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

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The excitation energies of $ns$, $np$, $nd$, and $nf$ ($n=6$) 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 ($2s\rightarrow np$), electric-quadrupole ($2s\rightarrow nd$), and electric-octupole ($2s\rightarrow nf$), 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 $-0.061 \pm 0.002$ Hz/(kV/cm)$^2$. Matrix elements used in evaluating polarizabilities, hyperfine constants, and the quadratic Stark shift are obtained using the all-order method.

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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 $2p\rightarrow2s$ transition close to 33.0$\pm0.002$ a.u. 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 Mifflé et al. [12]. The measured value $\alpha=164.2\pm1.1$ a.u. illustrated the sensitivity of atom interferometry and is in agreement with the theoretical result $\alpha=164.111\pm0.002$ 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 $(F=2\ M=0)\rightarrow(F=1\ M=0)$ ground-state hyperfine interval in Li $[-0.061\pm0.002$ 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 $n\leq6$, reduced matrix elements, oscillator strengths, transition rates, and lifetimes for levels with $n\leq4$, 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 $n=4$. We use $B$-splines [22] to generate a complete set of basis orbitals for use in the evaluation of energies and matrix elements.
TABLE I. Zeroth-order (DHF), second-order, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies $E^{(SD)}$ and $E^{(3)}$, first-order and second-order Breit corrections $B^{(1)}$, and Lamb shift $E_{LS}$ and recoil $E_{rec}$ corrections in $^7$Li. The total energies $E^{(3)}_n = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E_{LS} + E_{rec}$ and $E^{(3)}_n = E^{(0)} + E^{(SD)} + E^{(3)} + B^{(1)} + B^{(2)} + E_{LS} + E_{rec}$ 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 $R_y = 10973.7316$.

<table>
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<tr>
<th>$nlj$</th>
<th>$E^{(0)}$</th>
<th>$E^{(2)}$</th>
<th>$E^{(3)}$</th>
<th>$B^{(1)}$</th>
<th>$B^{(2)}$</th>
<th>$E_{LS}$</th>
<th>$E_{rec}$</th>
<th>$E^{(3)}_n$</th>
<th>$E^{(SD)}_n$</th>
<th>$E^{(3)}_n$</th>
<th>$E^{(SD)}_n$</th>
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<th>$E^{(SD)}_n$</th>
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<td>$2s_1/2$</td>
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<td>-362.03</td>
<td>-26.94</td>
<td>1.16</td>
<td>-0.48</td>
<td>0.24</td>
<td>3.59</td>
<td>-43471.8</td>
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<td>2.14</td>
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<td>0.56</td>
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II. THIRD-ORDER AND ALL-ORDER MANY-BODY PERTURBATION THEORY CALCULATIONS OF ENERGIES

Energies of $nlj$ 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 $E_{rec}$. The sum of these contributions $E^{(3)}_n$, 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 ($X_n = 2/3$ case) given by Sapsirstein and Cheng [24] with $1/n^2$. 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 $E^{(3)}_{SD}$. The sum of the seven terms $E^{(0)}$, $E^{(SD)}$, $E^{(3)}_{SD}$, $B^{(1)}$, $B^{(2)}$, $E_{LS}$, and $E_{rec}$ is our final all-order result $E^{(3)}_n$, 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, $\Delta E^{(3)} = E^{(3)}_n - E^{(3)}_n$ and $\Delta E^{(SD)} = E^{(SD)}_n - E^{(SD)}_n$, 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. [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 \( l_{\text{max}} = 6 \) and 8 yield \( E^{(2)}(2s_{1/2}) = -361.046 \) and \( -361.596 \) \( \text{cm}^{-1} \), respectively. Extrapolation of these calculations yields \(-362.025\) and \(-362.066\)\( \text{cm}^{-1} \), respectively. Thus, in this particular case, we have a numerical uncertainty in \( E^{(2)}(2s_{1/2}) \) of 0.041 \( \text{cm}^{-1} \). It should be noted that the 1.02 \( \text{cm}^{-1} \) 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 \( \text{cm}^{-1} \)) contribution is obtained for the two other \( n = 2 \) states and a much smaller contribution (0.01–0.32 \( \text{cm}^{-1} \)) for \( n = 3 \) states.

Owing to numerical complexity, we restrict \( l \leq l_{\text{max}} = 6 \) 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 \( E^4 \)), we use the second-order remainder as a guide to estimate the remainder in the third-order contribution. The term \( E^{(3)}_{\text{extr}} \) 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 \( 6E^{(SD)} \) in Table I gives differences between our \textit{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 \( \text{cm}^{-1} \)) and \( 5f \) (6.9 \( \text{cm}^{-1} \)) states. However, we agree very well (0.0 \( \text{cm}^{-1} \)) for the \( 4f \) states and 0.2 \( \text{cm}^{-1} \) for the \( 5f \) states) with more recent measurement of Radziemska 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 \( l \geq 1 \), 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 \( nl_j \rightarrow n{l'}_j \) electric-dipole transitions with \( n \leq 4 \) and \( l \leq 3 \) 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\%) transition are

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

<table>
<thead>
<tr>
<th>Lower</th>
<th>Upper</th>
<th>( f^{(SD)} )</th>
<th>( f )</th>
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<td>( 3p^2P )</td>
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<tr>
<td>( 2s^2S )</td>
<td>( 4p^2P )</td>
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</tr>
<tr>
<td>( 2p^2P )</td>
<td>( 3s^2S )</td>
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<td>0.110554 [31]</td>
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<tr>
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<td>( 4s^2S )</td>
<td>0.012833</td>
<td>0.012835 [31]</td>
</tr>
<tr>
<td>( 2p^2P )</td>
<td>( 3d^2D )</td>
<td>0.638615</td>
<td>0.638546 [31]</td>
</tr>
<tr>
<td>( 2p^2P )</td>
<td>( 4d^2D )</td>
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<td>0.123008 [33]</td>
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<tr>
<td>( 3s^2S )</td>
<td>( 3p^2P )</td>
<td>1.214724</td>
<td>1.215881 [31]</td>
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<td>( 4d^2D )</td>
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<tr>
<td>( 4d^2D )</td>
<td>( 4f^2F )</td>
<td>0.003130</td>
<td></td>
</tr>
</tbody>
</table>
tions were those obtained by Yan and Drake [7] who used
variationally constructed wave functions in Hylleraas coordi-
nates. Another Hylleraas-type calculation of the properties of
lithium was presented by Pestka and Wózniacki [33], where
superposition of correlated configurations was used to evalu-
ate the nonrelativistic energies and lifetimes of the ns 2S,
np 2P, and nd 2D states with n ≤ 4 together with the oscilla-
tor strengths of the transitions between such states. The
multiconfiguration Hartree-Fock (MCHF) method was used rec-
cently by Godefroid et al. [31] to calculate the atomic prop-
erties 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 val-
ues from [7] is about 0.002% for the 2s 2S-2p 2P transition
and 0.006% for the 2p 2P-3d 2D transition. These differ-
ences 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 dif-
fences between the SD all-order oscillator strengths and the
oscillator strengths presented by Pestka and Wózniacki [33]
(see Table II) are much larger; the smallest difference is
0.003% for the 2s 2S–2p 2P transition and the largest differ-
ence 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 tran-
sitions.

We also calculate the lifetimes of ns 2S 1/2, np 2P 1/2, nd 2D 1/2,
and nf 2F 1/2 states for n ≤ 4 in neutral lithium using SD all-
order dipole matrix elements and experimental energies [23].
We list the lifetimes τ(SD) in Table III. The difference be-
tween 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, illus-
trating the size of relativistic effects. In Table III, we compare
times τ(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 2s, 4p 2P 2s, or
4f 2F 2s states.) Our SD all-order results agree well with mea-
surements when experimental uncertainties are taken into
account. We also compare our lifetime calculations with theo-
roretical results from Refs. [7,31–33] in Table III. We find
excellent agreement (0.008% and 0.002%) between the pres-
ent lifetime data and the high-precision results [7] for
2p 2P and 3d 2D states. Differences between our values of
τ(SD) and the results from Refs. [31,32] for the 2p 2P, 3d 2D
3s 2S 1/2, 3p 2P 1/2, 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
2p 2P states are unexpected since we have excellent agree-
ment 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 τ = 375 ns which agrees much
better with our value τ(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^E_k of Li in its 2s
ground state can be separated into two terms: a dominant
first term from intermediate valence-excited states |nlj(1s)^2|
and a smaller second term from intermediate core-excited
|nlj(2s1s)| 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 con-
tribution is calculated using the sum-over-state approach,

\[
α_v^E_k = \frac{1}{2k+1} \sum_n \frac{|\langle nlj | r^k C_{2s} | 2s \rangle|^2}{E_{nlj} - E_{2s}},
\]

where \( C_{2s}(r) \) is a normalized spherical harmonic and where
\( nlj \) is npj, ndj, and nfj 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 ≤ 26 and in the DHF approximation for the remaining
states.

Contributions to dipole, quadrupole, and octupole polariz-
abilities of the 2s ground state are presented in Table IV.
The first two terms in the sum-over-states for \( α_v^E_1, α_v^E_2, \)
and \( α_v^E_3 \) contribute 98.8%, 74%, and 29%, respectively, of the

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<th>( nlj=3d_{3/2} )</th>
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<th>( nlj=4f_{5/2} )</th>
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<td>( n=[3p−2p] )</td>
<td>1.915</td>
<td>( n=[4d−2d] )</td>
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<td>Tail</td>
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<td>163.895</td>
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<td>( α_v^{E_3} )</td>
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TABLE V. Multipole polarizabilities $\alpha^{E1}$, $\alpha^{E2}$, and $\alpha^{E3}$ of the 2s ground state of Li are compared with other calculations and with experiment.

<table>
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<tr>
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<th>$\alpha^{E2}$</th>
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<td>39624.2</td>
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<td>Yan et al. [13]</td>
<td>164.111(2)</td>
<td>1423.266(5)</td>
<td>39650.49(8)</td>
</tr>
<tr>
<td>Porsev and Derevianko [16]</td>
<td>1424(4)</td>
<td>39570</td>
<td></td>
</tr>
<tr>
<td>Derevianko et al. [40]</td>
<td>164.0(1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Experiment [12]</td>
<td>164.2(1.1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The rapid convergence of the sum over states for $\alpha$, has been emphasized in many publications (for example, [33,44]). 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 $13 < n \leq 26$. The remaining contributions to $\alpha^{E2}$ 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 $\alpha^{E2}$ and $\alpha^{E3}$ 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 $1s$ 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 $\alpha^{E1}$, $\alpha^{E2}$, and $\alpha^{E3}$, 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 polarizability 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

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

$$\alpha_2(v) = (-1)^{j_v} \sqrt{\frac{40j_v(2j_v - 1)}{3(j_v + 1)(2j_v + 1)(2j_v + 3)}} \times \sum_{nlj} (-1)^{j_v} \frac{j_v}{j_v+1} \frac{1}{j_v+2} \frac{|\langle v| r C_{2l} |nlj \rangle|^2}{E_{nlj} - E_v}. \quad (3)$$

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 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%. Contributions from excited $ns$ and $nd$ states with $n > 26$ are very small $\alpha_{ns > 26} = 0.007 \alpha_0$ and are calculated in the DHF approximation. We evaluate the contribution from the scalar dipole polarizability to the excited $2p_{1/2}$ and $2p_{3/2}$ states by 0.189. A counterterm $\alpha_{c}(2p_j)$ 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 $0.003 \alpha_0$. The above values were combined to obtain our final result for the scalar polarizability of the first two excited states in Li: $\alpha_{0}^{(SD)}(2p_{1/2}) = 126.980 \alpha_0^3$ and $\alpha_{0}^{(SD)}(2p_{3/2}) = 126.995 \alpha_0^3$.

We present the details of our calculation of the tensor polarizability $\alpha_2$ 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 $Z_{nm} = \langle v | r C_{1l} |nlj \rangle$. The corresponding contributions to the tensor polarizability are given in the columns labeled $I_{nmj}$. The sum of contributions from $nd_{3/2}$ and $ns_{1/2}$ intermediate states is almost compensated for by the contribution from the $nd_{3/2}$ states. The resulting contribution to $\alpha_2(2p_{3/2})$ from states with $n \leq 26$ is 1.590$\alpha_0^3$. Contributions from states with $n > 26$ are $-0.001 \alpha_0^3$.

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 $\alpha_{2}^{(SD)}(2p_{3/2}) = 1.590 \alpha_0^3$.

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 $\alpha_{n=26}(2p_{3/2})=\sum_{n=2}^{70}I_{n=(2p_{3/2})}(nd)/(n+1)$, SD all-order dipole matrix elements $Z_{vn}=(\langle v|\delta|n\rangle)/n[7]$, are given. All values are in a.u.

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

Theoretical results for $\alpha_{n}(2p_{3/2})$ are taken from 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 ($\alpha_{0}$) and tensor ($\alpha_{2}$) polarizabilities nonrelativistically. As can be seen from Table VIII, the present SD all-order results 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 $2s^2 S_{1/2}$ (0.07%), $2p^2 P_{1/2}$ (0.004%), and $3s^2 S_{1/2}$ (0.03%). The largest disagreements between our SD all-order data and the experimental values occur for the $np^2 P_{3/2}$ states (1.4%, 1.6%, etc.).
and 7% for \( n=2, 3, \) and 4, respectively). The correlation correction for \( np^2 \) 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 \( A(np^3) \) accurately. Moreover, as was noted in Ref. [31], experimental values of \( A \) for the \( 2p^2 \) 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 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 \(^7\text{Li}\) 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 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

\[
\alpha_F^{(3)}(0) = \frac{1}{3} \frac{\langle 0 \| T \| F \rangle}{(2I)(2I+1)(2F+2)} \begin{pmatrix} j_v & I & F \\ 1 & j_v & 1 \\ 1 & j_v & 1 \end{pmatrix} \times g_I \mu_n (-1)^{F+I+j_v} (2T+C+R),
\]

where \( g_I \) is the nuclear gyromagnetic ratio, \( \mu_n \) is the nuclear magneton equal to 3.256 424 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

\[
T = \frac{(-1)^{j_v}}{2j_v + 1} \sum_{m,n \neq v} (-1)^{j_m} \frac{\langle v \| C_I \| m \rangle \langle m \| C_j \| v \rangle \langle v \| T \| u \rangle}{(E_m - E_v)(E_n - E_v)} \delta_{j_m,j_v},
\]

\[
C = \sum_{m,n \neq v} (-1)^{j_m} \frac{1}{1} \begin{pmatrix} j_v & j_v & j_v \\ 1 & j_m & j_m \end{pmatrix},
\]

\[
\langle v \| T \| u \rangle = \frac{\langle v \| C_I \| m \rangle \langle m \| T \| n \rangle \langle n \| C_j \| v \rangle}{(E_m - E_v)(E_n - E_v)},
\]

\[
R = \frac{\langle v \| T \| u \rangle}{2j_v + 1} \sum_n |\langle v \| C_j \| u \rangle|^2 \frac{(E_m - E_v)(E_n - E_v)}{2}.
\]

In the above equations, \( T \) is the dipole hyperfine operator.

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

\[
27^{DF} = 5.51 \times 10^{-5},
\]

\[
C^{DF} = 3.36 \times 10^{-10},
\]

\[
R^{DF} = 9.06 \times 10^{-5}.
\]

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 \( \alpha_F^{(3)}(0) \) [compare Eqs. (1) and (7)]. The difference is an additional factor in Eq. (7) of the diagonal hyperfine matrix element.
We evaluate the matrix elements \( \langle v | r C_i | n \rangle \) in the SD all-order approximation for \( n \geq 26 \). We use recommended NIST energies [23] for \( n = 13 \) and SD all-order energies for \( 14 \leq n \leq 26 \). The sum of terms for \( n \geq 26 \) is \( R_{n=26} = 1.2367 \times 10^{-3} \). 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 \( n = 26 \):

\[
T_{m=3}^{n=26} = -\frac{1}{2} \sum_{n=3s}^{26} \frac{\langle nS | T(1) | 2s \rangle}{(E_{ns} - E_{2s})} \left( \frac{\langle 2s | rC_1 | 2p_{1/2} \rangle \langle 2p_{1/2} | rC_1 | ns \rangle}{(E_{2p_{1/2}} - E_{2s})} \right) + \frac{\langle 2s | rC_1 | 3p_{1/2} \rangle \langle 3p_{1/2} | rC_1 | ns \rangle}{(E_{3p_{1/2}} - E_{2s})} \right) - \frac{\langle 2s | rC_1 | 2p_{3/2} \rangle \langle 2p_{3/2} | rC_1 | ns \rangle}{(E_{2p_{3/2}} - E_{2s})} - \frac{\langle 2s | rC_1 | 3p_{3/2} \rangle \langle 3p_{3/2} | rC_1 | ns \rangle}{(E_{3p_{3/2}} - E_{2s})} \right).
\]

(9)

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

\[
2T^{(SD)} + C^{DP} + R^{(SD)} = 1.9807 \times 10^{-4} \text{a.u.}
\]

(10)

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

\[
A(F) = \frac{g_1 \mu_0}{3} \sqrt{(2I)(2I+1)(2I+2)} \left( \frac{|j_v|}{I} \frac{I}{|j_v|} F \right) (-1)^{F+|j_v|}
\]

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

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

The Stark shift coefficient \( k \), defined as \( \Delta \nu = kE^2 \), is

\[
k = -\frac{1}{2} \left[ \alpha_{F=2}^{(3)}(0) - \alpha_{F=1}^{(3)}(0) \right].
\]

The Stark shift coefficient \( k \) is defined as \( \Delta \nu = kE^2 \). Converting from atomic units, we obtain

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

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

<table>
<thead>
<tr>
<th>References</th>
<th>( k ) in ( 10^{-10} \text{ Hz/(V/m)}^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present</td>
<td>(-0.05824)</td>
</tr>
<tr>
<td>Theory</td>
<td>(-0.0595)</td>
</tr>
<tr>
<td>Expt.</td>
<td>(-0.061 \pm 0.002)</td>
</tr>
</tbody>
</table>

In summary, a systematic MBPT study of the energies of the \( ns_{1/2}, np_j, nd_j, \) and \( nf_j (n \geq 6) \) 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 \( E_1, E_2, \) and \( E_3 \) static polarizabilities. Scalar and tensor polarizabilities for the \( 2p_j \) excited state in \( Li \) are calculated including \( 2p_j - nd_j \) and \( 2p_j - ns \) 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 \( ^7Li \) is also evaluated. These calculations provide a theoretical benchmark for comparison with experiment and theory.

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