

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

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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 $-0.0582 \text{ Hz}/(\text{kV}/\text{cm})^2$, in slight disagreement with the experimental value $-0.061 \pm 0.002 \text{ Hz}/(\text{kV}/\text{cm})^2$. Matrix elements used in evaluating polarizabilities, hyperfine constants, and the quadratic Stark shift are obtained using all-order method.

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I. INTRODUCTION

Investigations of 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 1980's and early 1990's [1–6] gave an accurate value of the line strength of the $2p - 2s$ transition close to $33.0 a_0^2$. 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, 10]. The difference between theory and experiment was ultimately resolved through measurements by Volz and Schmoranzler [11] and McAlexander et al. [10].

Very recently, measurements of the electric polarizability of lithium by atom interferometry were pre-

sented 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 later 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 [$-0.061 \pm 0.002 \text{ Hz}/(\text{kV}/\text{cm})^2$] were carried out by Mowat in Ref. [19] and evaluated theoretically to be $-0.0627 \text{ Hz}/(\text{kV}/\text{cm})^2$ by Kaldor [20] and $-0.0595 \text{ Hz}/(\text{kV}/\text{cm})^2$ 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 evalu-

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ate 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.

II. THIRD-ORDER AND ALL-ORDER MBPT 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 all-order (SD) 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 $E_{\text{tot}}^{(3)}$, 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. We list the all-order SD energies in the column labeled $E^{(\text{SD})}$ and list that part of the third-order energies missing from $E^{(\text{SD})}$ in the column labeled $E_{\text{extra}}^{(3)}$. The sum of the seven terms $E^{(0)}$, E^{SD} , $E_{\text{extra}}^{(3)}$, $B^{(1)}$, $B^{(2)}$, E_{LS} and E_{recoil} is our final all-order result $E_{\text{tot}}^{\text{SD}}$, listed in the twelfth 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, $\delta E^{(3)} = E_{\text{tot}}^{(3)} - E_{\text{NIST}}$ and $\delta E^{(\text{SD})} = E_{\text{tot}}^{\text{SD}} - E_{\text{NIST}}$, 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 $l_{\text{max}} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [24, 25]). 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 $l_{\text{max}} = 6$ 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 $l \leq l_{\text{max}} = 6$ in the $E^{(\text{SD})}$ calculation. As noted above, the second-order contribution dominates $E^{(\text{SD})}$, 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 -dependence 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 $E_{\text{extra}}^{(3)}$ in Table I, which accounts for that part of the third-order MBPT energy missing from the SD expression for the energy, is smaller than $E^{(3)}$ by an order of magnitude for the states considered here.

The column labeled $\delta E^{(\text{SD})}$ in Table I gives differences between our *ab initio* results and the experimental values [23]. The SD 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 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. [26]. We refer the reader to Ref. [27] and references therein for detailed discussion on 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 $R = 220 \text{ a.u.}$. 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 of 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 $n \leq 4$ and $l \leq 3$ in the SD approximation [2]. Our results are compared with other theoretical calculations [7, 28–31], and with experimental measurements [11, 32–36] in Tables II and III. Numerous theoretical calculations concerning properties of neutral lithium have been published over the past 30 years. In Table II, we compare our SD oscillator strengths with the accurate calculations given in Refs. [7, 28–31]. The highest ac-

TABLE I: Zeroth-order (DHF), second-order and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies $E^{(\text{SD})}$, $E_{\text{extra}}^{(3)}$, first-order and second-order Breit corrections $B^{(n)}$, Lamb-Shift E_{LS} and recoil E_{recoil} corrections in ${}^7\text{Li}$. The total energies ($E_{\text{tot}}^{(3)} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E_{\text{LS}} + E_{\text{recoil}}$, $E_{\text{tot}}^{(\text{SD})} = E^{(0)} + E^{\text{SD}} + E_{\text{extra}}^{(3)} + B^{(1)} + B^{(2)} + E_{\text{LS}} + E_{\text{recoil}}$) are compared with experimental energies E_{NIST} [23], $\delta E = E_{\text{tot}} - E_{\text{NIST}}$. Units: cm^{-1} .

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	E_{recoil}	$E_{\text{tot}}^{(3)}$	$E^{(\text{SD})}$	$E_{\text{extra}}^{(3)}$	$E_{\text{tot}}^{(\text{SD})}$	E_{NIST}	$\delta E^{(3)}$	$\delta E^{(\text{SD})}$
$2s_{1/2}$	-43087.3	-362.03	-26.94	1.16	-0.48	0.13	3.59	-43471.9	-407.02	2.35	-43487.6	-43487.2	15.2	-0.5
$2p_{1/2}$	-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	0.02	1.32	-16278.1	-85.52	0.38	-16281.1	-16281.0	2.9	-0.1
$3p_{1/2}$	-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	0.00	0.68	-8474.1	-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	0.00	0.41	-5187.2	-14.99	0.06	-5187.7	-5187.7	0.4	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	0.00	0.27	-3499.3	-8.28	0.03	-3499.6	-3499.5	0.2	-0.1
$6p_{1/2}$	-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

curacy oscillator strengths for $2s\ {}^2S - 2p\ {}^2P$ (0.0001%) and $2p\ {}^2P - 3d\ {}^2D$ (0.0005%) transitions were those obtained by Yan and Drake [7] who used variationally constructed wave functions in Hylleraas coordinates. Another Hylleraas-type calculations of properties of lithium was presented by Pestka and Wolźnicki [30], where superposition of correlated configurations was used to evaluate nonrelativistic energies and lifetimes of the $ns\ {}^2S$, $np\ {}^2P$, and $nd\ {}^2D$ states with $n \leq 4$ together with oscillator strengths of transitions between such states. The multi-configuration Hartree-Fock (MCHF) method was used recently by Godefroid et al. [28] to calculate 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 [28] was assessed by analysis of convergence patterns as the approximate wave function was systematically improved. In order to compare our relativistic SD oscillator strengths $f(nlj, n'l'j')$ with the nonrelativistic results given in Refs. [7, 28–31], 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 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 oscillator strengths and the MCHF [28] values listed in Table II is 0.17% ($2s\ {}^2S - 3p\ {}^2P$ transition) and 0.001% ($3p\ {}^2P - 4s\ {}^2S$ transition), respectively. The differences between the SD oscillator strengths and the oscillator strengths presented by Pestka and Wolźnicki [30] (see Table II) are much larger; the smallest difference is 0.003% for the $2s\ {}^2S - 2p\ {}^2P$ transition and the largest differences is and 73% for the $3s\ {}^2S - 4p\ {}^2P$ transition. It should be noted the oscillator strength of the $3s\ {}^2S - 4p\ {}^2P$ transition is 3-4 orders of magnitude smaller than for other transitions.

We also calculate 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 dipole matrix elements and experimental energies [23]. We list the lifetimes $\tau^{(\text{SD})}$ 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 $\tau^{(\text{SD})}$ with available experimental measurements [11, 32–36]. Experimental results have changed with time and we present only the most recent results in Table III. (We found no exper-

TABLE II: Oscillator strengths f averaged over j . The SD data ($f^{(\text{SD})}$) are compared with other theoretical data.

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

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imental measurements for $3d\ ^2D_J$, $4p\ ^2P_J$, or $4f\ ^2F_J$ states.) Our SD results agree well with measurements when experimental uncertainties are taken into account. We also compare our lifetime calculations with theoretical results from Refs. [7, 28–30] 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 $\tau^{(\text{SD})}$ and the results from Refs. [28, 29] 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. [30]. (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 4 of Ref. [30], we obtain the value $\tau = 375$ ns which agrees much better with our value $\tau^{(\text{SD})} = 388$ ns than the value 357 ns given in Table 5 of Ref. [30].)

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

The static multipole polarizability α_k 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 $|nl_j2s1s\rangle$ states. The latter term is smaller than the former by several orders of magnitude and is here evaluated in the random-phase approximation [38].

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

Level	$\tau^{(\text{SD})}$	$\tau^{\text{th.}}$	τ^{expt}
$2p\ ^2P$	27.108	$27.109804(36)^a$	$27.102(9)^e$
$2p\ ^2P_{1/2}$	27.109	27.106^b	$27.102(9)^e$
$2p\ ^2P_{3/2}$	27.107	27.104^b	$27.102(9)^e$
$3d\ ^2D$	14.583	$14.583687(68)^a$	$14.60(13)^f$
$3d\ ^2D_{3/2}$	14.584	14.591^b	
$3d\ ^2D_{5/2}$	14.583	14.592^b	
$3s\ ^2S_{1/2}$	29.856	29.886^b	$29.72(7)^g$
$3p\ ^2P_{1/2}$	211.11	210.94^c	$203(8)^h$
$3p\ ^2P_{3/2}$	211.15	210.93^c	
$4d\ ^2D_{3/2}$	33.382	33.315^d	$31.0(1.0)^i$
$4d\ ^2D_{5/2}$	33.381	33.315^d	
$4s\ ^2S_{1/2}$	56.037	56.084^c	$56(1.7)^j$
$4f\ ^2F_{5/2}$	72.278		
$4f\ ^2F_{7/2}$	72.279		
$4p\ ^2P_{1/2}$	388.17	357.2^d	
$4p\ ^2P_{3/2}$	388.30	357.2^d	

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The dominant valence contribution is calculated using the sum-over-state approach

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

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 [39]. The reduced matrix elements in the above sum are evaluated using the SD 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 totals. The rapid convergence of the sum over states for α_1 has been emphasized in many publications (for example, [40, 41]). We use recommended energies from [23] and SD wave functions to evaluate

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 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

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. [37]	164.0(1)		
Experiment [12]	164.2(1.1)		

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

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
$\alpha_{\text{main}}^{(SD)}(2p_j)$	126.787	126.802
$\alpha_{\text{tail}}^{(DF)}(2p_j)$	0.007	0.007
$\alpha_{\text{core}}(2p_j)$	0.189	0.189
$\alpha_{\text{vc}}(2p_j)$	-0.003	-0.003
$\alpha^{(SD)}(2p_j)$	126.980	126.995

terms in the sum with $n \leq 13$, and we use theoretical SD 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 ground state Li I are compared in Table V with high-precision calculations given in Refs. [13, 16, 37] 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. [37] for the dipole polarizability within the uncertainty quoted in [37]. 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

$$\alpha_0(v) = \frac{2}{3(2j_v + 1)} \sum_{nlj} \frac{|\langle v || r C_1 || nlj \rangle|^2}{E_{nlj} - E_v} \quad (2)$$

$$\alpha_2(v) = (-1)^{j_v} \sqrt{\frac{40j_v(2j_v - 1)}{3(j_v + 1)(2j_v + 1)(2j_v + 3)}} \times \sum_{nlj} (-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} \frac{|\langle v || r C_1 || nlj \rangle|^2}{E_{nlj} - E_v}. \quad (3)$$

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 wave functions. 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%. Contribution from excited ns and nd states $n > 26$ are very

TABLE VII: Contributions to tensor polarizability of Li in the excited state $v = 2p_{3/2}$ calculated using all-order SD method $\alpha_2(2p_{3/2}) = \sum_{n=3}^{70} I_{2p_{3/2}}(nd_j) + \sum_{n=1}^{70} I_{2p_{3/2}}(ns_{1/2})$. SD dipole matrix elements $Z_{vn} = \langle v || r C_1 || nlj \rangle$ 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

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

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

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

small $\alpha_{n > 26} = 0.007 a_0^3$ and are calculated in the DHF approximation. We evaluate contribution from ionic core α_{core} in the RPA and find $\alpha_{core} = 0.1894 a_0^3$. A counter term $\alpha_{vc}(2p_j)$ compensating for excitation from the core to the valence shell which violate the Pauli principle is also evaluated in the RPA and found to be $\alpha_{vc}(2p_j) = -0.003 a_0^3$. The above values were combined to obtain our final result for the scalar polarizability of the first two excited states in Li I: $\alpha_0^{(SD)}(2p_{1/2}) = 126.980 a_0^3$ and $\alpha_0^{(SD)}(2p_{3/2}) = 126.995 a_0^3$.

We present 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 approximations are given in columns labeled $Z_{vn} \equiv \langle v || r C_1 || nlj \rangle$. The corresponding contributions to the tensor polarizability are given in columns labeled I_{nlj} . The sum of contributions from $nd_{3/2}$ and $ns_{1/2}$ intermediate states is almost compensated 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 $1.590 a_0^3$. Contributions from states with $n > 26$ are $-0.001 a_0^3$.

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 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 wave functions for dipole matrix elements and energies. For $n \leq 13$, we use SD matrix elements and NIST energies [23] in the sums. Our final result is $\alpha_2^{(SD)}(2p_{3/2}) = 1.59 a_0^3$.

Our results for scalar and tensor polarizabilities of the $2p_j$ excited state of Li are compared in Table VIII with recent calculations by Cohen and Themells [15] and with experimental measurements reported by Windholz et al. [14]. The Rydberg-Klein-Rees inversion method com-

TABLE IX: Hyperfine constants A (in MHz) in ${}^7\text{Li}$ ($I=3/2$, $\mu=3.256427(2)$ [42]). The SD 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^a , 401.76^b	$401.7520433(5)^b$
$2p\ {}^2P_{1/2}$	32.295	45.916	45.96^a , 45.945^b	$45.914(25)^c$
$2p\ {}^2P_{3/2}$	6.457	-3.014	-3.03^a , -3.06^b	$-3.055(14)^c$
$3s\ {}^2S_{1/2}$	66.88	93.130	93.24^a , 93.084^b	$93.106(11)^d$
$3p\ {}^2P_{1/2}$	9.745	13.875	13.892^a	$13.5(2)^c$
$3p\ {}^2P_{3/2}$	1.9484	-1.0198	-1.045^a	$-1.036(16)^e$
$3d\ {}^2D_{3/2}$	0.8206	0.8376	0.8384^a	$0.843(41)^f$
$3d\ {}^2D_{5/2}$	0.3517	0.3441	0.3431^a	$0.343(10)^f$
$4s\ {}^2S_{1/2}$	25.34	35.12	35.09^a	$36.4(4)^g$
$4p\ {}^2P_{1/2}$	4.116	5.852		
$4p\ {}^2P_{3/2}$	0.8230	-0.4399		$-0.41(2)^h$
$4d\ {}^2D_{3/2}$	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		

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

VI. HYPERFINE CONSTANTS FOR ${}^7\text{Li}$

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition matrix elements. In Table IX, we list hyperfine constants A for ${}^7\text{Li}$ and compare our values with calculations by Godefroid et al. [28] and with available experimental data from Refs. [34, 43–47].

In this table, we present the lowest-order $A^{(\text{DHF})}$ and all-order $A^{(\text{SD})}$ values for the ns , np , nd , and nf levels up to $n = 4$. The magnetic moment and nuclear spin of ${}^7\text{Li}$ used here are taken from [42]. Our SD 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 data

TABLE X: Comparison of values of k in $10^{-10}\text{Hz}/(\text{v}/\text{m})^2$.

		References
present	-0.05824	
theory	-0.0595	Ref. [21]
theory	-0.0627	Ref. [20]
expt.	-0.061 ± 0.002	Ref. [19]

and the experimental values occur for the $np\ {}^2P_{3/2}$ states (1.4%, 1.6%, 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 $A(np\ {}^2P_{3/2})$ accurately. Moreover, as was noted in Ref. [28], 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 values obtained by Blundell et al. [2] for two reasons: firstly, 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; secondly, 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 ${}^7\text{Li}$ GROUND STATE

We now turn to the calculation of the quadratic Stark shift of the ground-state hyperfine interval ($F = 2 - F = 1$) in ${}^7\text{Li}$. The quadratic Stark shift is closely related to the black-body radiation shift discussed, for example, in Ref. [48] and our calculation follows the procedure outlined in [48] 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 the third-order F -dependent polarizability $\alpha_F^{(3)}(0)$. The expression for the $\alpha_F^{(3)}(0)$ is [48]:

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

where g_I is the nuclear gyromagnetic ratio, μ_n is the nuclear magneton equal to 3.256424 in ${}^7\text{Li}$, $I = 3/2$ is the nuclear spin, and $j_v = 1/2$ is the total angular momentum of the atomic ground state. The F -independent sums are ($|v\rangle \equiv |2s_{1/2}\rangle$)

$$T = \frac{(-1)^{j_v}}{2j_v + 1} \\ \times \sum_{m,n \neq v} (-1)^{j_m} \frac{\langle v || r C_1 || m \rangle \langle m || r C_1 || n \rangle \langle n || T || v \rangle}{(E_m - E_v)(E_n - E_v)} \delta_{j_n, j_v} \quad (5)$$

$$C = \sum_{m,n \neq v} (-1)^{j_m - j_n} \begin{Bmatrix} 1 & j_v & j_v \\ 1 & j_m & j_n \end{Bmatrix} \quad (6)$$

$$\times \frac{\langle v \| rC_1 \| m \rangle \langle m \| \mathcal{T} \| n \rangle \langle n \| rC_1 \| v \rangle}{(E_m - E_v)(E_n - E_v)}$$

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

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

$$\begin{aligned} 2T^{\text{DF}} &= 5.51 \times 10^{-5}, & C^{\text{DF}} &= 3.36 \times 10^{-10}, \\ R^{\text{DF}} &= 9.06 \times 10^{-5}. \end{aligned} \quad (8)$$

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

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

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

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

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

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 $T - T_{m \leq 3}^{n \leq 26} =$

0.0831×10^{-5} is evaluated in the DHF approximation, leading to a final value $T^{(\text{SD})} = 3.72018 \times 10^{-5}$. Combining these contributions, we obtain

$$2T^{\text{SD}} + C^{\text{DF}} + R^{\text{SD}} = 1.9807 \times 10^{-4} \text{ a.u.} \quad (10)$$

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

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

is equal to -1.477144 for $F = 1$ and 0.886286 for $F = 2$. Using these values and the result from Eq. (10), we obtain

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

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

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

In Table X, we compare our SD value of k with available theoretical [20, 21] and experimental [19] results. Our result is in the 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 , nd_j , and nf_j ($n \leq 6$) 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 first 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 high n up to $n = 26$. All of the above-mentioned matrix elements are determined using an all-order method. Hyperfine A -values are presented the first low-lying levels up to $n = 4$. The quadratic Stark shift of the ground-state hyperfine interval in ${}^7\text{Li I}$ is also evaluated. These calculations provide a theoretical benchmark for comparison with experiment and theory.

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