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Relativistic configuration-interaction calculations of the energy levels of the $1s^22l$ and $1s2l2l'$ states in lithiumlike ions: Carbon through chlorine

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We present systematic calculations of energy levels of the $1s^22l$ and $1s2l2l'$ states of ions along the lithium isoelectronic sequence from carbon to chlorine. The calculations are performed by using the relativistic configuration-interaction method adapted to the treatment of autoionizing core-excited states. The relativistic energies are supplemented with the QED energy shifts calculated within the model QED operator approach. A systematic estimation of the theoretical uncertainties is performed for every electronic state and every nuclear charge. The results are in agreement with existing high-precision theoretical and experimental data for the ground and first excited states. For the core-excited states, our theory is much more accurate than the presently available measurements.

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I. INTRODUCTION

Lithiumlike ions are among the simplest atomic systems. Their spectra can be described in *ab initio* theoretical calculations very accurately. For light atoms, the most powerful calculational approach presently available is based on the nonrelativistic quantum electrodynamics (NRQED) expansion of energy levels in powers of α and $Z\alpha$ (where α is the fine-structure constant and Z is the nuclear charge number). High-precision NRQED calculations were performed by Puchalski and Pachucki for the lowest lying states of Li and Be$^+$ [1–3]. In the region of heavy ions, the best results are presently obtained within the alternative approach that accounts for all orders in the nuclear binding strength parameter $Z\alpha$ but expands in the electron-electron interaction parameter $1/Z$. Calculations by this method were performed by Shabaev and coworkers [4–7] for the ground and first excited states of Li-like ions with $Z \geqslant 10$. It is important to point out that both these methods were able to produce *predictive* results; i.e., their results contain estimates of theoretical errors obtained without referring to experimental data.

For the core-excited states of Li-like ions, there have been no rigourous QED calculations accomplished so far. Previous calculations were performed using various methods, notably, the multiconfigurational Dirac-Fock method [8,9], the variational nonrelativistic approach with inclusion of leading relativistic effects [10], and many-body perturbation theory (MBPT) [11]. None of these calculations were able to provide estimations of theoretical errors.

In our previous investigation [12], we obtained predictive results for energies of the $1s2l2l'$ core-excited states of Li-like ions in the nuclear charge region $Z = 18$–36. By combining results obtained by the relativistic configuration-interaction method with the one-loop QED effects calculated in effective screening potentials, we were able to produce theoretical predictions with an accuracy better than what is presently achievable in experiments; see, e.g., the recent measurement of the $K\alpha$ transitions in iron [13]. Such accuracy opens possibilities of using theoretical energies of Li-like ions for calibration of experimental x-ray spectra for ions with a larger number of electrons, for which accurate calculations are presently not possible.

With the range of Z computed in Ref. [12], possible calibrations are restricted to the x-ray energies beyond 3 keV. The energy range of most third- and fourth-generation synchrotron light sources, however, lies in the region of smaller x-ray energies [14]. High-quality calibration sources are urgently needed for the energy range between the carbon and the chlorine K edges.

The present situation with calibration standards in the soft-x-ray regime has recently been examined by Müller and coworkers [15] with emphasis on photon energies near the neon K edge at approximately 870 eV. In numerous experiments performed by various techniques (see Table I of Ref. [15]), the $1s \to 3p$ dipole transition energy in neutral neon has been measured, with results ranging between 867.05 and 867.69 eV with quoted uncertainties of typically 50 to 80 meV but discrepancies reaching up to 640 meV. This situation clearly shows the need for new and reliable calibration standards in the soft-x-ray energy region.

Precise knowledge of the satellite transition energies are also required for the diagnostics of hot laboratory plasmas, particularly those in the magnetically confined fusion research. High-quality theoretical energies are considered to be critical for a proper fit of spectral lines and, accordingly, a better plasma diagnostics [16,17].

TABLE I. The convergence of the CI energies for the $1s2p^2\,{}^2D_{3/2}$ state (in a.u.) with respect to the number of one-electron orbitals in the basis, for the standard and for the balanced B-spline basis (see text). For illustration purposes, the one-electron basis is restricted to contain orbitals with $l \leqslant 2$ only and only the Coulomb interaction is included into the Hamiltonian. n_a is the number of B splines, $N_{\rm orb}$ is the number of one-electron orbitals, and E is the energy value.

	Standard basis			Balanced basis		
n_a	$N_{\rm orb}$	E	Increment	$N_{\rm orb}$	E	Increment
$Z = 6$						
30	81	−23.536 9		86	−23.519 37	
40	98	−23.519 1	0.017 8	101	−23.519 31	0.000 06
50	118	−23.523 4	−0.004 4	113	−23.519 28	0.000 03
60	141	−23.514 7	0.008 7	148	−23.519 25	0.000 03
70	161	−23.517 8	−0.003 1	166	−23.519 24	0.000 01
80	178	−23.517 4	0.000 4	183	−23.519 23	0.000 01
Result		−23.517 (15)			−23.519 23 (5)	
$Z = 17$						
30	81	−206.754 8		81	−206.754 26	
40	101	−206.753 0	0.001 8	102	−206.754 11	0.000 15
50	118	−206.759 0	−0.006 0	116	−206.754 05	0.000 06
60	146	−206.749 5	0.009 5	138	−206.754 01	0.000 04
70	163	−206.752 7	−0.003 3	153	−206.753 98	0.000 03
80	181	−206.752 7	0.000 0	170	−206.753 96	0.000 02
Result		−206.752 (15)			−206.754 0 (2)	

Partly motivated by the needs described above, the goal of the present work was to extend our previous calculation of the $n = 2$ valence and core-excited states of Li-like ions [12] to the lower-Z region. This task turned out to be less straightforward than it seemed and required significant alterations of our original computational approach, for two reasons. First, the interaction of the autoionizing core-excited reference states with closely lying continuum states became more pronounced for low-Z ions than it was for heavier ions, which led to poor convergence of the results with respect to the basis size. Second, the computation of the QED effects for the nuclear charges as low as $Z = 6$ in the same way as was done in Ref. [12] turned out to be not possible because of technical difficulties and numerical cancellations, which grow quickly as Z is decreased. Our ways for overcoming these problems are discussed in the next two sections.

II. CONFIGURATION-INTERACTION METHOD FOR CORE EXCITED STATES

We start with outlining the main features of the configuration-interaction (CI) method, which is by now one of the standard approaches in atomic structure calculations; see, e.g., Refs. [18,19]. The CI N-electron wave function $\Psi(PJM)$ with a definite parity P, total angular momentum J, and angular momentum projection M is represented as a finite sum of configuration-state functions (CSFs) with the same P, J, and M,

$$\Psi(PJM) = \sum_r c_r\,\Phi(\gamma_r PJM), \tag{1}$$

where γ_r denotes the set of additional quantum numbers that determine the CSF. The CSFs are constructed as linear combinations of antisymmetrized products of one-electron orbitals ψ_n, which are *positive-energy* eigenfunctions of some one-particle Dirac Hamiltonian (which corresponds to the so-called no-pair approximation). In our implementation of the CI method, we used the one-particle Dirac Hamiltonian with the frozen-core Dirac-Fock potential.

The eigenvalues and eigenfunctions of the Dirac Hamiltonian are constructed by the dual-kinetic-balance (DKB) method [20] from a finite set of B-spline basis functions. This approach yields a discrete representation of the continuum part of the Dirac spectrum, in which the density of the continuum states increases as the number of basis functions is enlarged. For a given number of B splines n_a, all Dirac eigenstates ψ_n with the energies $0 < \varepsilon_n \leqslant mc^2(1 + Z\alpha\,\epsilon)$ and the orbital quantum number $l \leqslant L_{\rm max}$ were included into the one-electron basis of our CI calculations. The dependence of the calculated results on the parameters n_a, ϵ, and $L_{\rm max}$ was carefully studied in order to provide estimates of the numerical uncertainty (see Tables I and II of Ref. [12] for examples of the analysis of the basis convergence).

The energies of electronic states and the corresponding expansion coefficients c_r are obtained as the eigenvalues and the eigenvectors of the matrix of the Dirac-Coulomb-Breit (DCB) Hamiltonian in the space of the CSFs,

$$\{H_{rs}\} \equiv \{\langle \gamma_r PJM | H_{\rm DCB} | \gamma_s PJM \rangle\}. \tag{2}$$

The DCB Hamiltonian is

$$H_{\rm DCB} = \sum_i h_{\rm D}(i) + \sum_{i<j} [V_C(i,j) + V_B(i,j)], \tag{3}$$

where the indices $i,j = 1,\ldots,N$ numerate the electrons, h_D is the one-particle Dirac-Coulomb Hamiltonian, and V_C and V_B are the Coulomb and the Breit parts of the electron-electron interaction. The matrix elements of the Hamiltonian are represented as linear combinations of one- and two-particle

TABLE II. The QED correction to the total energy of the $1s^22s$ and $1s^22p_{1/2}$ states: comparison of results of rigourous QED calculations ("exact") with ones obtained by the QEDMOD package. The "exact" results for the ionization energies of Li-like ions are taken from Ref. [1] for Li and Be$^+$ and from Ref. [7] for Mg^{9+} and Ar^{15+}. In order to obtain QED shifts to the total energies, we added results from Refs. [26,27] for the ionization energy of the corresponding He-like ions and results from Ref. [28] for the ionization energy of H-like ions. Units are a.u.

Z		$1s^22s$	$1s^22p_{1/2}$	$2s$-$2p_{1/2}$
3	Exact	0.000 114 53 (5)	0.000 113 14 (7)	0.000 001 388 (4)
	QEDMOD	0.000 115 3	0.000 113 9	0.000 001 42
4	Exact	0.000 350 9 (4)	0.000 342 1 (6)	0.000 008 83 (4)
	QEDMOD	0.000 353	0.000 345	0.000 008 45
12	Exact	0.020 27	0.019 21	0.001 06
	QEDMOD	0.020 38	0.019 33	0.001 05
18	Exact	0.084 10	0.079 29	0.004 81
	QEDMOD	0.084 42	0.079 64	0.004 78

radial integrals,

$$\langle \gamma_r PJM | H_{\mathrm{DCB}} | \gamma_s PJM \rangle = \sum_{ab} d_{rs}(ab)\, I(ab) + \alpha \sum_{k} \sum_{abcd} v_{rs}^{(k)}(abcd)\, R_k(abcd), \tag{4}$$

where a, b, c, and d numerate the one-electron orbitals, d_{rs} and $v_{rs}^{(k)}$ are the angular coefficients, $I(ab)$ are the one-electron radial integrals, and $R_k(abcd)$ are the two-electron radial integrals. We refer the reader to our previous papers for formulas and details of the implementation of the method [12,21].

In the present work, we would like to use the CI method for computing energy levels of core-excited states with energies above the autoionization threshold. For such states, the interaction of the reference state with the closely lying continuum $1s^2\varepsilon l$ states (with energy $\varepsilon > mc^2$) might be significant and should be properly accounted for. In our previous calculations [12,21,22], we addressed this issue by using increasingly large sets of one-electron orbitals and by studying the convergence of the results. In the present work, however, we are interested in the lower-Z ions where the interaction with the continuum states is more significant and the convergence of the results for such a straightforward approach often becomes unsatisfactory.

Let us consider the $1s2s^2\,{}^2S$ state as an example. It is the lowest lying core-excited state and its energy is significantly influenced by the interaction with the closely lying continuum $1s^2\varepsilon p_{1/2}$ states. If we increase our basis of one-electron orbitals in a straightforward way, we observe that at a certain level of precision our results stop to converge but start to oscillate instead. We would like to emphasize that this problem reveals itself only when we increase the *density* of the continuum states in the problematic region near the energy of the reference state. If we had not changed the density, we might have not even become aware of this problem.

It turns out that the instabilities of the convergence of energies can be traced back to the situations when a continuum $1s^2\varepsilon p_{1/2}$ state happens to be closely degenerate in energy with the reference state. We found out that the convergence with respect to the basis can be drastically improved if we balance our discrete representation of the continuum spectrum in such a way that the energies of the two nearest continuum states are on the same distance from the energy of the reference state (one continuum state below the reference state, and the other above).

The same situation occurs for other core-excited states, but the degree of the coupling to the continuum and, therefore, the magnitude of instabilities differ for different states. In particular, the $1s2s2p\,{}^4P^o$ state is rather insensitive to the interaction with the continuum. On the contrary, the ${}^2D$ state is very much so. Moreover, the latter couples not only with the $l = 1$ continuum states (as is the case for the S and P states), but also to the $l = 2$ ones. Table I presents a comparison of the convergence of the CI energies of the $1s2p^2\,{}^2D_{3/2}$ state for $Z = 6$ and $Z = 17$, as obtained by different methods. The left part of the table contains results obtained with the standard one-electron basis, whereas the right part displays results obtained with the balanced basis. We observe that the proposed balancing of the spectrum of one-electron orbitals significantly improves the convergence of the calculated CI energies, which entails an improvement of the estimated accuracy by up to two orders of magnitude.

Let us now discuss how we produce a balanced discrete representation of the one-electron continuum spectrum. In our approach, the one-electron orbitals are taken from the finite basis set representation of the Dirac Hamiltonian with the frozen-core Dirac-Fock potential, obtained by the DKB B-spline method [20]. The B splines are defined on a radial grid, whose form outside of the nucleus is exponential,

$$t_i = t_0 e^{A\,i/N}, \quad i = 0 \ldots N,$$

where $A = \ln(t_{\max}/t_0)$, $t_{\max}$ is the radial cutoff parameter, and t_0 is the nuclear radius. In the present work, we introduce a continuous parameter γ in the definition of the radial grid,

$$t_i = t_0 e^{A\,(i/N)^{\gamma}}.$$

After that, the energies of the continuum states of the B-spline representation of the one-electron Dirac Hamiltonian spectrum become functions of the parameter γ, $\varepsilon_n \equiv \varepsilon_n(\gamma)$. By varying γ (typically by 10–20% from the standard value $\gamma = 1$), we were able to adjust the energy positions of the two nearest continuum states to be symmetrical with respect to the reference-state energy. In practice, we repeated our CI calculations for different values of the parameter γ, adjusting this parameter until the separation energies of the two closest

TABLE III. Energy levels of Li-like ions, in Rydbergs. The labeling is as follows: "Coul" stands for the Dirac-Coulomb energies, "Breit" denotes the correction due to the Breit interaction, "NMS" is the normal mass shift, "SMS" is the specific mass shift, and "QED" denotes the QED correction. Further quantities are μ, the reduced mass; R, the root-mean-square nuclear charge radius; and c.g., the center-of-gravity energy of the multiplet level.

Term		J	Coul	Breit	NMS	SMS	QED	Total
C ($Z = 6$), $1 - \mu/m = 0.00004573$, $R = 2.470$ fm								
$1s^22s$	^2S	1/2	−4.74074	0.000 22	0.000 22	0.000 01	0.000 11	−4.740 19(10)
$1s^22p$	$^2P^o$	1/2	0.587 74	0.000 13	−0.000 03	−0.000 11	−0.000 12	0.587 61(11)
		3/2–1/2	0.001 18	−0.000 23	0.0	0.0	0.0	0.000 96(8)
$1s2s^2$	^2S	1/2	21.438 15	−0.003 87	−0.000 98	−0.000 08	−0.001 24	21.432 0(6)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	21.622 00	−0.003 83	−0.000 99	−0.000 22	−0.001 37	21.615 59(8)
		3/2–1/2	0.000 70	−0.000 66	0.0	0.0	0.0	0.000 04
		5/2–3/2	0.001 17	−0.000 29	0.0	0.0	0.0	0.000 88
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	22.053 27	−0.003 91	−0.001 01	0.000 05	−0.001 33	22.047 07(10)
		3/2–1/2	0.000 82	0.000 07	0.0	0.0	0.0	0.000 89(5)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	22.299 87	−0.003 56	−0.001 02	−0.000 37	−0.001 52	22.293 41(8)
		3/2–1/2	0.000 68	0.000 02	0.0	0.0	0.0	0.000 69(2)
		5/2–3/2	0.001 12	−0.000 76	0.0	0.0	0.0	0.000 36(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	22.306 98	−0.003 63	−0.001 02	−0.000 19	−0.001 37	22.300 8(4)
		3/2–1/2	0.000 62	−0.000 69	0.0	0.0	0.0	−0.000 1(4)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	22.533 10	−0.003 82	−0.001 03	−0.000 23	−0.001 51	22.526 5(3)
		5/2–3/2	0.000 10	−0.001 08	0.0	0.0	0.0	−0.001 0(3)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	22.625 11	−0.004 15	−0.001 03	0.000 08	−0.001 50	22.618 51(13)
		3/2–1/2	0.001 34	−0.000 01	0.0	0.0	0.0	0.001 33(10)
$1s(^2S)2p^2(^1S)$	^2S	1/2	22.983 52	−0.003 66	−0.001 05	−0.000 18	−0.001 47	22.977 2(7)
N ($Z = 7$), $1 - \mu/m = 0.000\,03918$, $R = 2.558$ fm								
$1s^22s$	^2S	1/2	−7.195 67	0.000 40	0.000 28	0.000 01	0.000 21	−7.194 76(11)
$1s^22p$	$^2P^o$	1/2	0.733 36	0.000 28	−0.000 03	−0.000 16	−0.000 24	0.733 21(11)
		3/2–1/2	0.002 77	−0.000 43	0.0	0.0	0.000 01	0.002 34(8)
$1s2s^2$	^2S	1/2	30.211 96	−0.006 52	−0.001 18	−0.000 09	−0.002 22	30.202 0(6)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	30.429 62	−0.006 46	−0.001 19	−0.000 27	−0.002 47	30.419 23(10)
		3/2–1/2	0.001 45	−0.001 14	0.0	0.0	0.0	0.000 31
		5/2–3/2	0.002 43	−0.000 50	0.0	0.0	0.0	0.001 93
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	30.973 33	−0.006 58	−0.001 21	0.000 08	−0.002 41	30.963 21(12)
		3/2–1/2	0.001 71	0.000 12	0.0	0.0	0.0	0.001 84(6)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	31.249 90	−0.005 98	−0.001 22	−0.000 45	−0.002 75	31.239 50(10)
		3/2–1/2	0.001 42	0.000 02	0.0	0.0	0.0	0.001 44(2)
		5/2–3/2	0.002 35	−0.001 32	0.0	0.0	0.0	0.001 03(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	31.271 35	−0.006 09	−0.001 23	−0.000 23	−0.002 46	31.261 3(4)
		3/2–1/2	0.001 26	−0.001 19	0.0	0.0	0.0	0.000 1(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	31.557 36	−0.006 42	−0.001 24	−0.000 27	−0.002 73	31.546 7(4)
		5/2–3/2	0.000 38	−0.001 91	0.0	0.0	0.0	−0.001 5(3)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	31.671 70	−0.006 99	−0.001 24	0.000 12	−0.002 72	31.660 87(15)
		3/2–1/2	0.002 84	0.0	0.0	0.0	0.0	0.002 84(11)
$1s(^2S)2p^2(^1S)$	^2S	1/2	32.105 33	−0.006 12	−0.001 26	−0.000 21	−0.002 69	32.095 1(8)
0 ($Z = 8$), $1 - \mu/m = 0.000\,03431$, $R = 2.701$ fm								
$1s^22s$	^2S	1/2	−10.152 93	0.000 68	0.000 35	0.000 01	0.000 37	−10.151 53(11)
$1s^22p$	$^2P^o$	1/2	0.878 33	0.000 50	−0.000 03	−0.000 20	−0.000 42	0.878 18(12)
		3/2–1/2	0.005 54	−0.000 73	0.0	0.0	0.000 02	0.004 82(9)
$1s2s^2$	^2S	1/2	40.490 94	−0.010 16	−0.001 39	−0.000 09	−0.003 67	40.475 6(6)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	40.742 92	−0.010 09	−0.001 40	−0.000 31	−0.004 08	40.727 04(14)
		3/2–1/2	0.002 69	−0.001 81	0.0	0.0	0.000 01	0.000 89
		5/2–3/2	0.004 53	−0.000 80	0.0	0.0	0.000 01	0.003 73

TABLE III. *(Continued.)*

Term		J	Coul	Breit	NMS	SMS	QED	Total
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	41.400 01	−0.010 27	−0.001 42	0.000 11	−0.003 99	41.384 44(15)
		3/2–1/2	0.003 20	0.000 18	0.0	0.0	0.000 01	0.003 40(6)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	41.706 27	−0.009 29	−0.001 43	−0.000 54	−0.004 55	41.690 46(13)
		3/2–1/2	0.002 65	0.000 03	0.0	0.0	0.0	0.002 69(2)
		5/2–3/2	0.004 36	−0.002 11	0.0	0.0	0.000 01	0.002 26(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	41.741 88	−0.009 48	−0.001 43	−0.000 26	−0.004 08	41.726 6(3)
		3/2–1/2	0.002 29	−0.001 88	0.0	0.0	0.000 01	0.000 4(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	42.088 43	−0.010 01	−0.001 44	−0.000 31	−0.004 53	42.072 1(4)
		5/2–3/2	0.000 34	−0.003 04	0.0	0.0	0.0	−0.002 7(3)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	42.226 21	−0.010 94	−0.001 45	0.000 16	−0.004 51	42.209 48(19)
		3/2–1/2	0.005 32	0.0	0.0	0.0	0.000 01	0.005 33(12)
$1s(^2S)2p^2(^1S)$	^2S	1/2	42.733 66	−0.009 47	−0.001 47	−0.000 25	−0.004 45	42.718 0(8)
F $(Z = 9)$, $1 - \mu/m = 0.000\,02888$, $R = 2.898$ fm								
$1s^22s$	^2S	1/2	−13.612 93	0.001 05	0.000 39	0.000 01	0.000 61	−13.610 87(12)
$1s^22p$	$^2P^o$	1/2	1.023 05	0.000 83	−0.000 03	−0.000 23	−0.000 68	1.022 95(13)
		3/2–1/2	0.009 98	−0.001 15	0.0	0.0	0.000 03	0.008 87(9)
$1s2s^2$	^2S	1/2	52.277 00	−0.014 97	−0.001 51	−0.000 09	−0.005 68	52.254 8(6)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	52.563 83	−0.014 88	−0.001 52	−0.000 34	−0.006 33	52.540 76(19)
		3/2–1/2	0.004 59	−0.002 70	0.0	0.0	0.000 01	0.001 90
		5/2–3/2	0.007 75	−0.001 20	0.0	0.0	0.000 01	0.006 56(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	53.334 93	−0.015 14	−0.001 54	0.000 14	−0.006 21	53.312 18(20)
		3/2–1/2	0.005 50	0.000 25	0.0	0.000 01	0.000 01	0.005 77(7)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	53.671 50	−0.013 66	−0.001 55	−0.000 59	−0.007 07	53.648 63(18)
		3/2–1/2	0.004 55	0.000 04	0.0	0.0	0.000 01	0.004 60(2)
		5/2–3/2	0.007 46	−0.003 16	0.0	0.0	0.000 01	0.004 31(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	53.720 50	−0.013 94	−0.001 55	−0.000 28	−0.006 32	53.698 4(3)
		3/2–1/2	0.003 85	−0.002 77	0.0	−0.000 01	0.000 01	0.001 1(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	54.128 80	−0.014 73	−0.001 56	−0.000 34	−0.007 04	54.105 1(4)
		5/2–3/2	0.000 61	−0.004 56	0.0	0.0	0.0	−0.004 0(4)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	54.290 63	−0.016 14	−0.001 57	0.000 19	−0.007 01	54.266 11(23)
		3/2–1/2	0.009 21	−0.000 01	0.0	0.0	0.000 02	0.009 21(13)
$1s(^2S)2p^2(^1S)$	^2S	1/2	54.870 79	−0.013 87	−0.001 58	−0.000 28	−0.006 92	54.848 1(8)
Ne $(Z = 10)$, $1 - \mu/m = 0.000\,02745$, $R = 3.005$ fm								
$1s^22s$	^2S	1/2	−17.576 29	0.001 55	0.000 48	0.000 01	0.000 93	−17.573 32(12)
$1s^22p$	$^2P^o$	1/2	1.167 78	0.001 27	−0.000 03	−0.000 28	−0.001 03	1.167 71(14)
		3/2–1/2	0.016 70	−0.001 70	0.0	0.0	0.000 05	0.015 05(9)
$1s2s^2$	^2S	1/2	65.571 42	−0.021 09	−0.001 80	−0.000 10	−0.008 36	65.540 1(7)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	65.894 54	−0.021 00	−0.001 81	−0.000 40	−0.009 33	65.862 0(3)
		3/2–1/2	0.007 34	−0.003 84	0.0	0.0	0.000 02	0.003 52(1)
		5/2–3/2	0.012 45	−0.001 72	0.0	0.0	0.000 02	0.010 75(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	66.780 12	−0.021 36	−0.001 83	0.000 18	−0.009 17	66.747 9(3)
		3/2–1/2	0.008 88	0.000 27	0.0	0.000 01	0.000 02	0.009 18(7)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	67.148 34	−0.019 21	−0.001 84	−0.000 71	−0.010 44	67.116 1(3)
		3/2–1/2	0.007 35	0.000 06	0.0	0.0	0.000 02	0.007 42(2)
		5/2–3/2	0.011 94	−0.004 51	0.0	0.0	0.000 02	0.007 46(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	67.209 36	−0.019 61	−0.001 84	−0.000 33	−0.009 32	67.178 3(4)
		3/2–1/2	0.006 10	−0.003 88	0.0	−0.000 01	0.000 02	0.002 2(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	67.681 07	−0.020 75	−0.001 86	−0.000 40	−0.010 40	67.647 7(8)
		5/2–3/2	0.001 08	−0.006 50	0.0	0.0	0.0	−0.005 4(8)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	67.867 44	−0.022 77	−0.001 86	0.000 24	−0.010 36	67.832 7(3)
		3/2–1/2	0.014 99	−0.000 02	0.0	0.0	0.000 04	0.015 00(14)
$1s(^2S)2p^2(^1S)$	^2S	1/2	68.519 39	−0.019 46	−0.001 88	−0.000 33	−0.010 22	68.487 5(9)

TABLE III. *(Continued.)*

Term		J	Coul	Breit	NMS	SMS	QED	Total
Na ($Z = 11$), $1 - \mu/m = 0.000\,02387$, $R = 2.994$ fm								
$1s^22s$	^2S	1/2	−22.043 76	0.002 13	0.000 53	0.000 01	0.001 36	−22.039 74(16)
$1s^22p$	$^2P^o$	1/2	1.312 70	0.001 88	−0.000 03	−0.000 31	−0.001 50	1.312 74(17)
		3/2–1/2	0.026 22	−0.002 38	0.0	0.0	0.000 10	0.023 94(10)
$1s2s^2$	^2S	1/2	80.376 39	−0.028 64	−0.001 92	−0.000 10	−0.011 82	80.333 9(8)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	80.737 55	−0.028 55	−0.001 93	−0.000 42	−0.013 21	80.693 4(4)
		3/2–1/2	0.011 15	−0.005 27	0.0	0.0	0.000 03	0.005 91(1)
		5/2–3/2	0.019 04	−0.002 35	0.0	0.0	0.000 04	0.016 72(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	81.737 97	−0.028 99	−0.001 95	0.000 21	−0.013 00	81.694 2(4)
		3/2–1/2	0.013 66	0.000 34	0.0	0.000 02	0.000 03	0.014 05(8)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	82.139 84	−0.026 06	−0.001 96	−0.000 76	−0.014 80	82.096 3(4)
		3/2–1/2	0.011 29	0.000 07	0.0	0.0	0.000 03	0.011 39(2)
		5/2–3/2	0.018 17	−0.006 19	0.0	0.0	0.000 03	0.012 01(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	82.210 98	−0.026 60	−0.001 96	−0.000 35	−0.013 19	82.168 9(5)
		3/2–1/2	0.009 18	−0.005 22	0.0	−0.000 02	0.000 03	0.004 0(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	82.748 22	−0.028 17	−0.001 98	−0.000 42	−0.014 75	82.702 9(6)
		5/2–3/2	0.001 89	−0.008 92	0.0	0.0	0.0	−0.007 0(5)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	82.959 57	−0.030 95	−0.001 98	0.000 27	−0.014 69	82.912 2(4)
		3/2–1/2	0.023 25	−0.000 03	0.0	0.0	0.000 05	0.023 27(15)
$1s(^2S)2p^2(^1S)$	^2S	1/2	83.682 59	−0.026 33	−0.002 00	−0.000 35	−0.014 48	83.639 4(9)
Mg ($Z = 12$), $1 - \mu/m = 0.000\,02288$, $R = 3.057$ fm								
$1s^22s$	^2S	1/2	−27.016 26	0.002 89	0.000 62	0.000 01	0.001 91	−27.010 83(17)
$1s^22p$	$^2P^o$	1/2	1.457 93	0.002 62	−0.000 03	−0.000 37	−0.002 10	1.458 05(19)
		3/2–1/2	0.039 39	−0.003 25	0.0	0.0	0.000 14	0.036 28(11)
$1s2s^2$	^2S	1/2	96.694 18	−0.037 87	−0.002 21	−0.000 11	−0.016 19	96.637 8(9)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	97.095 61	−0.037 78	−0.002 22	−0.000 48	−0.018 10	97.037 0(5)
		3/2–1/2	0.016 26	−0.007 02	0.0	0.0	0.000 04	0.009 28(1)
		5/2–3/2	0.027 99	−0.003 12	0.0	0.0	0.000 06	0.024 92(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	98.211 19	−0.038 34	−0.002 25	0.000 25	−0.017 83	98.153 0(5)
		3/2–1/2	0.020 20	0.000 32	0.0	0.000 03	0.000 04	0.020 58(12)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	98.649 30	−0.034 42	−0.002 26	−0.000 88	−0.020 30	98.591 4(5)
		3/2–1/2	0.016 67	0.000 08	0.0	0.0	0.000 04	0.016 79(2)
		5/2–3/2	0.026 53	−0.008 26	0.0	0.0	0.000 05	0.018 32(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	98.728 11	−0.035 11	−0.002 26	−0.000 41	−0.018 08	98.672 3(6)
		3/2–1/2	0.013 27	−0.006 79	0.0	−0.000 03	0.000 05	0.006 5(4)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	99.333 57	−0.037 24	−0.002 27	−0.000 48	−0.020 24	99.273 3(8)
		5/2–3/2	0.003 24	−0.011 85	0.0	0.0	0.000 01	−0.008 6(6)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	99.570 34	−0.040 93	−0.002 28	0.000 33	−0.020 16	99.507 3(5)
		3/2–1/2	0.034 73	−0.000 04	0.0	0.0	0.000 08	0.034 77(16)
$1s(^2S)2p^2(^1S)$	^2S	1/2	100.363 72	−0.034 71	−0.002 30	−0.000 41	−0.019 86	100.306 4(10)
Al ($Z = 13$), $1 - \mu/m = 0.000\,02034$, $R = 3.061$ fm								
$1s^22s$	^2S	1/2	−32.494 80	0.003 82	0.000 66	0.000 01	0.002 60	−32.487 71(19)
$1s^22p$	$^2P^o$	1/2	1.603 61	0.003 45	−0.000 03	−0.000 39	−0.002 85	1.603 79(23)
		3/2–1/2	0.056 95	−0.004 23	0.0	0.0	0.000 19	0.052 91(13)
$1s2s^2$	^2S	1/2	114.527 13	−0.048 90	−0.002 33	−0.000 11	−0.021 57	114.454 2(9)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	114.971 76	−0.048 83	−0.002 34	−0.000 51	−0.024 13	114.895 9(6)
		3/2–1/2	0.022 92	−0.009 13	0.0	0.0	0.000 06	0.013 85(1)
		5/2–3/2	0.039 83	−0.004 04	0.0	0.0	0.000 09	0.035 88(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	116.202 76	−0.049 49	−0.002 36	0.000 27	−0.023 80	116.127 4(6)
		3/2–1/2	0.028 94	0.000 19	0.0	0.000 04	0.000 05	0.029 22(9)

TABLE III. *(Continued.)*

Term		J	Coul	Breit	NMS	SMS	QED	Total
$1s(^2S)2p^2(^3P)$	^4P	c.g.	116.680 38	−0.044 41	−0.002 37	−0.000 93	−0.027 10	116.605 6(6)
		3/2–1/2	0.023 84	0.000 09	0.0	0.0	0.000 05	0.023 98(2)
		5/2–3/2	0.037 43	−0.010 75	0.0	0.0	0.000 08	0.026 76(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	116.764 10	−0.045 29	−0.002 37	−0.000 42	−0.024 10	116.691 9(7)
		3/2–1/2	0.018 56	−0.008 56	0.0	−0.000 04	0.000 07	0.010 0(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	117.440 75	−0.048 08	−0.002 39	−0.000 50	−0.027 02	117.362 8(8)
		5/2–3/2	0.005 43	−0.015 33	0.0	−0.000 01	0.000 01	−0.009 9(5)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	117.703 49	−0.052 84	−0.002 39	0.000 35	−0.026 92	117.621 7(6)
		3/2–1/2	0.050 29	−0.000 02	0.0	−0.000 01	0.000 12	0.050 38(16)
$1s(^2S)2p^2(^1S)$	^2S	1/2	118.566 58	−0.044 72	−0.002 41	−0.000 43	−0.026 51	118.492 5(11)
Si ($Z = 14$), $1 - \mu/m = 0.000\,01961$, $R = 3.122$ fm								
$1s^22s$	^2S	1/2	−38.480 53	0.004 93	0.000 75	0.000 01	0.003 46	−38.471 38(21)
$1s^22p$	$^2P^o$	1/2	1.749 78	0.004 52	−0.000 03	−0.000 45	−0.003 76	1.750 0(3)
		3/2–1/2	0.079 95	−0.005 47	0.0	0.0	0.000 25	0.074 73(12)
$1s2s^2$	^2S	1/2	133.878 51	−0.061 89	−0.002 63	−0.000 12	−0.028 09	133.785 8(11)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	134.369 29	−0.061 86	−0.002 64	−0.000 57	−0.031 44	134.272 8(8)
		3/2–1/2	0.031 40	−0.011 64	0.0	0.0	0.000 08	0.019 84(1)
		5/2–3/2	0.055 16	−0.005 10	0.0	0.0	0.000 13	0.050 19(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	135.715 92	−0.062 64	−0.002 66	0.000 32	−0.031 05	135.619 9(8)
		3/2–1/2	0.040 40	−0.000 09	0.0	0.000 06	0.000 06	0.040 44(9)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	136.236 98	−0.056 18	−0.002 67	−0.001 06	−0.035 34	136.141 7(8)
		3/2–1/2	0.033 22	0.000 09	0.0	0.0	0.000 08	0.033 40(2)
		5/2–3/2	0.051 27	−0.013 70	0.0	0.0	0.000 10	0.037 67(2)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	136.322 17	−0.057 27	−0.002 67	−0.000 48	−0.031 40	136.230 3(9)
		3/2–1/2	0.025 20	−0.010 50	0.0	−0.000 06	0.000 10	0.014 7(3)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	137.073 77	−0.060 87	−0.002 69	−0.000 56	−0.035 24	136.974 4(10)
		5/2–3/2	0.008 85	−0.019 38	0.0	−0.000 01	0.000 02	−0.010 5(6)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	137.363 14	−0.066 82	−0.002 69	0.000 40	−0.035 11	137.258 9(8)
		3/2–1/2	0.070 98	0.000 04	0.0	−0.000 01	0.000 17	0.071 17(17)
$1s(^2S)2p^2(^1S)$	^2S	1/2	138.295 35	−0.056 51	−0.002 71	−0.000 48	−0.034 57	138.201 1(12)
P ($Z = 15$), $1 - \mu/m = 0.000\,01772$, $R = 3.189$ fm								
$1s^22s$	^2S	1/2	−44.974 69	0.006 23	0.000 80	0.000 01	0.004 49	−44.963 17(24)
$1s^22p$	$^2P^o$	1/2	1.896 55	0.005 79	−0.000 03	−0.000 48	−0.004 87	1.896 9(3)
		3/2–1/2	0.109 14	−0.006 94	0.0	0.000 01	0.000 33	0.102 54(13)
$1s2s^2$	^2S	1/2	154.750 79	−0.077 00	−0.002 74	−0.000 12	−0.035 86	154.635 1(13)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	155.291 80	−0.077 03	−0.002 75	−0.000 60	−0.040 17	155.171 2(10)
		3/2–1/2	0.041 97	−0.014 59	0.0	0.0	0.000 10	0.027 49(1)
		5/2–3/2	0.074 68	−0.006 33	0.0	0.0	0.000 17	0.068 53(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	156.754 24	−0.077 93	−0.002 78	0.000 34	−0.039 70	156.634 2(10)
		3/2–1/2	0.055 19	−0.000 59	0.0	0.000 08	0.000 08	0.054 76(9)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	157.323 33	−0.069 88	−0.002 79	−0.001 11	−0.045 18	157.204 4(10)
		3/2–1/2	0.045 27	0.000 09	0.0	0.0	0.000 11	0.045 48(3)
		5/2–3/2	0.068 49	−0.017 15	0.0	0.0	0.000 13	0.051 47(3)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	157.406 22	−0.071 19	−0.002 79	−0.000 50	−0.040 11	157.291 6(11)
		3/2–1/2	0.033 33	−0.012 56	0.0	−0.000 08	0.000 14	0.020 8(4)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	158.236 99	−0.075 77	−0.002 80	−0.000 58	−0.045 06	158.112 8(12)
		5/2–3/2	0.014 05	−0.024 00	0.0	−0.000 02	0.000 04	−0.009 9(6)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	158.553 82	−0.083 02	−0.002 81	0.000 43	−0.044 90	158.423 5(10)
		3/2–1/2	0.097 99	0.000 16	0.0	−0.000 02	0.000 23	0.098 36(18)
$1s(^2S)2p^2(^1S)$	^2S	1/2	159.554 65	−0.070 24	−0.002 83	−0.000 51	−0.044 20	159.436 9(14)

TABLE III. *(Continued.)*

Term		J	Coul	Breit	NMS	SMS	QED	Total
S ($Z = 16$), $1 - \mu/m = 0.000\,01716$, $R = 3.261$ fm								
$1s^22s$	^2S	1/2	−51.978 65	0.007 74	0.000 89	0.000 01	0.005 73	−51.964 3(3)
$1s^22p$	$^2P^o$	1/2	2.043 99	0.007 27	−0.000 04	−0.000 54	−0.006 20	2.044 5(3)
		3/2–1/2	0.145 70	−0.008 64	0.0	0.000 01	0.000 43	0.137 49(13)
$1s2s^2$	^2S	1/2	177.147 37	−0.094 40	−0.003 04	−0.000 13	−0.045 01	177.004 8(15)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	177.743 15	−0.094 52	−0.003 05	−0.000 66	−0.050 46	177.594 5(13)
		3/2–1/2	0.054 90	−0.018 02	0.0	0.0	0.000 13	0.037 02(1)
		5/2–3/2	0.099 14	−0.007 71	0.0	0.0	0.000 23	0.091 67(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	179.321 54	−0.095 52	−0.003 08	0.000 39	−0.049 90	179.173 4(13)
		3/2–1/2	0.074 00	−0.001 40	0.0	0.000 11	0.000 10	0.072 81(10)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	179.943 94	−0.085 67	−0.003 09	−0.001 23	−0.056 80	179.797 2(13)
		3/2–1/2	0.060 56	0.000 09	0.0	0.0	0.000 13	0.060 77(3)
		5/2–3/2	0.089 48	−0.021 16	0.0	0.000 01	0.000 18	0.068 50(3)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	180.020 38	−0.087 21	−0.003 09	−0.000 55	−0.050 38	179.879 2(14)
		3/2–1/2	0.043 09	−0.014 68	0.0	−0.000 11	0.000 19	0.028 5(4)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	180.935 11	−0.092 96	−0.003 11	−0.000 64	−0.056 66	180.781 8(14)
		5/2–3/2	0.021 71	−0.029 19	0.0	−0.000 04	0.000 07	−0.007 4(6)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	181.280 48	−0.101 59	−0.003 11	0.000 47	−0.056 45	181.119 8(13)
		3/2–1/2	0.132 74	0.000 40	0.0	−0.000 03	0.000 31	0.133 42(18)
$1s(^2S)2p^2(^1S)$	^2S	1/2	182.349 57	−0.086 07	−0.003 13	−0.000 56	−0.055 56	182.204 3(16)
Cl ($Z = 17$), $1 - \mu/m = 0.000\,01569$, $R = 3.365$ fm								
$1s^22s$	^2S	1/2	−59.493 86	0.009 48	0.000 93	0.000 01	0.007 18	−59.476 3(3)
$1s^22p$	$^2P^o$	1/2	2.192 18	0.008 98	−0.000 03	−0.000 57	−0.007 75	2.192 8(4)
		3/2–1/2	0.190 77	−0.010 61	0.0	0.000 01	0.000 55	0.180 72(13)
$1s2s^2$	^2S	1/2	201.071 72	−0.114 24	−0.003 16	−0.000 13	−0.055 65	200.898 6(17)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	c.g.	201.727 47	−0.114 51	−0.003 17	−0.000 68	−0.062 44	201.546 7(16)
		3/2–1/2	0.070 47	−0.021 98	0.0	0.0	0.000 16	0.048 66(1)
		5/2–3/2	0.129 42	−0.009 25	0.0	0.0	0.000 31	0.120 48(1)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	c.g.	203.421 91	−0.115 57	−0.003 19	0.000 41	−0.061 79	203.241 8(16)
		3/2–1/2	0.097 69	−0.002 64	0.0	0.000 15	0.000 13	0.095 31(11)
$1s(^2S)2p^2(^3P)$	^4P	c.g.	204.103 61	−0.103 70	−0.003 20	−0.001 28	−0.070 34	203.925 1(15)
		3/2–1/2	0.079 74	0.000 07	0.0	0.0	0.000 16	0.079 97(3)
		5/2–3/2	0.114 62	−0.025 78	0.0	0.000 01	0.000 23	0.089 07(4)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	c.g.	204.169 16	−0.105 48	−0.003 20	−0.000 56	−0.062 33	203.997 6(16)
		3/2–1/2	0.054 59	−0.016 76	0.0	−0.000 14	0.000 25	0.037 9(4)
$1s(^2S)2p^2(^1D)$	^2D	c.g.	205.173 24	−0.112 62	−0.003 22	−0.000 66	−0.070 16	204.986 6(17)
		5/2–3/2	0.032 72	−0.034 93	0.0	−0.000 05	0.000 11	−0.002 2(6)
$1s(^2S)2p^2(^3P)$	^2P	c.g.	205.548 47	−0.122 63	−0.003 23	0.000 49	−0.069 91	205.353 2(16)
		3/2–1/2	0.176 85	0.000 79	0.0	−0.000 05	0.000 41	0.178 00(19)
$1s(^2S)2p^2(^1S)$	^2S	1/2	206.685 68	−0.104 16	−0.003 24	−0.000 58	−0.068 81	206.508 9(18)

lying continuum states from the reference state were equal. In these calculations, it was sufficient to restrict the basis by $L_{\max} = 1$ for the S and P states and by $L_{\max} = 2$ for the D states, since the higher L continuum states do not cause any problems.

III. QED EFFECTS

In the present work, we evaluated the leading QED effects to the energy levels by means of the model QED operator approach [23]. We used the implementation of this method in the form of the QEDMOD package [24]. Since the published version of the package had a restriction of the nuclear charge $Z \geqslant 10$, we had to extend it to the lower values of Z. We did this by performing numerical calculations of the one-loop self-energy matrix elements for the ns, np_j, and nd_j states for $Z = 3$–9 by the method described in Ref. [25] (extending Tables I–IV of Ref. [23]).

In order to establish the level of accuracy of the model QED operator approach in the region of low nuclear charges,

TABLE IV. Theoretical wavelengths of the $1s2l2l' \rightarrow 1s^22l$ transitions in lithlium-like ions, in Å. Transitions are labeled as by Gabriel [29].

Key	Transition	$Z = 6$	$Z = 7$	$Z = 8$	$Z = 9$	$Z = 10$	$Z = 11$
a	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.3660(3)	29.467 0(2)	22.050 3(1)	17.117 55(8)	13.671 79(6)	11.170 04(5)
b	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	41.364 2(3)	29.464 7(1)	22.047 7(1)	17.114 70(8)	13.668 70(6)	11.166 77(5)
c	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.368 5(3)	29.469 7(2)	22.053 1(1)	17.120 51(8)	13.674 86(6)	11.173 23(5)
d	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	41.366 7(2)	29.467 4(2)	22.050 5(1)	17.117 66(7)	13.671 78(6)	11.169 95(5)
e	$1s(^2S)2p^2(^3P)\,^4P_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.985 9(2)	29.874 2(1)	22.330 80(8)	17.318 47(6)	13.820 37(5)	11.282 87(5)
f	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.986 6(2)	29.875 2(1)	22.332 04(8)	17.319 89(6)	13.821 93(5)	11.284 55(5)
g	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	41.984 7(2)	29.872 9(1)	22.329 40(8)	17.316 97(6)	13.818 78(5)	11.281 20(5)
h	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.987 9(2)	29.876 6(1)	22.333 51(8)	17.321 40(6)	13.823 49(5)	11.286 14(5)
i	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	41.986 0(2)	29.874 3(1)	22.330 87(8)	17.318 49(6)	13.820 33(5)	11.282 79(5)
j	$1s(^2S)2p^2(^1D)\,^2D_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.541 0(6)	29.577 6(3)	22.125 3(2)	17.171 0(1)	13.711 3(1)	11.200 23(9)
k	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	41.537 3(6)	29.573 9(4)	22.121 3(2)	17.166 8(1)	13.707 1(2)	11.195 97(9)
l	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	41.539 2(6)	29.576 2(4)	22.123 9(2)	17.169 7(1)	13.710 2(2)	11.199 26(9)
m	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	40.704(1)	29.059 9(7)	21.783 2(4)	16.933 4(3)	13.539 8(2)	11.072 4(1)
n	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	40.702(1)	29.057 7(7)	21.780 6(4)	16.930 6(3)	13.536 8(2)	11.069 2(1)
o	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	43.722(1)	30.926 8(6)	23.016 9(3)	17.790 7(2)	14.159 9(2)	11.535 7(1)
p	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	43.720(1)	30.924 4(6)	23.014 1(3)	17.787 6(2)	14.156 6(2)	11.532 2(1)
q	$1s(^2S)2s2p(^3P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	41.334 1(2)	29.431 2(1)	22.019 71(8)	17.092 91(6)	13.652 11(6)	11.154 23(5)
r	$1s(^2S)2s2p(^3P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	41.335 8(2)	29.433 0(1)	22.021 52(8)	17.094 76(6)	13.653 99(6)	11.156 15(5)
s	$1s(^2S)2s2p(^1P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	40.864 5(7)	29.151 1(3)	21.839 7(2)	16.970 5(1)	13.565 13(8)	11.090 26(6)
t	$1s(^2S)2s2p(^1P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	40.864 3(7)	29.151 1(3)	21.839 9(2)	16.970 8(1)	13.565 58(8)	11.090 80(6)
u	$1s(^2S)2s2p(^3P^o)\,^4P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	42.160 6(2)	29.959 0(1)	22.376 70(7)	17.345 48(6)	13.837 39(5)	11.294 25(5)
v	$1s(^2S)2s2p(^3P^o)\,^4P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	42.160 7(2)	29.959 3(1)	22.377 19(7)	17.346 11(6)	13.838 13(5)	11.295 08(5)
Key	Transition	$Z = 12$	$Z = 13$	$Z = 14$	$Z = 15$	$Z = 16$	$Z = 17$
a	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.296 53(5)	7.857 14(4)	6.727 44(4)	5.824 50(4)	5.091 47(3)	4.488 21(3)
b	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.293 09(5)	7.853 56(4)	6.723 73(4)	5.820 69(4)	5.087 56(3)	4.484 22(3)
c	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.299 83(5)	7.860 56(4)	6.730 98(4)	5.828 17(4)	5.095 27(3)	4.492 15(3)
d	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.296 38(5)	7.856 97(4)	6.727 27(4)	5.824 35(4)	5.091 35(3)	4.488 15(3)
e	$1s(^2S)2p^2(^3P)\,^4P_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.384 17(4)	7.926 55(4)	6.783 35(4)	5.870 23(4)	5.129 38(3)	4.520 03(3)
f	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.385 94(4)	7.928 39(4)	6.785 26(4)	5.872 17(4)	5.131 35(3)	4.522 03(3)
g	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.382 43(4)	7.924 75(4)	6.781 48(4)	5.868 29(4)	5.127 39(3)	4.517 98(3)
h	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.387 56(4)	7.930 05(4)	6.786 94(4)	5.873 89(4)	5.133 11(3)	4.523 83(3)
i	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.384 06(4)	7.926 40(4)	6.783 17(4)	5.870 01(4)	5.129 14(3)	4.519 77(3)
j	$1s(^2S)2p^2(^1D)\,^2D_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.320 20(8)	7.876 14(6)	6.742 99(5)	5.837 47(4)	5.102 46(4)	4.497 66(4)
k	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.315 92(8)	7.871 86(6)	6.738 74(5)	5.833 27(4)	5.098 32(4)	4.493 61(4)
l	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.319 38(8)	7.875 46(6)	6.742 47(5)	5.837 10(4)	5.102 25(4)	4.497 62(4)
m	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.222 43(9)	7.799 71(7)	6.682 14(6)	5.788 23(5)	5.062 06(4)	4.464 10(4)
n	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.219 05(9)	7.796 18(7)	6.678 48(6)	5.784 46(5)	5.058 19(4)	4.460 15(4)
o	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	9.578 04(9)	8.078 95(6)	6.905 71(6)	5.970 32(5)	5.212 61(4)	4.590 26(4)
p	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	9.574 39(9)	8.075 16(6)	6.901 80(6)	5.966 31(5)	5.208 51(4)	4.586 08(4)
q	$1s(^2S)2s2p(^3P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.283 71(5)	7.846 64(4)	6.718 74(4)	5.817 23(4)	5.085 35(4)	4.483 03(4)
r	$1s(^2S)2s2p(^3P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.285 66(5)	7.848 61(4)	6.720 74(4)	5.819 26(4)	5.087 42(4)	4.485 13(4)
s	$1s(^2S)2s2p(^1P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.235 30(6)	7.809 11(5)	6.689 05(4)	5.793 33(4)	5.065 82(4)	4.466 84(4)
t	$1s(^2S)2s2p(^1P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.235 91(5)	7.809 78(5)	6.689 78(4)	5.794 10(4)	5.066 62(4)	4.467 67(4)
u	$1s(^2S)2s2p(^3P^o)\,^4P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.392 19(5)	7.932 48(4)	6.787 92(4)	5.873 88(4)	5.132 40(4)	4.522 61(4)
v	$1s(^2S)2s2p(^3P^o)\,^4P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	9.393 09(5)	7.933 43(4)	6.788 92(4)	5.874 92(4)	5.133 47(4)	4.523 70(4)

we compared values obtained with the QEDMOD package with results of rigourous QED calculations for the $1s^22s$ and $1s^22p_{1/2}$ states. Such calculations were accomplished for the lightest Li-like atoms within the NRQED approach [1] and for heavier Li-like ions within the all order in $Z\alpha$ method [5,7]. The comparison is presented in Table II. From this comparison,

TABLE V. Ionization potential of the ground state of Li-like ions, in eV.

Z	This work	Rigorous QED [4,6,7,30]	NIST [31]
10	239.097 (2)	239.097 (1)	239.097 (2)
12	367.501 (2)	367.500 (1)	367.489 (7)
15	611.755 (3)	611.752 (1)	611.741 (7)

we conclude that the QEDMOD package reproduces results of rigorous QED calculations for the total energies to accuracy of better than 1%.

IV. RESULTS AND DISCUSSION

Numerical results of our calculations of the energy levels for the ground $1s^22s$ state, the first two valence-excited $1s^22p_j$ states, and the core-excited $1s2l2l'$ states of Li-like ions are listed in Table III. The results are given for ions along the lithium isoelectronic sequence starting from carbon ($Z = 6$) and ending with chlorine ($Z = 17$). For the ground state, the table presents ionization energies, i.e., energies relative to the ground state of the corresponding He-like ion. For the valence-excited states, we present energies of the $1s^22p_{1/2}$ state relative to the ground $1s^22s$ state and the $2p_{3/2}$-$2p_{1/2}$ fine-structure interval, since they usually appear in the literature in this form. For the core-excited levels, the center-of-gravity (c.g.) energies relative to the ground state and the fine-structure intervals (J-J') are listed.

Table III presents the total theoretical energies as well as individual theoretical contributions. For each level, the Dirac-Coulomb energy and corrections to it due to the Breit interaction, the normal mass shift (NMS), the specific mass shift (SMS), and the QED effects are provided. The theoretical uncertainty comes from two main sources: the Dirac-Coulomb-Breit (DCB) energy and the QED correction. The uncertainty of the DCB energies was estimated by performing a series of CI calculations with 20–30 different

TABLE VI. Comparison of theory and experiment for the $2p_{1/2}$-$2s$ transition energy, in a.u.

Z	This work	Other theory	Experiment
6	0.29380 (5)		0.293811 (5)[a]
			0.293823 (7)[b]
7	0.36660 (6)	0.36663[c]	0.366616 (5)[a]
8	0.43909 (6)	0.43911[c]	0.439117 (5)[a]
9	0.51147 (6)	0.51150[c]	0.51150 (1)[a]
10	0.58385 (7)	0.58387[c]	0.58390 (1)[a]
		0.58388 (1)[d]	
11	0.65637 (9)	0.65637[c]	0.65640 (1)[a]
12	0.72903 (9)		0.72907 (1)[a]
13	0.80189 (12)	0.80190[c]	0.80197 (1)[a]
14	0.87502 (13)		0.87509 (1)[a]
15	0.94847 (14)	0.94846[c]	0.94849 (5)[a]
		0.94854 (1)[d]	
16	1.02224 (16)		1.02232 (3)[a]
17	1.09640 (19)	1.09638[c]	1.09652 (5)[a]

[a] Reference [32].
[b] Reference [33].
[c] MBPT results from Ref. [34] and QED results from Ref. [35].
[d] Reference [7].

TABLE VII. Comparison of theory and experiment for the fine-structure splitting intervals of the $1s^22p\,^2P$, $1s2s2p\,^4P$, and $1s2p^2\,^4P$ states, in cm^{-1}.

Z	State	$J - J'$	This work	Experiment	Ref.
6	$1s^22p\,^2P$	3/2-1/2	106 (8)	107.3	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	97 (1)	100 (5)	[36]
				96 (2)	[37]
		3/2-1/2	4	0 (7)	[36]
				4 (3)	[37]
	$1s2p^2\,^4P^e$	5/2-3/2	40 (2)	41 (5)	[36]
				44 (2)	[37]
		3/2-1/2	76 (2)	83 (7)	[36]
				76 (3)	[37]
7	$1s^22p\,^2P$	3/2-1/2	257 (9)	259 (1)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	212	212 (3)	[36]
		3/2-1/2	35	35 (4)	[36]
	$1s2p^2\,^4P^e$	5/2-3/2	113 (2)	115 (3)	[36]
		3/2-1/2	158 (2)	160 (4)	[36]
8	$1s^22p\,^2P$	3/2-1/2	529 (10)	531 (1)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	409 (1)	418 (4)	[36]
		3/2-1/2	98	102 (5)	[36]
	$1s2p^2\,^4P^e$	5/2-3/2	248 (2)	252 (4)	[36]
		3/2-1/2	295 (2)	295 (5)	[36]
9	$1s^22p\,^2P$	3/2-1/2	973 (10)	976 (2)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	719 (1)	716 (10)	[38]
		3/2-1/2	209 (1)	220 (5)	[38]
	$1s2p^2\,^4P^e$	5/2-3/2	473 (2)	487 (5)	[38]
		3/2-1/2	505 (2)	523 (10)	[38]
10	$1s^22p\,^2P$	3/2-1/2	1652 (10)	1649 (2)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	1180 (1)	1102 (15)	[39]
				1196 (60)	[40]
		3/2-1/2	386 (1)	444 (15)	[39]
				368 (60)	[40]
	$1s2p^2\,^4P^e$	5/2-3/2	818 (2)	856 (15)	[39]
				832 (60)	[40]
		3/2-1/2	815 (2)	746 (15)	[39]
				816 (60)	[40]
11	$1s^22p\,^2P$	3/2-1/2	2627 (11)	2631 (5)	[32]
12	$1s^22p\,^2P$	3/2-1/2	3981 (12)	3975 (3)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	2735 (1)	2708 (20)	[41]
		3/2-1/2	1019 (1)	1010 (20)	[41]
	$1s2p^2\,^4P^e$	5/2-3/2	2011 (2)	1955 (25)	[41]
		3/2-1/2	1843 (2)	1824 (35)	[41]
13	$1s^22p\,^2P$	3/2-1/2	5806 (15)	5796 (5)	[32]
	$1s2s2p\,^4P^o$	5/2-3/2	3937 (1)	3900 (40)	[42]
				3885 (60)	[43]
		3/2-1/2	1520 (1)	1584 (40)	[42]
				1543 (60)	[43]
	$1s2p^2\,^4P^e$	5/2-3/2	2937 (2)	2884 (60)	[42]
		3/2-1/2	2632(2)	2588 (60)	[42]
				2625 (60)	[43]
14	$1s^22p\,^2P$	3/2-1/2	8201 (14)	8177 (4)	[32]
15	$1s^22p\,^2P$	3/2-1/2	11252 (14)	11253 (15)	[32]
16	$1s^22p\,^2P$	3/2-1/2	15088 (14)	15063 (5)	[32]
17	$1s^22p\,^2P$	3/2-1/2	19832 (14)	19770 (15)	[32]

TABLE VIII. Comparison of theory and experiment for the center-of-gravity multiplet separation wavelengths, in Å.

Z	This work	Experiment	Ref.
$1s2p^2\,{}^4P^e - 1s2s2p\,{}^4P^o$			
6	1344.41 (21)	1344.2 (3)	[36]
		1344.49 (4)	[37]
7	1110.94 (15)	1111.1 (1)	[36]
8	945.87 (11)	946.8 (1)	[36]
9	822.54 (9)	822.47 (8)	[38]
10	726.62 (8)	726.51 (5)	[39]
		726.71 (20)	[40]
12	586.24 (8)	586.04 (5)	[41]
13	533.03 (7)	532.83 (9)	[43]
		533.11 (9)	[42]
$1s2s2p\,({}^1P^o)\,{}^2P^o - 1s2s2p\,({}^3P^o)\,{}^2P^o$			
6	3592.(6)	3582. (4)	[44]

TABLE IX. Comparison of theory and experiment for the center-of-gravity level energies, relative to the ground $(1s)^2\,2s$ state, in eV.

Z	State	This work	Experiment	Ref.
6	$1s2s^2\,{}^2S$	291.597 (8)	291.59 (10)	[45][†,a]
			291.49 (10)	[46][a]
	$1s2s2p\,({}^3P^o)\,{}^2P^o$	299.966 (1)	299.98 (3)	[44]
			299.98 (5)	[45][†,a]
			299.91 (7)	[47]
	$1s2s2p\,({}^1P^o)\,{}^2P^o$	303.418 (5)	303.44 (3)	[44]
			303.48 (5)	[45][†,a]
			303.76 (7)	[47]
	$1s2p^2\,{}^2D$	306.489 (4)	306.54 (5)	[45][†,a]
	$1s2p^2\,{}^2S$	312.62 (1)	312.67 (5)	[45][†,a]
7	$1s2s2p\,({}^3P^o)\,{}^2P^o_{3/2}$	421.284 (2)	421.52 (5)	[48]
	$1s2s2p\,({}^3P^o)\,{}^2P^o$	421.276 (2)	421.47 (3)	[49]
			421.23 (4)	[47]
			421.12 (7)	[46]
	$1s2s2p\,({}^1P^o)\,{}^2P^o$	425.332 (5)	425.45 (3)	[49]
			425.62 (30)	[47]
			424.89 (15)	[46]
	$1s2p^2\,{}^2D$	429.215 (5)	429.07 (13)	[46][a]
	$1s2p^2\,{}^2S$	436.675 (10)	436.61 (10)	[46][a]
8	$1s2s^2\,{}^2S$	550.699 (8)	550.79 (8)	[46][a]
	$1s2s2p\,({}^3P^o)\,{}^2P^o$	563.064 (2)	562.93 (8)	[46][a]
			563.05 (15)	[47]
			562.94 (15)	[50]
			563.07 (4)	[51]
	$1s2s2p\,({}^1P^o)\,{}^2P^o$	567.720 (5)	567.50 (15)	[46][a]
			567.56 (26)	[47]
			567.62 (16)	[50]
	$1s2p^2\,{}^2D$	572.421 (5)	572.43 (8)	[46][a]
	$1s2p^2\,{}^2S$	581.21 (1)	581.04 (8)	[46][a]
10	$1s2s^2\,{}^2S$	891.72 (1)	891.52 (10)	[52]
	$1s2s2p\,({}^3P^o)\,{}^4P^o$	896.098 (4)	895.98 (4)	[52]
	$1s2s2p\,({}^3P^o)\,{}^2P^o$	908.152 (4)	907.90 (9)	[52]
	$1s2p^2({}^3P)\,{}^4P$	913.161 (3)	913.05 (4)	[52]
	$1s2s2p\,({}^1P^o)\,{}^2P^o$	914.007 (5)	913.91 (20)	[52]
	$1s2p^2\,{}^2D$	920.39 (1)	920.38 (6)	[52]
	$1s2p^2\,{}^2S$	931.82 (1)	932.19 (27)	[52]

[†] The statistical uncertainty as given in Table IV of Ref. [45] is added quadratically to the energy scale uncertainty of 0.05 eV mentioned in the text.

[a] Using the ionization energy of the ground state of the corresponding ion from Table III.

basis sets and by analyzing consecutive increments of the results as the basis set was increased in different directions (see Ref. [12] for details). The uncertainty of the QED energy shifts was estimated on the basis of the analysis presented in Sec. III. For single energy levels, we assume the uncertainty of the QED correction to be 1%. For the energy differences, we take the smallest of the two values, 4% of the QED correction to the energy difference and the two QED uncertainties for the two states added quadratically.

For the fine-structure intervals, the QED correction and its uncertainty largely cancel in the difference, so our theoretical values are more accurate for these intervals than for the center-of-gravity energies. The remaining theoretical uncertainty is dominated by the estimated error of the DCB energies, obtained by adding quadratically the uncertainties for the two levels.

Our final theoretical results for the wavelengths of the 22 strongest $1s2l2l' \rightarrow 1s^2 2l$ transitions are summarized in Table IV. The transitions are labeled from "a" to "v", following the widely used notations by Gabriel [29].

We now turn to analyzing the obtained results. We start with comparing our predictions with benchmark theoretical and experimental results available for the ground and first excited states of Li-like ions. Rigorous QED calculations to all orders in the nuclear binding strength parameter $Z\alpha$ were performed in Refs. [4,6,7,30], yielding the presently best theoretical results for the $1s^2 2s$, $1s^2 2p_{1/2}$, and $1s^2 2p_{3/2}$ states of Li-like ions with $Z \geqslant 10$. The ionization potential of the $1s^2 2s$ state was not presented explicitly but can be extracted. The corresponding comparison is presented in Table V. Excellent agreement with the results of the rigorous QED calculations confirms that we were able to keep the electron-correlation and QED effects in our calculations well under control.

Table VI presents a comparison of our predictions for the $2p_{1/2}$-$2s$ transition energies with the best theoretical and experimental data. There are remarkably many experimental results with accuracy significantly better than that of our predictions, most of them produced decades ago and summarized in Ref. [32]. The rigorous QED calculations [7] provide results only for $Z = 10$ and 15 in the region of Z relevant for the present work. Because of this, we also compare our values against the MBPT results of Ref. [34] supplemented by the QED correction evaluated separately in Ref. [35]. Although these results do not have estimations of uncertainties, they reproduce the experimental data remarkably well. We observe agreement within the estimated error bars for all cases listed in the table.

Table VII compares our theoretical results for the fine-structure splitting intervals of the $1s^2 2p\,{}^2P$, $1s2s2p\,{}^4P^o$, and $1s2p^2\,{}^4P^e$ states with the available experimental data. We observe that for the $1s^2 2p\,{}^2P$ state, the fine structure has been measured up to an accuracy significantly higher than that of our theoretical predictions. The agreement between theory and experiment is very good for $Z \leqslant 13$, but for $Z = 14-17$ we observe deviations on the level of $2-3\,\sigma$. For the $1s2s2p\,^4P^o$ and $1s2p^2\,^4P^e$ fine structure, our theory is more accurate than experiment.

In Table VIII, we compare our theoretical results with the experimental data on the multiplet separation center-of-gravity energies of the core-excited P levels. In this case, theory and experiment are on a similar level of accuracy. The agreement is very good for $Z \leqslant 10$ and deteriorates somewhat for $Z = 12$ and 13.

Finally, in Table IX we present a comparison of theoretical and experimental results for the center-of-gravity energies of different levels relative to the ground state. In this case, the accuracy of our theory is significantly higher than that of the experimental data. The agreement is good in the case of carbon. For higher Z ions, however, we observe numerous deviations between theory and experiment and between different experiments. We attribute these discrepancies to difficulties to reliably assign the energy scale in such x-ray measurements.

V. CONCLUSION

We performed extensive relativistic calculations of the energy levels and the fine-structure splitting of the $n = 2$ valence and core-excited states of Li-like ions. The Dirac-Coulomb-Breit energies were obtained by the configuration-interaction method adapted for treatment of autoionizing core-excited states. By using specially balanced basis sets, we were able to improve the convergence of our results and enhance the numerical accuracy of the calculated energy levels by up to two orders of magnitude as compared to that for the standard basis. The uncertainty of the Dirac-Coulomb-Breit energies was evaluated by analyzing the convergence of the results with respect to the number of partial waves included and the size of the one-electron basis.

The relativistic energies were supplemented with the QED energy shifts. To this end, the model QED operator approach as implemented by the QEDMOD package was used. In order to cover the range of the nuclear charge numbers Z aimed at in the present work, we extended the QEDMOD package (originally limited to $Z \geqslant 10$) to the lower values of Z. The uncertainty estimation of the QED energy shifts was based on the comparison with results of rigorous QED calculations available for the ground and first excited states of Li-like ions.

The main result of the present work is the tabulation of theoretical energy levels and transition wavelengths for the $1s^22l$ and $1s2l2l'$ states of ions along the lithium isoelectronic sequence from carbon to chlorine. All our theoretical predictions are supplied with uncertainties that include estimations of effects omitted in the theoretical treatment. For the $1s^22l$ states, our results agree well with the benchmark theoretical and experimental results available in the literature. For the core-excited $1s2l2l'$ energy levels, our theory is by an order of magnitude more accurate than the measurements performed so far, which opens possibilities for using theoretical predictions for calibrating experimental x-ray and electron spectra.

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[1] M. Puchalski and K. Pachucki, Phys. Rev. A **78**, 052511 (2008).

[2] M. Puchalski and K. Pachucki, Phys. Rev. Lett. **113**, 073004 (2014).

[3] M. Puchalski and K. Pachucki, Phys. Rev. A **92**, 012513 (2015).

[4] V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, M. M. Sysak, O. M. Zherebtsov, and G. Soff, Phys. Rev. A **64**, 032109 (2001).

[5] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **97**, 253004 (2006).

[6] V. A. Yerokhin, A. N. Artemyev, and V. M. Shabaev, Phys. Rev. A **75**, 062501 (2007).

[7] Y. S. Kozhedub, A. V. Volotka, A. N. Artemyev, D. A. Glazov, G. Plunien, V. M. Shabaev, I. I. Tupitsyn, and T. Stöhlker, Phys. Rev. A **81**, 042513 (2010).

[8] M. H. Chen, At. Data Nucl. Data Tables **34**, 301 (1986).

[9] J. Nilsen, At. Data Nucl. Data Tables **38**, 339 (1988).

[10] K. T. Chung, Phys. Rev. A **29**, 682 (1984).

[11] U. Safronova and M. Safronova, Can. J. Phys. **82**, 743 (2004).

[12] V. A. Yerokhin and A. Surzhykov, Phys. Rev. A **86**, 042507 (2012).

[13] J. K. Rudolph, S. Bernitt, S. W. Epp, R. Steinbrügge, C. Beilmann, G. V. Brown, S. Eberle, A. Graf, Z. Harman, N. Hell, M. Leutenegger, A. Müller, K. Schlage, H.-C. Wille, H. Yavaş, J. Ullrich, and J. R. Crespo López-Urrutia, Phys. Rev. Lett. **111**, 103002 (2013).

[14] M. Couprie, J. Electron Spectrosc. Relat. Phenom. **196**, 3 (2014).

[15] A. Müller, D. Bernhardt, A. Borovik, Jr., T. Buhr, J. Hellhund, K. Holste, A. L. D. Kilcoyne, S. Klumpp, M. Martins, S. Ricz *et al.*, Astrophys. J. **836**, 166 (2017).

[16] Y. Ralchenko (private communication).

[17] R. Piron, F. Gilleron, Y. Aglitskiy, H.-K. Chung, C. Fontes, S. Hansen, O. Marchuk, H. Scott, E. Stambulchik, and Y. Ralchenko, High Energy Density Phys. **23**, 38 (2017).

[18] M. H. Chen, K. T. Cheng, and W. R. Johnson, Phys. Rev. A **47**, 3692 (1993).

[19] M. H. Chen, K. T. Cheng, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **52**, 266 (1995).

[20] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. Lett. **93**, 130405 (2004).

[21] V. A. Yerokhin, A. Surzhykov, and S. Fritzsche, Phys. Rev. A **90**, 022509 (2014).

[22] V. A. Yerokhin, A. Surzhykov, and S. Fritzsche, Phys. Scr. **90**, 054003 (2015).

[23] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Phys. Rev. A **88**, 012513 (2013).

[24] V. Shabaev, I. Tupitsyn, and V. Yerokhin, Comput. Phys. Commun. **189**, 175 (2015).

[25] V. A. Yerokhin, K. Pachucki, and V. M. Shabaev, Phys. Rev. A **72**, 042502 (2005).

[26] V. A. Yerokhin and K. Pachucki, Phys. Rev. A **81**, 022507 (2010).

[27] A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A **71**, 062104 (2005).
[28] V. A. Yerokhin and V. M. Shabaev, J. Phys. Chem. Ref. Data **44**, 033103 (2015).
[29] A. H. Gabriel, Mon. Not. R. Astron. Soc. **160**, 99 (1972).
[30] V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, M. M. Sysak, O. M. Zherebtsov, and G. Soff, Phys. Rev. Lett. **85**, 4699 (2000).
[31] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team, *NIST Atomic Spectra Database* (ver. 5.3) (National Institute of Standards and Technology, Gaithersburg, MD, 2015) [http://physics.nist.gov/asd].
[32] B. Edlén, Phys. Scr. **28**, 51 (1983).
[33] U. Schramm, M. Bussmann, D. Habs, M. Steck, T. Kühl, K. Beckert, P. Beller, B. Franzke, F. Nolden, G. Saathoff, S. Reinhardt, and S. Karpuk, Hyperfine Interact. **162**, 181 (2005).
[34] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 2764 (1988).
[35] D. K. McKenzie and G. W. F. Drake, Phys. Rev. A **44**, R6973 (1991); **48**, 4803(E) (1993).
[36] A. E. Livingston and H. G. Berry, Phys. Rev. A **17**, 1966 (1978).
[37] L. Engström, R. Hutton, N. Reistad, I. Martinson, S. Huldt, S. Mannervik, and E. Träbert, Phys. Scr. **36**, 250 (1987).
[38] I. Martinson, B. Denne, J. O. Ekberg, L. Engström, S. Huldt, C. Jupn, U. Litzn, S. Mannervik, and A. Trigueiros, Phys. Scr. **27**, 201 (1983).
[39] A. E. Livingston, J. E. Hardis, L. J. Curtis, R. L. Brooks, and H. G. Berry, Phys. Rev. A **30**, 2089 (1984).
[40] E. J. Knystautas and M. Druetta, Phys. Rev. A **31**, 2279 (1985).
[41] E. Träbert, H. Hellmann, P. Heckmann, S. Bashkin, H. Klein, and J. Silver, Phys. Lett. A **93**, 76 (1982).
[42] J. P. Buchet, M. C. Buchet-Poulizac, A. Denis, J. Desesquelles, M. Druetta, S. Martin, J. P. Grandin, D. Hennecart, X. Husson, and D. Lecler, J. Phys. (Paris) **45**, 361 (1983).
[43] E. Träbert, H. Hellmann, and P. H. Heckmann, Z. Phys. A **313**, 373 (1983).
[44] A. Müller, S. Schippers, R. A. Phaneuf, S. W. J. Scully, A. Aguilar, A. M. Covington, I. Álvarez, C. Cisneros, E. D. Emmons, M. F. Gharaibeh *et al.*, J. Phys. B **42**, 235602 (2009).
[45] S. Mannervik, S. Asp, L. Broström, D. R. DeWitt, J. Lidberg, R. Schuch, and K. T. Chung, Phys. Rev. A **55**, 1810 (1997).
[46] M. Mack and A. Niehaus, Nucl. Instrum. Methods B **23**, 291 (1987).
[47] P. Nicolosi and G. Tondello, J. Opt. Soc. Am. **67**, 1033 (1977).
[48] P. Beiersdorfer, J. R. C. López-Urrutia, P. Springer, S. B. Utter, and K. L. Wong, Rev. Sci. Instrum. **70**, 276 (1999).
[49] M. M. Al Shorman, M. F. Gharaibeh, J. M. Bizau, D. Cubaynes, S. Guilbaud, N. E. Hassan, C. Miron, C. Nicolas, E. Robert, I. Sakho, C. Blancard, and B. M. McLaughlin, J. Phys. B **46**, 195701 (2013).
[50] B. M. McLaughlin, J.-M. Bizau, D. Cubaynes, S. Guilbaud, S. Douix, M. M. A. Shorman, M. O. A. E. Ghazaly, I. Sakho, and M. F. Gharaibeh, Mon. Not. R. Astron. Soc. **465**, 4690 (2017).
[51] M. Schmidt, P. Beiersdorfer, H. Chen, D. B. Thorn, E. Träbert, and E. Behar, Astrophys. J. **604**, 562 (2004).
[52] A. E. Kramida and M.-C. Buchet-Poulizac, Eur. Phys. J. D **39**, 173 (2006).