QED calculation of the $2p_{1/2}$-$2s$ and $2p_{3/2}$-$2s$ transition energies and the ground-state hyperfine splitting in lithiumlike scandium

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We present the most accurate up-to-date theoretical values of the $2p_{1/2}$-$2s$ and $2p_{3/2}$-$2s$ transition energies and the ground-state hyperfine splitting in Sc^{18+}. All two- and three-electron contributions to the energy values up to the two-photon level are treated in the framework of bound-state QED without αZ expansion. The interelectronic interaction beyond the two-photon level is taken into account by means of the large-scale configuration-interaction Dirac-Fock-Sturm (CI-DFS) method. The relativistic recoil correction is calculated with many-electron wave functions in order to take into account the electron-correlation effect. The accuracy of the transition energy values is improved by a factor of 5 compared to the previous calculations. The CI-DFS calculation of interelectronic-interaction effects and the evaluation of the QED correction in an effective screening potential provide significant improvement for the $2s$ hyperfine splitting. The results obtained are in good agreement with recently published experimental data.

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I. INTRODUCTION

The dielectronic recombination process has proven to be a useful tool in high-precision measurements of the excitation energy of low-lying levels in middle-Z lithiumlike systems [1,2]. By this method the energy of the $2p_{3/2}$-$2s$ transition in Sc^{18+} was determined to be 44.3107(19) eV [2]. A significant improvement of the accuracy was announced recently by Lestinsky *et al.* [3,4], with the preliminary value of 44.3096(4) eV, and work on further improvement of this value is in progress [5]. In these experiments the energy of the Rydberg resonances E_{res} was measured. The Rydberg state energy E_{bind} was evaluated by means of relativistic many-body perturbation theory (RMBPT). Then the excitation energy of the ion was determined as $E_{\mathrm{exc}}=E_{\mathrm{res}}+E_{\mathrm{bind}}$. In Ref. [2] the theoretical value of E_{exc} for both $2p_{1/2}$-$2s$ and $2p_{3/2}$-$2s$ transitions was obtained by means of RMBPT, while for the quantum electrodynamic (QED) correction the result of Ref. [6] was taken into account. The energy resolution achieved in these experiments also allowed for resolving the $2s$ hyperfine structure. As a result, the $2s$ hyperfine splitting of lithiumlike scandium was measured to be 6.21(20) meV [4].

The main goal of the present investigation is to evaluate the $2p_{1/2}$-$2s$ and $2p_{3/2}$-$2s$ transition energies and the ground-state hyperfine splitting in lithiumlike scandium to the utmost accuracy, aiming at a stringent test of the present state-of-the-art theoretical description of many-electron effects. Various contributions to the energy of the $2p$-$2s$ transitions are considered in the next section. In order to meet the experimental accuracy, rigorous quantum electrodynamic calculations of the first two orders of perturbation theory are combined with large-scale configuration-interaction Dirac-Fock-Sturm (CI-DFS) calculations of the third- and higher-order contributions within the Breit approximation. The relativistic nuclear recoil corrections are calculated as well. The evaluation of the hyperfine splitting is accomplished in Sec. III. The CI-DFS method is employed to obtain correlation effects of order $1/Z^2$ and higher. The radiative correction to hyperfine splitting is calculated with an effective local screening potential.

Relativistic units are used throughout the paper ($\hbar=c=1$).

II. $2p_{1/2}$-$2s$ AND $2p_{3/2}$-$2s$ TRANSITION ENERGIES

We start with the Furry picture, where in the zeroth-order approximation noninteracting electrons are bound by the Coulomb field of the nucleus. The Dirac equation yields zeroth-order energies of the one-electron states. The homogeneously-charged-sphere model of the nucleus is employed with the value of rms radius $\langle r^2\rangle^{1/2}=3.5443(23)$ fm [7].

In leading order of the perturbation theory, diagrams of self-energy, vacuum polarization, and one-photon exchange arise. Techniques for the evaluation of these corrections nonperturbative in αZ have been described in numerous publications (see, e.g., Ref. [8]). For the self-energy correction we interpolate the values presented in Ref. [9] for the $2s$ and $2p_{1/2}$ states and those presented in Ref. [10] for the $2p_{3/2}$ state. The vacuum-polarization and one-photon exchange corrections are recalculated in the present work with inclusion of finite-nuclear-size effects.

The second-order contributions can be classified as one-electron two-loop QED corrections, two-electron QED corrections, and two-photon exchange. Rigorous calculation of all two-loop QED corrections is a challenging problem. To date, the dominant part of these corrections was calculated in a wide range of $Z=10-92$ for the $1s$ state only (see Ref. [11] and references therein). Recently, the corresponding results for $2s$, $2p_{1/2}$, and $2p_{3/2}$ states were presented for high-Z ions [12]. However, since for low values of Z the numerical evaluation of the second-order self-energy correction be-

comes rather difficult, so far one has to rely on the αZ expansion, which reads

$$\Delta E_{\text{two loop}} = m\left(\frac{\alpha}{\pi}\right)^2 \frac{(\alpha Z)^4}{n^3}[B_{40} + (\alpha Z)B_{50} + (\alpha Z)^2\{B_{63}L^3 + B_{62}L^2 + B_{61}L + B_{60}\} + \cdots], \tag{1}$$

where $L=\ln[(\alpha Z)^{-2}]$. The values of the coefficients for the $2s$ state can be found in Appendix A of Ref. [13] and for the $2p_{1/2}$ and $2p_{3/2}$ states in Ref. [14]. Since the convergence of the expansion in αZ is known to be rather bad, we assume the uncertainty to be about 50% in our case.

The two-electron QED corrections are represented by the diagrams of the screened self-energy and the screened vacuum polarization. Rigorous evaluation of the screened self-energy in Li-like ions was performed in Ref. [15] for $2s$ and $2p_{1/2}$ states and in Ref. [16] for the $2p_{3/2}$ state. The screened vacuum-polarization correction was calculated in Ref. [17]. We obtain the corresponding values for $Z=21$ employing the procedure presented in these works. In order to estimate higher-order (in $1/Z$) terms of the screened QED correction, the following approximate scheme is used. The first-order QED correction is evaluated in an effective screening potential and the higher-order terms are extracted by subtracting the zeroth- and first-order terms. The uncertainty of the higher-order screened QED correciton obtained in this way is assumed to be 100%.

The two-photon exchange correction is evaluated within the framework of QED, following our previous investigations [18,19].

In order to evaluate the interelectronic-interaction corrections of third and higher orders we proceed as follows. The Dirac-Coulomb-Breit equation within the no-pair approximation is solved by means of the large-scale CI-DFS method [20,21] yielding the many-electron wave functions and the energy values. The interelectronic-interaction operator employed in the Dirac-Coulomb-Breit equation reads

$$V_{\text{Breit}} = \lambda\alpha\sum_{i>j}\left(\frac{1}{r_{ij}} - \frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{2r_{ij}} - \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_{ij})(\boldsymbol{\alpha}_j\cdot\boldsymbol{r}_{ij})}{2r_{ij}^3}\right), \tag{2}$$

where a scaling parameter λ is introduced in order to separate terms of different order in $1/Z$ from the numerical results with different λ. Here i,j enumerate the electrons and $\boldsymbol{\alpha}$ is a vector incorporating the Dirac matrices. In this way, for small λ, the total energy of the system can be expanded in powers of λ,

$$E(\lambda) = E_0 + E_1\lambda + E_2\lambda^2 + \sum_{k=3}^{\infty} E_k\lambda^k, \tag{3}$$

where

$$E_k = \frac{1}{k!}\frac{d^k}{d\lambda^k}E(\lambda)|_{\lambda=0}. \tag{4}$$

The higher-order contribution $E_{\geqslant 3}\equiv\Sigma_{k=3}^{\infty}E_k$ is calculated as $E_{\geqslant 3}=E(\lambda=1)-E_0-E_1-E_2$, where the low-order terms E_0, E_1, and E_2 are determined numerically according to Eq. (4). Comparison of E_1 and E_2 with the corresponding QED results allows us to conclude that the uncertainty of the higher-order contribution due to the Breit approximation is less than 0.1%.

The full relativistic theory of the nuclear recoil effect can be formulated only in the framework of QED [22]. To evaluate the recoil effect within the lowest-order relativistic approximation one can use the operator (see, e.g., Ref. [22])

$$H_M = \frac{1}{2M}\sum_{i,j}\left[\boldsymbol{p}_i\cdot\boldsymbol{p}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\right)\cdot\boldsymbol{p}_j\right], \tag{5}$$

where M is the nuclear mass and $\boldsymbol{p}_i$ is the momentum operator acting on the ith electron. The expectation value of H_M on the many-electron wave function of the system, obtained by the CI-DFS method, yields the recoil correction to the energy levels in all orders of $1/Z$ within the $(\alpha Z)^4 m^2/M$ approximation. The electron-correlation effects contribute to about 20% of the total value and have to be taken into account in order to achieve the desirable accuracy. The one- and two-electron recoil corrections of higher orders in αZ are taken from Refs. [23,24]. The recoil correction of the next order in m/M is negligible in the case under consideration.

All contributions to the transition energies considered above are collected in Table I. For comparison, previous theoretical results and available experimental data are presented as well. As one can see from the table, the theoretical values of the transition energies reported in this paper are about five times more precise than those in Ref. [2] and agree well with the experiments. Further improvement of the theoretical accuracy can be achieved by more accurate calculations of the higher-order screened QED effects.

III. HYPERFINE SPLITTING

The ground-state hyperfine splitting of a lithiumlike ion is conveniently written as

$$\Delta E_\mu = \frac{1}{6}\alpha(\alpha Z)^3\frac{m}{m_p}\frac{\mu}{\mu_N}\frac{2I+1}{2I}\frac{1}{(1+m/M)^3}mc^2 \times\left(A(\alpha Z)(1-\delta)(1-\varepsilon) + \frac{1}{Z}B(\alpha Z) + \frac{1}{Z^2}C(Z,\alpha Z) + x_{\text{rad}}\right), \tag{6}$$

where m_p is the mass of the proton, μ and I are the nuclear magnetic moment and spin, and μ_N denotes the nuclear magneton. The one-electron relativistic factor $A(\alpha Z)$ can easily be derived from the Dirac equation utilizing virial relations [26]. The finite-nuclear-size correction δ is evaluated numerically employing the homogeneously-charged-sphere model for the nuclear-charge distribution. The Bohr-Weisskopf correction ε, arising due to the nonpointlike nuclear magnetization distribution, is evaluated within the single-particle nuclear model [27,28].

The first-order interelectronic-interaction correction described by the function $B(\alpha Z)$ is evaluated in the rigorous QED approach [29]. The dual-kinetic-balance (DKB) ap-

TABLE I. Individual contributions to the $2p_{1/2}-2s$ and $2p_{3/2}-2s$ transition energies in Li-like scandium, in eV. For comparison, the theoretical result from Ref. [2] and the experimental values, obtained via optical spectroscopy [25] and via the dielectronic recombination process [2,3], are presented.

	$2p_{1/2}-2s$	$2p_{3/2}-2s$
Dirac value (extended nucleus)	−0.00237	8.93553
One-photon exchange	41.89788	38.90847
Self-energy	−0.2871(3)	−0.2679(3)
Vacuum polarization	0.01979	0.01989
Two-photon exchange	−3.5683(2)	−3.2388(2)
Screened QED	0.0387(20)	0.0331(20)
Three- and more-photon exchange	−0.0594(3)	−0.0713(3)
Two-loop QED	0.00011(5)	0.00008(4)
Recoil	−0.00991(2)	−0.01001(2)
Theory: This work	38.0294(21)	44.3091(21)
S. Kieslich *et al.* [2]	38.0261(100)	44.3089(100)
Experiment: S. Suckewer *et al.* [25]	38.02(4)	44.312(35)
S. Kieslich *et al.* [2]		44.3107(19)
M. Lestinsky *et al.* [3]		44.3096(4)

proach [30] is employed to construct the complete set of one-electron wave functions from the B splines. The finite distributions of the nuclear charge and the nuclear magnetization are taken into account. The latter is introduced via the replacement of $1/r^2$ with $F(r)/r^2$ in the hyperfine interaction matrix elements. The explicit form of the function $F(r)$ can be found in Refs. [31,32]. The higher-order correction $C(Z,\alpha Z)/Z^2$ is obtained in the framework of the large-scale CI-DFS method.

The QED correction x_{rad} is evaluated in one-loop approximation with an effective non-Coulomb binding potential V_{eff}, which partly takes into account the interelectronic-interaction effects. It is taken in the following form [33,34]:

$$V_{\mathrm{eff}}(r) = V_{\mathrm{nuc}}(r) + \alpha \int_0^\infty dr' \frac{1}{r_>} \rho(r') - x_\alpha \frac{\alpha}{r} \left(\frac{81}{32\pi^2} r\rho(r) \right)^{1/3}. \tag{7}$$

Here ρ is the total electron density, including the $(1s)^2$ shell and the $2s$ electron. The parameter x_α is taken to be $x_\alpha = 2/3$, which corresponds to the Kohn-Sham potential. To provide a proper asymptotic behavior, the potential V_{eff} should be corrected at large r [35]. The one-electron spectrum of the Dirac equation with V_{eff} is constructed by means of the DKB method [30]. Since the potential V_{eff} is assumed to be self-consistent, the standard iteration procedure is employed. The calculations performed are very similar to our recent calculations of the one-loop QED corrections to the g factor of Li-like ions [36]. We mention also that the evaluation of the QED corrections to the hyperfine structure with an effective screening potential was performed in the past for the case of lithiumlike bismuth [37].

The individual contributions to the hyperfine splitting in litiumlike scandium are listed in Table II. For each contribution the corresponding term in the square brackets in Eq. (6) is explicitly written. For comparison, the experimental value from Ref. [4] as well as the previously published results by Shabaev *et al.* [38] and by Boucard and Indelicato [39] are presented. The accuracy of the present result is twice better than that of Ref. [38] and about two orders of magnitude higher than the experimental one.

IV. CONCLUSION

In this paper we have presented *ab initio* QED evaluations of the $2p_{1/2}$-$2s$ and $2p_{3/2}$-$2s$ transition energies in lithiumlike scandium, where the most accurate experimental data for middle-Z lithiumlike ions have been achieved. All presently available contributions to the transition energies are collected. Except for the one-electron two-loop correction, all other terms up to the two-photon level are treated within the

TABLE II. Individual contributions to the ground-state hyperfine splitting of lithiumlike scandium, in meV. Comparison with the available theoretical and experimental values in terms of the wavelength λ is presented.

Dirac value	6.9650
Finite-nuclear-size correction	−0.0224(3)
Bohr-Weisskopf correction	−0.0064(32)
Interelectronic interaction, $1/Z$	−0.8817
Interelectronic interaction, $1/Z^2$ and higher	0.0150(2)
QED (with screening)	−0.0061(6)
Total theory, this work	6.0633(33)
Wavelength, this work	0.020448(10) cm
Theory: Shabaev *et al.* [38]	0.020450(20) cm
Boucard and Indelicato [39]	0.020403 cm
Experiment: Lestinsky *et al.* [4]	0.0200(7) cm

framework of bound-state QED to all orders in αZ. The third- and higher-order interelectronic-interaction effects are accounted for within the Breit approximation using large-scale CI-DFS calculations. The relativistic recoil corrections are evaluated as well. As a result, the total theoretical accuracy is improved by a factor of 5 compared to the previous calculations.

The ground-state hyperfine splitting of lithiumlike scandium has been calculated. The interelectronic-interaction correction to the first order in $1/Z$ is evaluated within the framework of QED. The higher-order electron-correlation effects are calculated using the large-scale CI-DFS method. The one-loop radiative corrections are calculated with an effective screening potential. The theoretical value of the hyperfine splitting is improved in comparison with the previous results.

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