Relativistic many-body calculation of energies, lifetimes, hyperfine constants, and polarizabilities in ^{7}Li

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The excitation energies of ns, np, nd, and nf ($n \leq 6$) states in neutral lithium are evaluated within the framework of relativistic many-body theory. First-, second-, third-, and all-order Coulomb energies and first- and second-order Breit corrections to energies are calculated. All-order calculations of reduced matrix elements, oscillator strengths, transition rates, and lifetimes are given for levels up to $n=4$. Electric-dipole ($2s$ $-np$), electric-quadrupole ($2s-nd$), and electric-octupole ($2s-nf$), matrix elements are evaluated to obtain the corresponding ground-state multipole polarizabilities using the sum-over-states approach. Scalar and tensor polarizabilities for the $2p_{1/2}$ and $2p_{3/2}$ states are also calculated. Magnetic-dipole hyperfine constants A are determined for low-lying levels up to $n=4$. The quadratic Stark shift for the $(F=2\ M=0) \leftrightarrow (F=1\ M=0)$ ground-state hyperfine transition is found to be -0.0582 Hz/(kV/cm)^2, in slight disagreement with the experimental value -0.061 ± 0.002 Hz/(kV/cm)^2. Matrix elements used in evaluating polarizabilities, hyperfine constants, and the quadratic Stark shift are obtained using the all-order method.

I. INTRODUCTION

Investigations of the properties of neutral lithium provide excellent illustrations of how disagreement between theory and experiment leads to the development of new techniques that improve both theory and experiment. For example, precise calculations of energies and matrix elements for Li carried out in the late 1980s and early 1990s [1–6] gave an accurate value of the line strength of the $2p$-$2s$ transition close to $33.0a_0^2$. These theoretical calculations were confirmed by a highly accurate (0.0001%) variational calculation by Yan and Drake [7]. The theoretical lifetime disagreed by about 1% with a precise (0.15%) measurement by Gaupp *et al.* [8], which was confirmed by subsequent measurements [9]. The difference between theory and experiment was ultimately resolved through measurements by Volz and Schmoranzer [11] and McAlexander *et al.* [10].

Very recently, measurements of the electric polarizability of lithium by atom interferometry were presented by Miffre *et al.* [12]. The measured value $\alpha = 164.2 \pm 1.1$ a.u. illustrated the sensitivity of atom interferometry and is in agreement with the theoretical result $\alpha = 164.111 \pm 0.002$ a.u. obtained using variational wave functions by Yan *et al.* [13].

Experimental measurements by Windholz *et al.* [14] of scalar and tensor polarizabilities of the $2p$ ^2P state of Li also compare well with recent model-potential calculations by Cohen and Themells [15]. Highly accurate variational calculations (0.0002%–0.00035%) of electric-quadrupole ($E2$) and electric-octupole ($E3$) polarizabilities of the Li ground state were carried out by Yan *et al.* [13] and relativistic many-body calculations of $E2$ and $E3$ polarizabilities for the Li ground state, accurate to 0.3%, were carried out by Porsev and Derevianko [16]. In the latter calculations, wave functions were determined from an effective many-body Schrödinger equation [17,18]. Measurements of the Stark shift of the $(F=2\ M=0) \leftrightarrow (F=1\ M=0)$ ground-state hyperfine interval in Li $[-0.061 \pm 0.002$ Hz/(kV/cm)$^2]$ were carried out by Mowat [19] and evaluated theoretically to be -0.0627 Hz/(kV/cm)^2 by Kaldor [20] and -0.0595 Hz/(kV/cm)^2 by Lee *et al.* [21].

In the present paper, we investigate all of the above properties of the ground state and low-lying excited states of neutral Li using the relativistic all-order method described by Blundell *et al.* [2]. In particular, we evaluate the excitation energies of ns, np, nd, and nf states with $n \leq 6$, reduced matrix elements, oscillator strengths, transition rates, and lifetimes for levels with $n \leq 4$, ground state $E1$, $E2$, and $E3$ static polarizabilities, scalar and tensor polarizabilities for $2p$ and $2p$ states, and magnetic-dipole hyperfine constants A for levels with $n \leq 4$. We use B-splines [22] to generate a complete set of basis orbitals for use in the evaluation of energies and matrix elements.

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TABLE I. Zeroth-order (DHF), second-order, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies $E^{(SD)}$ and $E^{(3)}_{extra}$, first-order and second-order Breit corrections $B^{(n)}$, and Lamb shift E_{LS} and recoil E_{recoil} corrections in ^{7}Li. The total energies $(E^{(3)}_{tot}=E^{(0)}+E^{(2)}+E^{(3)}+B^{(1)}+B^{(2)}+E_{LS}+E_{recoil}$ and $E^{(SD)}_{tot}=E^{(0)}+E^{SD}+E^{(3)}_{extra}+B^{(1)}+B^{(2)}+E_{LS}+E_{recoil})$ are compared with experimental energies E_{NIST} [23], $\delta E=E_{tot}-E_{NIST}$. Units: cm^{-1}. The value of the infinite-mass Rydberg constant used to convert numerical data from a.u. to cm^{-1} is Ry=10 973.7316.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	E_{recoil}	$E^{(3)}_{tot}$	$E^{(SD)}$	$E^{(3)}_{extra}$	$E^{(SD)}_{tot}$	E_{NIST}	$\delta E^{(3)}$	$\delta E^{(SD)}$
$2s_{1/2}$	−43087.3	−362.03	−26.94	1.16	−0.48	0.24	3.59	−43471.8	−407.02	2.35	−43487.5	−43487.2	15.3	−0.4
$2p_{1/2}$	−28232.9	−301.77	−29.69	0.61	−0.18	0.00	1.52	−28562.4	−353.11	2.14	−28581.9	−28583.5	21.1	1.6
$2p_{3/2}$	−28232.3	−301.67	−29.69	0.31	−0.16	0.00	1.52	−28562.0	−352.99	2.13	−28581.5	−28583.2	21.1	1.6
$3s_{1/2}$	−16197.4	−76.72	−5.48	0.26	−0.12	0.07	1.32	−16278.1	−85.52	0.38	−16281.0	−16281.0	2.9	0.0
$3p_{1/2}$	−12460.0	−88.63	−8.36	0.20	−0.06	0.00	0.76	−12556.1	−102.58	0.56	−12561.2	−12561.8	5.6	0.6
$3p_{3/2}$	−12459.9	−88.60	−8.36	0.11	−0.06	0.00	0.76	−12556.0	−102.54	0.56	−12561.0	−12561.8	5.8	0.7
$3d_{3/2}$	−12194.4	−8.93	−1.24	0.00	0.00	0.00	0.95	−12203.7	−10.67	0.13	−12204.0	−12204.1	0.4	0.1
$3d_{5/2}$	−12194.4	−8.93	−1.24	0.00	0.00	0.00	0.95	−12203.6	−10.67	0.13	−12204.0	−12204.0	0.4	0.0
$4s_{1/2}$	−8444.5	−28.33	−2.00	0.11	−0.04	0.03	0.68	−8474.0	−31.51	0.13	−8475.1	−8475.1	1.0	0.0
$4p_{1/2}$	−6975.1	−37.16	−3.46	0.09	−0.03	0.00	0.45	−7015.2	−42.84	0.23	−7017.2	−7017.6	2.4	0.4
$4p_{3/2}$	−6975.0	−37.15	−3.46	0.04	−0.02	0.00	0.45	−7015.2	−42.83	0.23	−7017.2	−7017.6	2.4	0.4
$4d_{3/2}$	−6859.4	−4.18	−0.56	0.00	0.00	0.00	0.54	−6863.6	−4.97	0.06	−6863.8	−6863.8	0.2	0.0
$4d_{5/2}$	−6859.4	−4.18	−0.56	0.00	0.00	0.00	0.54	−6863.6	−4.97	0.06	−6863.8	−6863.8	0.2	0.0
$4f_{5/2}$	−6858.6	−0.64	−0.10	0.00	0.00	0.00	0.54	−6858.8	−0.78	0.01	−6858.8	−6857.0	−1.9	−1.9
$4f_{7/2}$	−6858.6	−0.64	−0.10	0.00	0.00	0.00	0.54	−6858.8	−0.78	0.01	−6858.8	−6857.0	−1.8	−1.9
$5s_{1/2}$	−5173.2	−13.49	−0.95	0.04	−0.02	0.01	0.41	−5187.2	−14.99	0.06	−5187.7	−5187.7	0.5	0.0
$5p_{1/2}$	−4450.0	−18.95	−1.76	0.04	−0.01	0.00	0.35	−4470.3	−21.80	0.11	−4471.3	−4471.6	1.3	0.3
$5p_{3/2}$	−4450.0	−18.94	−1.76	0.02	−0.01	0.00	0.35	−4470.3	−21.79	0.11	−4471.3	−4471.6	1.3	0.3
$5d_{3/2}$	−4390.0	−2.24	−0.30	0.00	0.00	0.00	0.34	−4392.2	−2.65	0.03	−4392.3	−4392.2	0.1	0.0
$5d_{5/2}$	−4390.0	−2.23	−0.30	0.00	0.00	0.00	0.34	−4392.1	−2.65	0.03	−4392.2	−4392.2	0.1	0.0
$5f_{5/2}$	−4389.5	−0.37	−0.06	0.00	0.00	0.00	0.34	−4389.6	−0.45	0.01	−4389.6	−4382.7	−6.9	−6.9
$5f_{7/2}$	−4389.5	−0.37	−0.06	0.00	0.00	0.00	0.34	−4389.6	−0.45	0.01	−4389.6	−4382.7	−6.9	−6.9
$6s_{1/2}$	−3491.6	−7.45	−0.53	0.02	−0.01	0.01	0.27	−3499.3	−8.28	0.03	−3499.6	−3499.5	0.2	0.0
$6p_{1/2}$	−3083.5	−10.94	−1.01	0.02	−0.01	0.00	0.24	−3095.2	−12.56	0.07	−3095.8	−3096.3	1.1	0.6
$6p_{3/2}$	−3083.5	−10.93	−1.01	0.02	−0.01	0.00	0.24	−3095.2	−12.56	0.07	−3095.7	−3096.3	1.1	0.6
$6d_{3/2}$	−3048.5	−1.32	−0.17	0.00	0.00	0.00	0.24	−3049.8	−1.57	0.02	−3049.9	−3049.8	0.0	0.0
$6d_{5/2}$	−3048.5	−1.32	−0.17	0.00	0.00	0.00	0.24	−3049.8	−1.57	0.02	−3049.9	−3049.8	0.0	0.0

II. THIRD-ORDER AND ALL-ORDER MANY-BODY PERTURBATION THEORY CALCULATIONS OF ENERGIES

Energies of nl_j states are evaluated for $n \leq 6$ and $l \leq 3$ using both third-order many-body perturbation theory (MBPT) and the single-double (SD) all-order method discussed in Ref. [2], in which single and double excitations of Dirac-Hartree-Fock (DHF) wave functions are iterated to all orders. Results of our energy calculations are summarized in Table I. Columns 2–8 of Table I give the lowest-order DHF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, first-order and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$, an estimated Lamb shift contribution E_{LS}, and a recoil correction E_{recoil}. The sum of these contributions $E^{(3)}_{tot}$, listed in the ninth column of Table I, is the final third-order MBPT result. The recoil correction, which is the sum of the reduced mass correction and the mass-polarization correction, is calculated through third-order in MBPT. The Lamb shift correction for ns states is estimated

by scaling the $2s$ Lamb shift ($X_\alpha=2/3$ case) given by Sapirstein and Cheng [24] with $1/n^3$. The $2s$ Lamb shift from [24] is consistent with values found in Refs. [25,26]. For states with $l>0$, the Lamb shift is estimated to be smaller than 0.01 cm^{-1} using scaled Coulomb values and is ignored. We list the all-order SD energies in the column labeled $E^{(SD)}$ and list that part of the third-order energies missing from $E^{(SD)}$ in the column labeled $E^{(3)}_{extra}$. The sum of the seven terms $E^{(0)}$, E^{SD}, $E^{(3)}_{extra}$, $B^{(1)}$, $B^{(2)}$, E_{LS} and E_{recoil} is our final all-order result E^{SD}_{tot}, listed in the 12th column of Table I. Recommended energies from the National Institute of Standards and Technology (NIST) database [23] are given in the column labeled E_{NIST}. Differences between our third-order and all-order calculations and experimental data, $\delta E^{(3)}=E^{(3)}_{tot}-E_{NIST}$ and $\delta E^{(SD)}=E^{(SD)}_{tot}-E_{NIST}$, are given in the two final columns of Table I, respectively.

As expected, the largest correlation contribution to the valence energy comes from the second-order term $E^{(2)}$. Therefore, we calculate $E^{(2)}$ with higher numerical accuracy.

The second-order energy includes partial waves up to l_{max} $=8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [27,28]). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $2s_{1/2}$ state. Calculations of $E^{(2)}$ with $l_{max}=6$ and 8 yield $E^{(2)}(2s_{1/2})=-361.046$ and -361.596 cm^{-1}, respectively. Extrapolation of these calculations yields -362.025 and -362.066 cm^{-1}, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(2s_{1/2})$ of 0.041 cm^{-1}. It should be noted that the 1.02 cm^{-1} contribution from partial waves with $l>8$ for the $2s$ state is the largest among all states considered in Table I; a smaller (1.00 cm^{-1}) contribution is obtained for the two other $n=2$ states and a much smaller contribution ($0.01–0.32$ cm^{-1}) for $n=3$ states.

Owing to numerical complexity, we restrict $l \le l_{max}=6$ in the $E^{(SD)}$ calculation. As noted above, the second-order contribution dominates $E^{(SD)}$; therefore, we can use the extrapolated value of $E^{(2)}$ described above to account for the contributions of the higher partial waves. Six partial waves are also used in the calculation of $E^{(3)}$. Since the asymptotic l dependences of the second- and third-order energies are similar (both fall off as l^{-4}), we use the second-order remainder as a guide to estimate the remainder in the third-order contribution. The term $E^{(3)}_{extra}$ in Table I, which accounts for that part of the third-order MBPT energy missing from the SD all-order expression for the energy, is smaller than $E^{(3)}$ by an order of magnitude for the states considered here.

The column labeled $\delta E^{(SD)}$ in Table I gives differences between our *ab initio* results and the experimental values [23]. The SD all-order results agree better with measured values than do the third-order MBPT results, illustrating the importance of fourth- and higher-order correlation corrections. It should be noted that the largest differences between our SD all-order data and the NIST data occur for $4f$ (1.9 cm^{-1}) and $5f$ (6.9 cm^{-1}) states. However, we agree very well (0.0 cm^{-1} for the $4f$ states and 0.2 cm^{-1} for the $5f$ states) with more recent measurement of Radziemski *et al.* [29]. We refer the reader to Ref. [30] and references therein for a detailed discussion of the $4f$ energy level.

Below, we give a few numerical details of our calculation. We use the B-spline method described in [22] to generate a complete set of DHF basis wave functions for use in the evaluation of MBPT expressions. For Li I, we use 70 splines of order $k=9$ for each angular momentum. The basis orbitals are constrained to a spherical cavity of radius $R=220$ a.u. The cavity radius is chosen large enough to accommodate all nl_j orbitals considered here and small enough that 70 splines can approximate inner-shell DHF wave functions with good precision. We use 65 out 70 basis orbitals for each partial wave in our third-order and all-order energy calculations, since contributions from the highest-energy orbitals are negligible.

III. OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES

We calculate oscillator strengths and transition probabilities for $nl_j-n'l'_{j'}$ electric-dipole transitions with $n \le 4$ and l

TABLE II. Oscillator strengths f averaged over j. The SD all-order data ($f^{(SD)}$) are compared with other theoretical data.

Lower	Upper	$f^{(SD)}$	f	f
$2s\ ^2S$	$2p\ ^2P$	0.746944	0.747042 [31]	0.7469572(10) [7]
$2s\ ^2S$	$3p\ ^2P$	0.004704	0.004712 [31]	0.0047242 [33]
$2s\ ^2S$	$4p\ ^2P$	0.004235		0.0042187 [33]
$2p\ ^2P$	$3s\ ^2S$	0.110595	0.110554 [31]	0.110505 [33]
$2p\ ^2P$	$4s\ ^2S$	0.012833	0.012835 [31]	0.012887 [33]
$2p\ ^2P$	$3d\ ^2D$	0.638615	0.638546 [31]	0.6385705(30) [7]
$2p\ ^2P$	$4d\ ^2D$	0.122731		0.123008 [33]
$3s\ ^2S$	$3p\ ^2P$	1.214724	1.215881 [31]	1.214925 [33]
$3s\ ^2S$	$4p\ ^2P$	0.000041		0.000024 [33]
$3p\ ^2P$	$3d\ ^2D$	0.074366	0.074336 [31]	0.074173 [33]
$3p\ ^2P$	$4d\ ^2D$	0.522086		0.522649 [33]
$3p\ ^2P$	$4s\ ^2S$	0.223285	0.223283 [31]	0.223392 [33]
$3d\ ^2D$	$4p\ ^2P$	0.018129		0.017963 [33]
$3d\ ^2D$	$4f\ ^2F$	1.015637		1.0153 [34]
$4s\ ^2S$	$4p\ ^2P$	1.640289		1.6359 [33]
$4p\ ^2P$	$4d\ ^2D$	0.135795		0.135305 [33]
$4d\ ^2D$	$4f\ ^2F$	0.003130		

≤ 3 in the SD all-order approximation [2]. Our results are compared with other theoretical calculations [7,31–34], and with experimental measurements [11,35–39] in Tables II and III. Numerous theoretical calculations concerning the properties of neutral lithium have been published over the past 30 years. In Table II, we compare our SD all-order oscillator strengths with the accurate calculations given in Refs. [7,31–34]. The highest-accuracy oscillator strengths for $2s\ ^2S$-$2p\ ^2P$ (0.0001%) and $2p\ ^2P$-$3d\ ^2D$ (0.0005%) transi-

TABLE III. Lifetimes of $nl\ ^2L_J$ states in neutral lithium. The SD all-order data ($\tau^{(SD)}$) are compared with theoretical and experimental data.

Level	$\tau^{(SD)}$	τ^{th}	τ^{expt}
$2p\ ^2P$	27.108	27.109804(36) [7]	27.102(9) [35]
$2p\ ^2P_{1/2}$	27.109	27.106 [31]	27.102(9) [35]
$2p\ ^2P_{3/2}$	27.107	27.104 [31]	27.102(9) [35]
$3d\ ^2D$	14.583	14.583687(68) [7]	14.60(13) [36]
$3d\ ^2D_{3/2}$	14.584	14.591 [31]	
$3d\ ^2D_{5/2}$	14.583	14.592 [31]	
$3s\ ^2S_{1/2}$	29.856	29.886 [31]	29.72(7) [11]
$3p\ ^2P_{1/2}$	211.11	210.94 [32]	203(8) [37]
$3p\ ^2P_{3/2}$	211.15	210.93 [32]	
$4d\ ^2D_{3/2}$	33.382	33.315 [33]	31.0(1.0) [38]
$4d\ ^2D_{5/2}$	33.381	33.315 [33]	
$4s\ ^2S_{1/2}$	56.037	56.084 [32]	56(1.7) [39]
$4f\ ^2F_{5/2}$	72.278		
$4f\ ^2F_{7/2}$	72.279		
$4p\ ^2P_{1/2}$	388.17	357.2 [33]	
$4p\ ^2P_{3/2}$	388.30	357.2 [33]	

TABLE IV. Contributions to multipole polarizabilities (a.u.) of the $2s$ state of Li. The two leading terms and those terms with $n \leq 26$ in the expression for α_v^{Ek} [Eq. (1)] are evaluated using SD all-order wave functions. The remainders ($n > 26$), labeled "Tail" below, are evaluated in the DHF approximation. Contributions from core-excited states α_c^{Ek} are evaluated in the random-phase approximation.

$nlj = 2p_{1/2}$	53.993	$nlj = 3d_{3/2}$	421.75	$nlj = 4f_{5/2}$	4949.3
$nlj = 2p_{3/2}$	107.986	$nlj = 3d_{5/2}$	632.60	$nlj = 4f_{7/2}$	6599.1
$nl = [3p - 26p]$	1.915	$nl = [4d - 26d]$	368.16	$nl = [5f - 26f]$	28074.8
Tail	0.001	Tail	0.12	Tail	0.9
α_v^{E1}	163.895	α_v^{E2}	1422.62	α_v^{E3}	39624.1
α_c^{E1}	0.189	α_c^{E2}	0.11	α_c^{E3}	0.2
α^{E1}	164.084	α^{E2}	1422.73	α^{E3}	39624.2

tions were those obtained by Yan and Drake [7] who used variationally constructed wave functions in Hylleraas coordinates. Another Hylleraas-type calculation of the properties of lithium was presented by Pestka and Wolźnicki [33], where superposition of correlated configurations was used to evaluate the nonrelativistic energies and lifetimes of the ns ^2S, np ^2P, and nd ^2D states with $n \leq 4$ together with the oscillator strengths of the transitions between such states. The multiconfiguration Hartree-Fock (MCHF) method was used recently by Godefroid *et al.* [31] to calculate the atomic properties of $[2s, 3s, 4s$ $^2S]$, $[2p, 3p$ $^2P]$, and $[3d$ $^2D]$ states in Li and Li-like ions. The reliability of expectation values in [31] was assessed by analysis of convergence patterns as the approximate wave function was systematically improved. In order to compare our relativistic SD all-order oscillator strengths $f(nlj, n'l'j')$ with the nonrelativistic results given in Refs. [7,31–34], we average our $f(nlj, n'l'j')$ data over j and j'. The contribution of relativistic effects is in the range 0.005%–0.01%. We can see from Table II that the difference between our SD all-order values and the high-precision values from [7] is about 0.002% for the $2s$ ^2S-$2p$ ^2P transition and 0.006% for the $2p$ ^2P-$3d$ ^2D transition. These differences are in part explained by relativistic effects omitted in Ref. [7]. The largest and smallest differences between the present SD all-order oscillator strengths and the MCHF [31] values listed in Table II are 0.17% ($2s$ ^2S-$3p$ ^2P transition) and 0.001% ($3p$ ^2P-$4s$ ^2S transition), respectively. The differences between the SD all-order oscillator strengths and the oscillator strengths presented by Pestka and Wolźnicki [33] (see Table II) are much larger; the smallest difference is 0.003% for the $2s$ ^2S-$2p$ ^2P transition and the largest difference is 73% for the $3s$ ^2S-$4p$ ^2P transition. It should be noted that the oscillator strength of the $3s$ ^2S-$4p$ ^2P transition is three to four orders of magnitude smaller than for other transitions.

We also calculate the lifetimes of ns $^2S_{1/2}$, np ^2P_J, nd ^2D_J, and nf ^2F_J states for $n \leq 4$ in neutral lithium using SD all-order dipole matrix elements and experimental energies [23]. We list the lifetimes $\tau^{(SD)}$ in Table III. The difference between lifetimes of np $^2P_{1/2}$ and np $^2P_{3/2}$ states is 0.01%, 0.02%, and 0.03% for $n = 2$, 3, and 4, respectively, illustrating the size of relativistic effects. In Table III, we compare lifetimes $\tau^{(SD)}$ with available experimental measurements [11,35–39]. Experimental results have changed with time, and we present only the most recent results in Table III. (We

found no experimental measurements for $3d$ ^2D_J, $4p$ ^2P_J, or $4f$ ^2F_J states.) Our SD all-order results agree well with measurements when experimental uncertainties are taken into account. We also compare our lifetime calculations with theoretical results from Refs. [7,31–33] in Table III. We find excellent agreement (0.008% and 0.002%) between the present lifetime data and the high-precision results [7] for $2p$ ^2P and $3d$ ^2D states. Differences between our values of $\tau^{(SD)}$ and the results from Refs. [31,32] for the $2p$ ^2P_J, $3d$ ^2D_J, $3s$ $^2S_{1/2}$, $3p$ ^2P_J, and $4s$ $^2S_{1/2}$ states are less than 0.1%. There is also good agreement, except for the $4p$ ^2P state, with results from Ref. [33]. (The differences found for $4p$ ^2P states are unexpected since we have excellent agreement for oscillator strengths for all transitions including the $4p$ ^2P state, as seen in Table II. When we recalculate the lifetime of the $4p$ ^2P state using data given in Table IV of Ref. [33], we obtain the value $\tau = 375$ ns which agrees much better with our value $\tau^{(SD)} = 388$ ns than the value 357 ns given in Table V of Ref. [33].)

IV. STATIC MULTIPOLE POLARIZABILITIES IN THE 2s GROUND STATE OF NEUTRAL LI

The static multipole polarizability α_v^{Ek} of Li in its $2s$ ground state can be separated into two terms: a dominant first term from intermediate valence-excited states $|nl_j(1s)^2\rangle$ and a smaller second term from intermediate core-excited $|nl_j 2s 1s\rangle$ states. The latter term is smaller than the former by several orders of magnitude and is here evaluated in the random-phase approximation [41]. The dominant valence contribution is calculated using the sum-over-state approach,

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 2s \rangle|^2}{E_{nlj} - E_{2s}}, \quad (1)$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and where nl_j is np_j, nd_j, and nf_j for $k = 1$, 2, and 3, respectively [42]. The reduced matrix elements in the above sum are evaluated using the SD all-order approximation for basis states with $n \leq 26$ and in the DHF approximation for the remaining states.

Contributions to dipole, quadrupole, and octupole polarizabilities of the $2s$ ground state are presented in Table IV. The first two terms in the sum-over-states for α^{E1}, α^{E2}, and α^{E3} contribute 98.8%, 74%, and 29%, respectively, of the

TABLE V. Multipole polarizabilities α^{E1}, α^{E2}, and α^{E3} of the $2s$ ground state of Li are compared with other calculations and with experiment.

Reference	α^{E1}	α^{E2}	α^{E3}
Present	164.084	1422.73	39624.2
Yan *et al.* [13]	164.111(2)	1423.266(5)	39650.49(8)
Porsev and Derevianko[16]		1424(4)	39570
Derevianko *et al.* [40]	164.0(1)		
Experiment [12]	164.2(1.1)		

totals. The rapid convergence of the sum over states for α_1 has been emphasized in many publications (for example, [43,44]). We use recommended energies from [23] and SD all-order wave functions to evaluate terms in the sum with $n \leq 13$, and we use theoretical SD all-order energies and wave functions to evaluate terms with $13 \leq n \leq 26$. The remaining contributions to α^{Ek} from basis functions with $27 \leq n \leq 70$ are evaluated in the DHF approximation. As can be seen from Table IV, sums over n for $n \leq 26$ in α^{E2} and α^{E3} essentially reproduce the final results, since the contribution from $27 \leq n \leq 70$ is smaller than 0.01% in all cases.

Final results for the multipole polarizabilities of the Li I ground state are compared in Table V with high-precision calculations given in Refs. [13,16,40] and a recent experimental measurement presented in Ref. [12]. Our results given in the first row of Table V differ from high-precision calculations presented by Yan *et al.* [13] by 0.016%, 0.03%, and 0.06% for α^{E1}, α^{E2}, and α^{E3}, respectively. Our results agree with values given by Porsev and Derevianko [16] for the quadrupole polarizability taking into account the uncertainty given in [16]; however, the difference for the octupole polarizability is equal to 0.13%. Also, we agree with theoretical results given by Derevianko *et al.* [40] for the dipole polarizabilty within the uncertainty quoted in [40]. The uncertainty in the experimental measurement [12] of the dipole polarizability is too large to reflect on the accuracy of the present calculations.

V. SCALAR AND TENSOR POLARIZABILITIES OF THE $2p_{1/2}$ AND $2p_{3/2}$ EXCITED STATES OF Li

The scalar $\alpha_0(v)$ and tensor $\alpha_2(v)$ polarizabilities of an excited state v of Li are given by

$$\alpha_0(v) = \frac{2}{3(2j_v+1)} \sum_{nlj} \frac{|\langle v\|rC_1\|nlj\rangle|^2}{E_{nlj} - E_v}, \quad (2)$$

$$\alpha_2(v) = (-1)^{j_v} \sqrt{\frac{40 j_v (2j_v - 1)}{3(j_v+1)(2j_v+1)(2j_v+3)}}$$
$$\times \sum_{nlj} (-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} \frac{|\langle v\|rC_1\|nlj\rangle|^2}{E_{nlj} - E_v}. \quad (3)$$

As before, our calculation of the sums is divided into three parts. The first part is the sum over valence states with $n \leq 26$, which is carried out using SD all-order wave func-

TABLE VI. Contributions to scalar polarizability of Li in the excited $2p_{1/2}$ and $2p_{3/2}$ states calculated with SD all-order wave functions $\alpha_0(2p_{1/2}) = \sum_{n=3}^{70} I_{2p_{1/2}}(nd_{3/2}) + \sum_{n=1}^{70} I_{2p_{1/2}}(ns_{1/2})$ and $\alpha_0(2p_{3/2}) = \sum_{n=3}^{70} I_{2p_{3/2}}(nd_j) + \sum_{n=1}^{70} I_{2p_{3/2}}(ns_{1/2})$.

Contribution	$j=1/2$	$j=3/2$
$\sum_{n=3}^{26} I_{2p_j}^{(SD)}(nd_{3/2})$	142.648	14.266
$\sum_{n=3}^{26} I_{2p_j}^{(SD)}(nd_{5/2})$	0	128.393
$\sum_{n=1}^{26} I_{2p_j}^{(SD)}(ns_{1/2})$	−15.860	−15.856
$\alpha_{main}^{(SD)}(2p_j)$	126.787	126.802
$\alpha_{tail}^{(DF)}(2p_j)$	0.007	0.007
$\alpha_{core}(2p_j)$	0.189	0.189
$\alpha_{vc}(2p_j)$	−0.003	−0.003
$\alpha^{(SD)}(2p_j)$	126.980	126.995

tions. The second part is the sum over basis states with $n > 26$, which is carried out in the DHF approximation. The third part is the contribution from core-excited states, which is carried out in the random-phase approximation (RPA).

A breakdown of contributions to the scalar dipole polarizability for the excited $2p_{1/2}$ and $2p_{3/2}$ states is presented in Table VI. Contributions from excited ns and nd states with $n \leq 26$ differ only by 0.001%. Contributions from excited ns and nd states $n > 26$ are very small $\alpha_{n>26} = 0.007a_0^3$ and are calculated in the DHF approximation. We evaluate the contribution from the ionic core α_{core} in the RPA and find $\alpha_{core} = 0.1894a_0^3$. A counterterm $\alpha_{vc}(2p_j)$ compensating for excitation from the core to the valence shell which violates the Pauli principle is also evaluated in the RPA and found to be $\alpha_{vc}(2p_j) = -0.003a_0^3$. The above values were combined to obtain our final result for the scalar polarizability of the first two excited states in Li I: $\alpha_0^{(SD)}(2p_{1/2}) = 126.980a_0^3$ and $\alpha_0^{(SD)}(2p_{3/2}) = 126.995a_0^3$.

We present the details of our calculation of the tensor polarizability α_2 of the $2p_{3/2}$ state in Table VII. Reduced electric-dipole matrix elements evaluated in the SD all-order approximation are given in the columns labeled $Z_{vn} \equiv \langle v\|rC_1\|nlj\rangle$. The corresponding contributions to the tensor polarizability are given in the columns labeled I_{nlj}. The sum of contributions from $nd_{3/2}$ and $ns_{1/2}$ intermediate states is almost compensated for by the contribution from the $nd_{5/2}$ states. The resulting contribution to $\alpha_2(2p_{3/2})$ from states with $n \leq 26$ is $1.590a_0^3$. Contributions from states with $n > 26$ are $-0.001a_0^3$.

States with $n > 13$ in our basis have positive energies and provide a discrete representation of the continuum. We find that the continuous part of the spectra is responsible for 6% of $\alpha_2(2p_{3/2})$. We evaluated the continuum contributions in the range $14 < n \leq 26$ using SD all-order wave functions for dipole matrix elements and energies. For $n \leq 13$, we use SD all-order matrix elements and NIST energies [23] in the sums. Our final result is $\alpha_2^{(SD)}(2p_{3/2}) = 1.59a_0^3$.

Our results for scalar and tensor polarizabilities of the $2p_j$ excited state of Li are compared in Table VIII with recent

TABLE VII. Contributions to tensor polarizability of Li in the excited state $v=2p_{3/2}$ calculated using all-order SD method $\alpha_2(2p_{3/2})=\Sigma_{n=3}^{70}I_{2p_{3/2}}(nd_j)+\Sigma_{n=1}^{70}I_{2p_{3/2}}(ns_{1/2})$. SD all-order dipole matrix elements $Z_{vn}=\langle v\|rC_1\|nlj\rangle$ are also given. All values are in a.u.

n	Z_{vn}	$I_v(nd_{3/2})$	n	Z_{vn}	$I_v(nd_{5/2})$	n	Z_{vn}	$I_v(ns_{1/2})$
						$2s_{1/2}$	4.690	53.994
$3d_{3/2}$	−2.266	9.173	$3d_{5/2}$	−6.798	−20.640	$3s_{1/2}$	3.441	−35.200
$4d_{3/2}$	0.863	1.003	$4d_{5/2}$	2.588	−2.256	$4s_{1/2}$	0.917	−1.529
$5d_{3/2}$	0.501	0.304	$5d_{5/2}$	1.504	−0.685	$5s_{1/2}$	−0.493	−0.380
$6d_{3/2}$	0.344	0.135	$6d_{5/2}$	−1.031	−0.304	$6s_{1/2}$	−0.327	−0.156
$7d_{3/2}$	0.257	0.073	$7d_{5/2}$	0.770	−0.164	$7s_{1/2}$	−0.240	−0.081
$8d_{3/2}$	−0.202	0.044	$8d_{5/2}$	−0.606	−0.100	$8s_{1/2}$	0.187	−0.048
$9d_{3/2}$	0.165	0.029	$9d_{5/2}$	0.496	−0.066	$9s_{1/2}$	0.151	−0.031
$10d_{3/2}$	0.148	0.023	$10d_{5/2}$	−0.445	−0.053	$10s_{1/2}$	0.130	−0.022
$11d_{3/2}$	0.158	0.026	$11d_{5/2}$	−0.473	−0.059	$11s_{1/2}$	−0.132	−0.023
$12d_{3/2}$	−0.171	0.031	$12d_{5/2}$	0.512	−0.069	$12s_{1/2}$	−0.144	−0.027
$13d_{3/2}$	−0.180	0.033	$13d_{5/2}$	−0.541	−0.075	$13s_{1/2}$	−0.145	−0.027
$14d_{3/2}$	−0.155	0.024	$14d_{5/2}$	−0.540	−0.074	$14s_{1/2}$	−0.189	−0.045
$15d_{3/2}$	−0.193	0.037	$15d_{5/2}$	0.549	−0.075	$15s_{1/2}$	0.143	−0.026
$16d_{3/2}$	0.144	0.021	$16d_{5/2}$	−0.565	−0.078	$16s_{1/2}$	−0.007	0.000
$17d_{3/2}$	−0.318	0.096	$17d_{5/2}$	0.984	−0.228	$17s_{1/2}$	−0.360	−0.154
$18d_{3/2}$	−0.079	0.006	$18d_{5/2}$	0.038	0.000	$18s_{1/2}$	0.414	−0.177
$19d_{3/2}$	−0.364	0.116	$19d_{5/2}$	1.093	−0.258	$19s_{1/2}$	0.003	0.000
$20d_{3/2}$	0.364	0.103	$20d_{5/2}$	−1.078	−0.222	$20s_{1/2}$	0.391	−0.127
$21d_{3/2}$	0.023	0.000	$21d_{5/2}$	−0.011	0.000	$21s_{1/2}$	−0.312	−0.060
$22d_{3/2}$	0.327	0.071	$22d_{5/2}$	0.957	−0.148	$22s_{1/2}$	−0.216	−0.020
$23d_{3/2}$	−0.265	0.038	$23d_{5/2}$	−0.767	−0.077	$23s_{1/2}$	−0.133	−0.005
$24d_{3/2}$	−0.196	0.016	$24d_{5/2}$	0.561	−0.032	$24s_{1/2}$	0.075	−0.001
$25d_{3/2}$	0.133	0.006	$25d_{5/2}$	−0.379	−0.011	$25s_{1/2}$	0.041	0.000
$26d_{3/2}$	0.085	0.002	$26d_{5/2}$	−0.240	−0.003	$26s_{1/2}$	−0.064	0.000
Sum		11.413			−25.679			15.856

$$\alpha_{n\leq26}^{(SD)}(2p_{3/2})=1.590$$
$$\alpha_{n>26}(2p_{3/2})=-0.001$$
$$\alpha^{(SD)}(2p_{3/2})=1.59$$

calculations by Cohen and Themells [15] and with experimental measurements reported by Windholz *et al.* [14]. The Rydberg-Klein-Rees inversion method combined with quantum defect theory was used in [15] to calculate the scalar (α_0) and tensor (α_2) polarizabilities nonrelativistically. As can be seen from Table VIII, the present SD all-order results

TABLE VIII. Values of scalar (α_0) and tensor (α_2) part of polarizability of the excited state $2p\ ^2P_J$ in Li I. The SD all-order data are compared with (a) theoretical [15] and (b) experimental [14] values.

	$\alpha^{(SD)}$	$\alpha_{th.}^a$	α_{expt}^b
$\alpha_2(2p\ ^2P_{3/2})$	1.59	1.75	1.64(4)
$\alpha_0(2p\ ^2P_{1/2})$	126.980		126.9(3)
$\alpha_0(2p\ ^2P_{3/2})$	126.995		126.7(4)
$\alpha_0(2p\ ^2P)$	126.990	126.4	

are in better agreement with measurements [14] than with the theoretical results given by Cohen and Themells [15].

VI. HYPERFINE CONSTANTS FOR ^{7}Li

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition matrix elements. In Table IX, we list the hyperfine constants A for ^{7}Li and compare our values with calculations by Godefroid *et al.* [31] and with available experimental data from Refs. [37,46–50].

In this table, we present the lowest-order $A^{(DHF)}$ and all-order $A^{(SD)}$ values for the ns, np, nd, and nf levels up to $n=4$. The magnetic moment and nuclear spin of ^{7}Li used here are taken from [45]. Our SD all-order values are in excellent agreement with high-precision measurements for the $2s\ ^2S_{1/2}$ (0.07%), $2p\ ^2P_{1/2}$ (0.004%), and $3s\ ^2S_{1/2}$ (0.03%). The largest disagreements between our SD all-order data and the experimental values occur for the $np\ ^2P_{3/2}$ states (1.4%, 1.6%,

TABLE IX. Hyperfine constants A (in MHz) in ^{7}Li ($I=3/2$, $\mu=3.256427(2)$ [45]). The SD all-order data are compared with theoretical and experimental results.

Level	$A^{(\text{DHF})}$	$A^{(\text{SD})}$	$A^{(\text{th})}$	$A^{(\text{expt})}$
$2s\ ^2S_{1/2}$	284.35	402.02	402.47 [2], 401.76 [31]	401.7520433(5) [31]
$2p\ ^2P_{1/2}$	32.295	45.916	45.96 [2], 45.945 [31]	45.914(25) [46]
$2p\ ^2P_{3/2}$	6.457	−3.014	−3.03 [2], −3.06 [31]	−3.055(14) [46]
$3s\ ^2S_{1/2}$	66.88	93.130	93.24 [2], 93.084 [31]	93.106(11) [47]
$3p\ ^2P_{1/2}$	9.745	13.875	13.892 [2]	13.5(2) [46]
$3p\ ^2P_{3/2}$	1.9484	−1.0198	−1.045 [2]	−1.036(16) [37]
$3d\ ^2D_{3/2}$	0.8206	0.8376	0.8384 [2]	0.843(41) [48]
$3d\ ^2D_{5/2}$	0.3517	0.3441	0.3431 [2]	0.343(10) [48]
$4s\ ^2S_{1/2}$	25.34	35.12	35.09 [2]	36.4(4) [49]
$4p\ ^2P_{1/2}$	4.116	5.852		
$4p\ ^2P_{3/2}$	0.8230	−0.4399		−0.41(2) [50]
$4d\ ^2D_{3/2}$	0.3465	0.3557		
$4d\ ^2D_{5/2}$	0.1485	0.1438		
$4f\ ^2F_{5/2}$	0.1057	0.1058		
$4f\ ^2F_{7/2}$	0.05871	0.05876		

and 7% for $n=2$, 3, and 4, respectively). The correlation correction for $np\ ^2P_{3/2}$ states is of the same order of magnitude as the DHF value and has an opposite sign. With such large cancellations, it is difficult to calculate $A(np_{3/2})$ accurately. Moreover, as was noted in Ref. [31], experimental values of A for the $2p\ ^2P_{3/2}$ state obtained in different experiments differ by 7%.

The present values of A for the $2s$, $2p$, and $3s$ states differ slightly from the earlier SD all-order values obtained by Blundell et al. [2] for two reasons: first, the present values are evaluated in the infinite-nuclear-mass limit, whereas the earlier values took into account the finite mass of the Li nucleus; second, the present calculations assume a Fermi distribution for the nuclear magnetism with parameters obtained from the charge distribution, while the previous calculation assumed a point nucleus.

VII. HYPERFINE-INDUCED TRANSITION POLARIZABILITY OF THE ^{7}Li GROUND STATE

We now turn to the calculation of the quadratic Stark shift of the ground-state hyperfine interval ($F=2-F=1$) in ^{7}Li. The quadratic Stark shift is closely related to the blackbody radiation shift discussed, for example, in Ref. [51], and our calculation follows the procedure outlined in [51], but includes some details omitted therein.

The dominant second-order contribution to the polarizability cancels between the two hyperfine components of the $2s$ state, so the Stark shift of the hyperfine interval is governed by the third-order F-dependent polarizability $\alpha_F^{(3)}(0)$. The expression for the $\alpha_F^{(3)}(0)$ is [51]

$$\alpha_F^{(3)}(0) = \frac{1}{3}\sqrt{(2I)(2I+1)(2I+2)}\begin{Bmatrix} j_v & I & F \\ I & j_v & 1 \end{Bmatrix}$$
$$\times g_I\mu_n(-1)^{F+I+j_v}(2T+C+R), \quad (4)$$

where g_I is the nuclear gyromagnetic ratio, μ_n is the nuclear

magneton equal to 3.256 424 in ^{7}Li, $I=3/2$ is the nuclear spin, and $j_v=1/2$ is the total angular momentum of the atomic ground state. The F-independent sums are ($|v\rangle \equiv |2s_{1/2}\rangle$)

$$T = \frac{(-1)^{j_v}}{2j_v+1}\sum_{m,n\neq v}(-1)^{j_m}\frac{\langle v\|rC_1\|m\rangle\langle m\|rC_1\|n\rangle\langle n\|\mathcal{T}\|v\rangle}{(E_m-E_v)(E_n-E_v)}\delta_{j_n,j_v},$$
$$(5)$$

$$C = \sum_{m,n\neq v}(-1)^{j_m-j_n}\begin{Bmatrix} 1 & j_v & j_v \\ 1 & j_m & j_n \end{Bmatrix}$$
$$\times \frac{\langle v\|rC_1\|m\rangle\langle m\|\mathcal{T}\|n\rangle\langle n\|rC_1\|v\rangle}{(E_m-E_v)(E_n-E_v)}, \quad (6)$$

$$R = \frac{\langle v\|\mathcal{T}\|v\rangle}{2j_v+1}\sum_n\frac{|\langle v\|rC_1\|n\rangle|^2}{(E_n-E_v)^2}. \quad (7)$$

In the above equations, $\mathcal{T}$ is the dipole hyperfine operator,

We note first that in the DHF approximation the values of T, C, and R in atomic units are

$$2T^{\text{DF}} = 5.51\times10^{-5},$$

$$C^{\text{DF}} = 3.36\times10^{-10},$$

$$R^{\text{DF}} = 9.06\times10^{-5}. \quad (8)$$

Since the value of C^{DF} is smaller than the value of T^{DF} and R^{DF} by five orders of magnitude, we do not recalculate the C term in the SD all-order approximation.

The expression for R is similar to that for $\alpha^{E1}(0)$ [compare Eqs. (1) and (7)]. The difference is an additional factor in Eq. (7) of the diagonal hyperfine matrix element:

$$\langle 2s_{1/2}\|\mathcal{T}\|2s_{1/2}\rangle^{(\mathrm{SD})} = 3.4447 \times 10^{-8} \ \ \mathrm{a.u.}$$

We evaluate the matrix elements $\langle v\|rC_1\|n\rangle$ in the SD all-order approximation for $n \le 26$. We use recommended NIST energies [23] for n up to $n=13$ and SD all-order energies for $14 \le n \le 26$. The sum of terms for $n \le 26$ is $R_{n \le 26} = 1.2367 \times 10^{-4}$. The remainder of the sum, evaluated in the DHF approximation, $R_{n > 26} = 1.0 \times 10^{-10}$ is insignificant.

The expression for T includes sums over two indices m and n. To calculate the dominant part of T, we limit the sum over m to four states ($m = 2p_{1/2}$, $3p_{1/2}$, $2p_{3/2}$, and $3p_{3/2}$) and sum over n up to $n = 26$:

$$
\begin{aligned}
T_{\substack{m \le 3 \\ n \le 26}} = -\frac{1}{2} \sum_{ns=3s}^{26s} \frac{\langle ns\|\mathcal{T}^{(1)}\|2s\rangle}{(E_{ns} - E_{2s})} & \left[\frac{\langle 2s\|rC_1\|2p_{1/2}\rangle\langle 2p_{1/2}\|rC_1\|ns\rangle}{(E_{2p_{1/2}} - E_{2s})} \right. \\
& + \frac{\langle 2s\|rC_1\|3p_{1/2}\rangle\langle 3p_{1/2}\|rC_1\|ns\rangle}{(E_{3p_{1/2}} - E_{2s})} \\
& - \frac{\langle 2s\|rC_1\|2p_{3/2}\rangle\langle 2p_{3/2}\|rC_1\|ns\rangle}{(E_{2p_{3/2}} - E_{2s})} \\
& \left. - \frac{\langle 2s\|rC_1\|3p_{3/2}\rangle\langle 3p_{3/2}\|rC_1\|ns\rangle}{(E_{3p_{3/2}} - E_{2s})} \right].
\end{aligned}
\tag{9}
$$

The sum of the four contributions from Eq. (9) is 3.6371×10^{-5}. Contributions to the sum from the $3p$ states are smaller than contributions from the $2p$ states by a factor of 30. The relatively small remainder $T - T_{\substack{m \le 3 \\ n \le 26}} = 0.0831 \times 10^{-5}$ is evaluated in the DHF approximation, leading to a final value $T^{(\mathrm{SD})} = 3.720\,18 \times 10^{-5}$. Combining these contributions, we obtain

$$2T^{\mathrm{SD}} + C^{\mathrm{DF}} + R^{\mathrm{SD}} = 1.9807 \times 10^{-4}\,\mathrm{a.u.} \tag{10}$$

The F-dependent factor [see Eq. (4)]

$$A(F) = \frac{g_I \mu_n}{3} \sqrt{(2I)(2I+1)(2I+2)} \begin{Bmatrix} j_v & I & F \\ I & j_v & 1 \end{Bmatrix} (-1)^{F+I+j_v}$$

is equal to $-1.477\,144$ for $F=1$ and $0.886\,286$ for $F=2$. Using these values and the result from Eq. (10), we obtain

$$\alpha^{(3)}_{F=2}(0) - \alpha^{(3)}_{F=1}(0) = 4.6814 \times 10^{-4} \ \ \mathrm{a.u.}$$

The Stark shift coefficient k defined as $\Delta\nu = kE^2$ is $k = -\frac{1}{2}[\alpha^{(3)}_{F=2}(0) - \alpha^{(3)}_{F=1}(0)]$. Converting from atomic units, we obtain

$$k = -2.3407 \times 10^{-4} \ \ \mathrm{a.u.} = -5.8244 \times 10^{-12} \ \ \mathrm{Hz/(V/m)^2}.$$

TABLE X. Comparison of values of k in 10^{-10} Hz/(V/m)^2.

		References
Present	-0.05824	
Theory	-0.0595	[21]
Theory	-0.0627	[20]
Expt.	-0.061 ± 0.002	[19]

In Table X, we compare our SD all-order value of k with available theoretical [20,21] and experimental [19] results. Our result is in better agreement with result by Lee *et al.* [21] than with the theoretical result by Kaldor [20] and the measurement performed by Mowat [19].

VIII. CONCLUSION

In summary, a systematic MBPT study of the energies of the $ns_{1/2}$, np_j, and nd_j, and nf_j ($n \le 6$) states in neutral lithium is presented. The energy calculations are in excellent agreement with existing experimental energy data. A systematic relativistic MBPT study of reduced matrix elements and oscillator strengths, transition rates, and lifetimes for the low-lying levels up to $n=4$ is conducted. Electric-dipole ($2s_{1/2}-np_j$, $n=2-26$), electric-quadrupole ($2s_{1/2}-nd_j$, $n=3-26$), and electric-octupole ($2s_{1/2}-nf_j$, $n=4-26$) matrix elements are calculated to obtain the ground-state $E1$, $E2$, and $E3$ static polarizabilities. Scalar and tensor polarizabilities for the $2p_j$ excited state in Li I are calculated including $2p_j-nd_j$ and $2p_j-ns_j$ matrix elements with n up to 26. All of the above-mentioned matrix elements are determined using an all-order method. Hyperfine A values are presented for the low-lying levels up to $n=4$. The quadratic Stark shift of the ground-state hyperfine interval in ^{7}Li I is also evaluated. These calculations provide a theoretical benchmark for comparison with experiment and theory.

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