202.164 63

^aExpectation value obtained from the GRASP code [22].

^bResults from Johnson and Soff [20] corrected for field shift since extended-nucleus effects are included in the Dirac-Fock- (Breit) value.

described in [16].

The energies of the berylliumlike systems are calculated relative to the corresponding lithiumlike systems. The result is obtained as the sum of one-particle contributions, i.e., the binding energies of the $2s$, $2p_{1/2}$, or $2p_{3/2}$ electrons in the lithiumlike system, and two-particle contributions which involve both the outer electrons. The former contribute only in the diagonal elements in Eq. (3) while the latter enter in all four elements.

III. RADIATIVE CORRECTIONS

The Lamb shift for hydrogenlike Mo and Fe is taken from [20], corrected for the field shift since the present calculation is done with an extended nucleus. The use of the hydrogenlike value, obtained with $Z=42$, respectively, $Z=26$, is, however, quite misleading for the outer electrons. An important neglected effect is that the two $1s$ electrons will shield approximately two units of charge of the nuclear field. To obtain a more realistic description, some estimation of this screening of the Lamb shift has to be made. There is still no method presented with which radiative corrections can be joined with a many-body calculation starting from first principles. Cheng *et al.* [21] have very recently published calculations of a few heavy ions where a first-principles Lamb shift calculation is performed with the nuclear potential replaced by a more realistic local potential. Although this procedure is not completely satisfying, it will certainly give the dominating part of the screening. In a number of calculations, Indelicato and Desclaux [1,8] have used the observation that, in the nonrelativistic limit, the Lamb shift for an s electron is proportional to the density of charge at the nucleus, to estimate the screened self-energy as the ratio between the expectation value of the charge density obtained with screened functions and with hydrogenlike functions multiplied with the hydrogenlike result from Ref. [20]. This approximation should at least give the correct order of magnitude of the effect. The vacuum po-

larization, which can be expressed as expectation values of conventional potentials, is calculated from first principles. Screening corrections to the Lamb shift are illustrated in Fig. 1(a).

A. Berylliumlike molybdenum

The dominating effect caused by the presence of the $1s$ electrons is given as a shift of the binding energy of the corresponding lithiumlike system. The results for $Z=42$ from [8] can then be added to the present work before comparing with experiment. When the hydrogenic results are subtracted from the QED effects given in [8], the screening is found to increase the energy difference with 0.00755 a.u. for the $2p_{1/2}-2s$ transition, which dominates the $2^3P_1-2^1S_0$ transition, and with 0.00673 a.u. for the $2p_{3/2}-2s$ transition, which instead dominates the $2^1P_1-2^1S_0$ transition.

The only lithiumlike system calculated in Ref. [21] is U^{89+} . If the screening of the self-energy and the vacuum polarization obtained for this system is compared with the result for the same system in Ref. [8], it is seen that the latter is about 17% larger. A difference of that order of magnitude could probably be expected for the systems considered here as well. Although none of the methods can be supposed to give a final answer for the screening, the difference can be viewed as a hint about the uncertainty in the predictions in Ref. [8]. Thus, the uncertainty is estimated to ± 0.00130 and ± 0.00115 a.u. for the $2p_{1/2}-2s$ and the $2p_{3/2}-2s$ transition, respectively, which is around twice the experimental accuracy for the $2^3P_1-2^1S_0$, but well below it for $2^1P_1-2^1S_0$.

There is, however, also many-body corrections to the Lamb shift in Be-like systems which are not present in Li-like systems. The most important of these applies to the 2^1S_0 state and is due to the large admixture of p^2 configurations in the wave function. Around 3% of the probability density comes from p^2 configurations which have a much smaller Lamb shift than the dominating $2s^2$ configuration and the Lamb shift contribution will decrease with the same fraction. Thus, a contribution of -0.00587 is added to the 2^1S_0 state. We note that this corresponds to the addition of certain backward diagrams, illustrated in Fig. 1(b), in the coupled-cluster expansion [23] and is not a departure from first principles. The uncertainty given for the screening effects above should also cover the uncertainty due to additional many-body effects.

B. Berylliumlike iron

For berylliumlike iron, the screening deduced from [8] is found to increase the energy difference with 0.00277 ± 40 a.u. for the $2^3P_1-2^1S_0$ transition and with 0.00204 ± 35 a.u. for the $2^1P_1-2^1S_0$ transition. The errors are estimated as for molybdenum. For both the transitions this uncertainty is larger than the experimental error.

The admixture of p^2 configurations in the 2^1S_0 ground-state configuration is larger than for berylliumlike molybdenum, around 5% of the probability density.

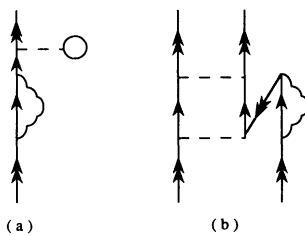


FIG. 1. Examples of diagrams which describe many-body corrections to the radiative effects. (a) illustrates an important contribution to the screening of the Lamb shift. (b) is a backward, or folded, diagram which involves the radiative corrections. It is only important for the 2^1S_0 state and accounts for the main part of the difference in the Lamb shift contribution to the true 2^1S_0 state as compared to when it is described by a pure $2s^2$ configuration. The large admixture of p^2 configurations into the 2^1S_0 state of berylliumlike systems explains the importance of this effect. Valence states are indicated with double arrows and excited states with single arrows. The dotted lines represent the Coulomb interaction.

This is mainly because the $2p$ orbital energies are relatively closer to the $2s$ energy in berylliumlike Fe. The Lamb shift is, however, smaller. This results in a contribution to the 2^1S_0 state of -0.00195 a.u. from correlation corrections to the Lamb shift.

IV. RESULTS

The results are summarized in Tables I–III. In Table I terms which involve only one of the valence electrons are listed. These terms are referred to as one-particle contributions and are the same as for the corresponding lithiumlike system. The two first lines give together the eigenvalue of H_0 ; the Breit interaction has been separated out for comparison. The retardation beyond the Breit interaction is the difference between the first-order expectation value of the energy-dependent form of the contribution from exchange of transverse photons [25,26] and the Breit interaction, which is the low-energy limit of the full expression. This difference is obtained with the GRASP code [22]. The Lamb shift is the value listed in [20]. The

correlation contributions in Table I are dominated by Brueckner effects which contribute in second order and beyond. Again, the Coulomb and Breit contributions are given separately.

The mass polarization is treated with the Hughes-Eckart formula [27]. Only the Dirac-Fock value is considered. There is no important contribution involving both the outer electrons since the lowest-order term is proportional to the square of the differences in orbital energy for the involved electrons. Due to the near degeneracy of the $2s$ and $2p$ states, the result is smaller than 1×10^{-5} . There is no first-order contribution for the 2^1S_0 state of either one- or two-particle type.

In Table II, terms involving two valence electrons, referred to as two-particle effects, are given. The result for the Coulomb part of the perturbation is evaluated with eigenstates to the Dirac-Fock Hamiltonian as well as the Dirac-Fock-Breit Hamiltonian in order to separate the effects. The interelectronic distance, $1/r_{12}$, in the Coulomb as well as in the Breit interaction is expanded in partial waves and angular momenta from zero to five are included for berylliumlike Mo. The contributions from

TABLE II. Two-particle contributions to $\langle \phi | V\Omega | \phi \rangle$, see Sec. II and especially Eq. (3) for explanation, to the $(2s^2)^1S_0$, $(2s2p_{1/2})^3P_1$, and $(2s2p_{3/2})^1P_1$ states of berylliumlike molybdenum and iron. Angular momenta up to six are included for the Coulomb interaction in Fe^{22+} , otherwise angular momenta up to five are used. Estimations of the contributions from higher angular momenta are indicated. Results are given in atomic units.

	Fe^{22+}		Mo^{18+}	
1S_0				
Coulomb interaction	3.469 64		5.980 61	
Difference obtained with DF-Breit orbitals	-0.000 30		0.000 79	
Breit interaction	0.001 94		0.011 57	
Correlation correction to the Lambshift ^a	-0.001 96		-0.006 05	
Difference obtained with DF-Breit orbitals	0.000 01		0.000 18	
Total	3.469 33		5.987 09	
Contributions from higher angular momenta	-0.000 10±0.000 05		-0.000 31±0.000 15	
$^{1,3}P_1$				
	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$
Coulomb interaction	3.739 80	-0.670 14	6.366 52	-1.134 60
Difference obtained with DF-Breit orbitals	-0.001 67	0.000 14	-0.004 66	0.000 36
Breit interaction	-0.000 32	-0.000 34	-0.001 35	-0.001 94
Total	3.737 80	-0.670 34	6.360 51	-1.136 18
Contributions from higher angular momenta	-0.000 12±0.000 06	0.000 17±0.000 09	-0.000 19±0.000 10	0.000 28±0.000 015
	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$	$\langle \phi^0 V\Omega \phi^0 \rangle$
Coulomb interaction	-0.670 43	4.195 89	-1.135 44	7.084 51
Difference obtained with DF-Breit orbitals	0.000 15	-0.001 17	0.000 38	-0.003 25
Breit interaction	-0.000 35	0.003 65	-0.002 00	0.018 07
Total	-0.670 63	4.198 36	-1.137 06	7.099 32
Contributions from higher angular momenta	0.000 16±0.000 08	-0.000 28±0.000 014	0.000 29±0.000 15	-0.000 46±0.000 025

^aIllustrated in Fig. 1(b).

TABLE III. Comparison of theory to experiment for the $2^1,3P_1-2^1S_0$ transition in berylliumlike iron and molybdenum.

	Fe^{22+}		Mo^{38+}	
	Theory	Experiment ^a	Theory	Experiment ^b
$2^3P_1-2^1S_0$				
This work (a.u.) ^c	1.725 13±0.000 07		3.299 24±0.000 20	
Screening of the Lamb shift (a.u.) ^d	0.002 27±0.000 40		0.007 55±0.001 30	
Total (a.u.)	1.727 40±0.000 41		3.306 79±0.001 35	
Total (cm ⁻¹)	379 118±90	379 140±20	725 751±300	725 758±158
$2^1P_2-2^1S_0$				
This work (a.u.) ^c	3.426 45±0.000 20		9.126 33±0.000 30	
Screening of the Lamb shift (a.u.) ^d	0.002 04±0.000 35		0.006 73±0.001 15	
Total (a.u.)	3.428 49±0.000 40		9.133 06±0.001 20	
Total (cm ⁻¹)	752 459±90	752 372±57	2 004 464±300	2 003 847±1200

^aHinnov [28].

^bDenne *et al.* [10].

^c1 a.u. (⁹⁸Mo)= $2.194\,734 \times 10^5 \text{ cm}^{-1}$ using the value $R_M=10\,9736.7 \text{ cm}^{-1}$ ($M=97.9055$) for the Rydberg constant. 1 a.u. (⁵⁶Fe)= $2.194\,725 \times 10^5 \text{ cm}^{-1}$ using the value $R_M=109\,736.2 \text{ cm}^{-1}$ ($M=55.9349$) for the Rydberg constant.

^dIndelicato and Desclaux [8].

higher angular momenta are of the order a few digits in the fourth decimal and can be approximated by extrapolation. Since this is a minor error compared to the uncertainty in the radiative effects and also smaller than the experimental error, only an estimate of the extrapolation contribution has been made. For berylliumlike iron, the experimental error bars are smaller [28] and, in addition, the Lamb shift is less important leading to a smaller uncertainty due to uncalculated many-body corrections to the Lamb shift. A more careful investigation has then been made of the effects on the Coulomb correlation from higher angular momenta. Angular momenta up to six are included and the results from calculations with angular

moment up to four, five, and six are used to extrapolate the result leading to an uncertainty of around five units in the fifth decimal, apart from the 2^1P_1 state where it is somewhat larger. The expected error in the given contributions from the partial-wave expansion is then of the same order of magnitude as the experimental error. It should be noted that this theoretical uncertainty can be further reduced if needed. The pure numerical uncertainty is well below the experimental accuracy, about one unit in the fifth decimal.

The effective Hamiltonian for the $2P_1$ states of the berylliumlike ions relative the $1s^2s$ state of the lithium-like ions can now be written

$$H_{\text{eff}}^{\text{Mo}^{38+}} = \begin{pmatrix} -206.791\,73 + 6.360\,51 - 0.000\,19 & -1.136\,18 + 0.000\,28 \\ -1.137\,06 + 0.000\,29 & -202.164\,63 + 7.099\,32 - 0.000\,46 \end{pmatrix} \quad (4)$$

and

$$H_{\text{eff}}^{\text{Fe}^{22+}} = \begin{pmatrix} -73.395\,13 + 3.737\,80 - 0.000\,12 & -0.670\,34 + 0.000\,17 \\ -0.670\,63 + 0.000\,16 & -72.808\,07 + 4.198\,36 - 0.000\,28 \end{pmatrix}, \quad (5)$$

where the results from Tables I and II have been inserted in Eq. (3). The first term in each of the diagonal elements is the sum of the one-particle contributions as given in Table I. The second term in the diagonal elements as well as the first term in the nondiagonal elements are the two-particle contributions from Table II. The last number in every element is the approximation of the contributions from higher angular momenta in the partial-wave expansion.

For berylliumlike molybdenum, diagonalization of (4) gives a binding energy of $-200.662\,13 \pm 0.000\,09$ a.u. for 2^3P_1 and $-194.835\,04 \pm 0.000\,25$ a.u. for the 2^1P_1 state relative to the first ionization limit, while the binding energy for the last electron is $-203.961\,37 \pm 0.000\,15$ for

the 2^1S_0 state. The errors refer to the partial-wave expansion.

Diagonalization of (5) gives the corresponding results from berylliumlike iron: $-69.984\,38 \pm 0.000\,03$ a.u. for 2^3P_1 and $-68.283\,06 \pm 0.000\,20$ a.u. for 2^1P_1 . The binding energy for the last electron in the 2^1S_0 state is $-71.709\,51 \pm 0.000\,06$.

Before a comparison can be made with experiment, we have to consider the uncalculated many-body corrections to the Lamb shift. The most important of these is the screening due to the presence of the $1s$ electrons, as discussed in Sec. III. An estimate of this effect can be found in [8]. The comparison with experiment is shown in Table III.

V. CONCLUSIONS

The calculation agrees well with experiment. The uncertainty in the theoretical value arises predominantly in the approximation of radiative many-body effects and a proper treatment of the screened self-energy would reduce the theoretical error bars significantly. What is needed is a Dirac-Fock value of the radiative effects and eventually an investigation of many-body corrections beyond that. The available estimations of the screening of the Lamb shift are useful approximations of the former

but fail to be even a first step towards an accomplishment of the latter.

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