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Dynamic polarizabilities and van der Waals coefficients for the ground $2\,^2S$ and excited $2\,^4P^o$ states of Li

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The dynamic dipole polarizabilities at real and imaginary frequencies have been determined for the ground $2\,^2S$ and excited $2\,^4P^o$ states of Li using our time dependent gauge invariant method. Accurate C_6 dispersion energy coefficients for the Li $(2\,^2S)$–H_2 and Li$(2\,^4P^o)$–H_2 systems and their dependence on the intramolecular H-H distance are reported.

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I. INTRODUCTION

The systematic study of the interaction of slow electrons with excited atoms and molecules is very important in both basic and applied chemical physics. Profound changes in the scattering [1–4] and electron attachment or detachment [5–7] cross sections have been reported when electronically excited states are considered. Qualitatively good agreement between experimental results and optical models [8–10] shows the dominant role played by the dipole polarizability in the scattering process. In the same way for processes involving excited atoms and various target molecules, quantum mechanical calculations based on an optical potential model [11] and classical trajectory calculations [12] have shown that the dipole-dipole interaction is the major contribution to autoionization process at large interatomic distances [13]. Although reliable values for dipole and dipole-dipole (C_6) dispersion coefficients are available for atoms and atom-atom or atom-diatom systems in which atoms are in their ground state, very little is known for excited atoms.

In this paper we present accurate dynamic polarizabilities calculations for the lithium open-shell atom in its ground $2\,^2S$ $(1s^22s)$ and excited $2\,^4P^o$ $(1s2s2p)$ states. We employ our time-dependent gauge-invariant (TDGI) method [14–17], which was successfully used for evaluating the same properties for the ground state $1\,^1S$ [17] and the metastable states $2\,^1S$, $2\,^3S$ [18] and $2\,^1P$, $2\,^3P$ of helium [19].

The aim of this paper is twofold. First we generate wave functions capable of giving accurate dipole and eventually quadrupole moments that can be used for precise calculations of the dynamic properties. When possible our values are compared with those obtained from the combined configuration-interaction (CI) Hylleraas method [20] used by Pipin and Bishop [21] for the ground state and with the variation perturbation approach used by Chung [22] for the metastable $2\,^4P^o$ state.

Second we calculate frequency-dependent polarizabilities at imaginary frequencies to compute two-body dispersion coefficients corresponding to the $2\,^2S$ and $2\,^4P^o$ states. With dynamic polarizabilities values of He and H_2 obtained in previous works [17–19], we have evaluated C_6 dispersion coefficients for all pairs which can be taken from Li $(2\,^2S, 2\,^4P^o)$ and He $(1\,^1S, 2\,^1S, 2\,^3S, 2\,^1P, 2\,^3P)$ and calculated the dependence of C_6 as a function of H_2 intramolecular coordinate for Li $(2\,^2S, 2\,^4P^o)$–H_2 systems.

Some methodological and computational details are given in Sec. II and results are presented and discussed in Sec. III. Atomic units are used throughout the paper.

II. METHOD AND COMPUTATIONAL DETAILS

The results presented in this work have been carried out according to the TDGI formalism [14–16] that uses a first-order wave function combining a polynomial function and both true spectral states and quasispectral series. This method applied with success to closed-shell systems in their ground state [14–17], then extended for their excited states [18,19], is applied here to calculate dynamic polarizabilities of the $2\,^2S$ and $2\,^4P^o$ states of Li at frequencies below and above the first excitation threshold.

For Li the basis set used consists in the $(14s8p3d)$ Gaussian-type orbital built from the $11s$ set of Van Duijneveldt [23] augmented by three additional diffuse s orbitals: $\alpha_s = 0.010\,335, 0.003\,845, 0.001\,431$. The exponential parameters of the p shell are $\alpha_p = 8.302, 1.488, 0.2667, 0.07201, 0.0237, 0.0078, 0.0026, 0.0008$. The exponents of the three d functions $\alpha_d = 0.20, 0.05, 0.017$ are chosen in the same way as those used in Ref. [14].

Using this basis set, CI calculations were carried out in order to obtain the ground $2\,^2S$ and the lowest excited states ($2\,^2P$ and $3\,^2D$) together with the quadruplet states $2\,^4P^o$ $(1s2s2p)$, $2\,^4P$ $(1s2p2p)$, and $3\,^4S$ $(1s2s3s)$. The term $(1s2s2p)$ $2\,^4P^o$ is the lowest quartet of Li-like ions. It is metastable for both radiative deexcitations and autoionizations but is known to have a long lifetime [24,25]. It could be a candidate for experimental measurements. All states studied here are obtained using the multireference second-order many body perturbation via the CIPSI algorithm [26,27]. To treat with the same accuracy all the states, only the diagonalization of the subspace built up from the most important determinants is considered. These determinants are chosen from an iteratively procedure taking into account all single and double excitations of a changing and increasing subspace generated with a fixed threshold.

The diagonalized subspace contains between 5000 and 7000 determinants for each state and leads to energies approximatively 2×10^{-3} a.u. above the nonrelativistic limits. These latter differencies decrease and are equal to 10^{-4} a.u. if we add the perturbative contribution to our variational energies. Although the differencies between our variational energies and the nonrelativistic limits appear important, the wave functions generated give good transition energies and accurate dipole and quadrupole moments which can be used for precise calculations of the dynamic and static properties (see Sec. III).

According to the definition of Orr and Ward [28], dipole (α_{zz}) and quadrupole ($C = C_{zz,zz}$) polarizabilities are calculated for the ground state $2\ ^2S$. The intermediate states in the perturbation expression for α and C must be of ^2P and ^2D symmetry, respectively.

Scalar α_0 and tensor α_2 polarizabilities, as defined by Chung [22] and calculated for the $2\ ^1P$ and $2\ ^3P$ states of He [19], are obtained for the quadruplet state $2\ ^4\mathrm{P}^o$ of Li: $\alpha_0 = (\alpha_{10} + \alpha_{11} + \alpha_{12})/9$ and $\alpha_2 = -(\alpha_{10} - \frac{1}{2}\alpha_{11} + \frac{1}{10}\alpha_{12})/9$ in which α_{10},α_{11} and α_{12} are, respectively, the contributions of the ^4S, ^4P and ^4D states to the polarizability of a $^4P^o$ state.

Dispersion coefficients C_6 (or C_8) for noninteracting systems are calculated via the so-called Casimir-Polder [29] formula linking them to imaginary frequency polarizabilities of each system. Dispersion coefficients are then obtained by combining our $\alpha(i\omega)$ [or $C(i\omega)$] values through a simple numerical integration [30].

III. RESULTS AND DISCUSSION

A. Transition energies and oscillator strengths

The results of our calculated transition energies and oscillator strengths are presented in Table I and compared with previous studies [31–38]. There is an excellent agreement between our values and the experimental ones [31–33] for the doublet states. Our dipole oscillator strength (0.7505) for the $2\ ^2S \rightarrow 2\ ^2P$ transition also agrees within: 0.5% with the theoretical results of Sims, Hagstrom, and Rumble [34] (0.7476) and Pipin and Bishop [21] (0.7470) carried out within the framework of the Hylleraas method; 0.2% with the many body perturbation theory (MBPT) value (0.7495) given by Johnson, Idrees, and Sapirstein [35].

Our dipole and quadrupole moments (2.2502 and 8.248) for the $2\ ^2P \rightarrow 3\ ^2D$ transition compare very well with the results of Pipin and Bishop [21] (2.2652 and 8.670).

We use the first excited states with ^4P, ^4S, and ^4D symmetry in order to describe the proper first-order wave function of the quadruplet state. Our transition energies ($1s2s2p \rightarrow 1s2p2p$ and $1s2s2p \rightarrow 1s2s3s$) agree within 1% with the results of Bunge and Bunge [36], Hsu, Chung, and Huang [37], and Chung [22]. In contrast to the doublet states, very little is known about transition dipole moment. Our oscillator strengths 0.3684 for $2\ ^4P^o \rightarrow 2\ ^4P$ and 0.0630 for $2\ ^4P^o \rightarrow 3\ ^4S$ transitions are in

TABLE I. Calculated transition energies ΔE and oscillator strengths f_{ik} involving $2\ ^2S$, $2\ ^2P$, $3\ ^2S$, $3\ ^2D$ and the first $^4P^o$ ($1s2s2p$), ^4P ($1s2p2p$), and ^4S ($1s2s3s$) states of Li. Comparison with some experimental and theoretical results. All results are in a.u.

Transition	ΔE		f_{ik}	
	Our results	Others	Our results	Others
$2\ ^2S \rightarrow 2\ ^2P$ $1s^22s \rightarrow 1s^22p$	0.06812	0.06791[a]	0.7505	0.753[a],0.742[b] 0.7476[d],0.7470[e] 0.754[f],0.748[g]
$2\ ^2P \rightarrow 3\ ^2S$ $1s^22p \rightarrow 1s^23s$	0.05559	0.05605[a]	0.1125	0.115[a],0.110[f]
$2\ ^2P \rightarrow 3\ ^2D$ $1s^22p \rightarrow 1s^23d$	0.07612	0.07463[a]	0.6339	0.667[a],0.643[c] 0.6382[e],0.64[f]
$2\ ^4P^o \rightarrow 2\ ^4P$ $1s2s2p \rightarrow 1s2p2p$	0.12391	0.122597[h]	0.3684	0.3593[h]
$2\ ^4P^o \rightarrow 3\ ^4S$ $1s2s2p \rightarrow 1s2s3s$	0.15406	0.155261[i]	0.0630	0.0640[h]

[a] Reference [31].
[b] Reference [32].
[c] Reference [33].
[d] Reference [35].
[e] Reference [21].
[f] Reference [38].
[g] Reference [34].
[h] Reference [36].
[i] Reference [37].

excellent agreement with those obtained by Bunge and Bunge [36] (0.3593 and 0.0640) from a CI method with Slater-type orbitals.

This agreement between our calculated transition energies and moments with the most accurate calculations is important since the more these properties are accurately described the more the results on computed dynamic dipole and quadrupole polarizabilities are expected to be good.

B. Dynamic polarizabilities

If accurate calculations of dynamic polarizabilities for atoms in their ground state is difficult and require elaborate wave functions, the most challenging task, however, is the calculation of these properties for excited states. There is a vast amount of theoretical [14,21,39–44] and experimental data [45] for the static dipole and quadrupole polarizability of the ground 2 ^2S state of lithium. The results range respectively between 163.8 and 164.8 a.u. for α and 1323 and 1428 a.u. for C. Our TDGI values (164.8 and 1430 a.u.) are in excellent agreement with the fourth-order Moller-Plesset results of Maroulis and Thakkar [43] (164.8 and 1428 a.u.) and with the values recently obtained by Pipin and Bishop [21] (164.1 and 1423 a.u.) from a combined configuration interaction Hylleraas method. Our dynamic dipole and quadrupole polarizabilities values calculated in the range 0.0–0.100 a.u. are listed in Table II. Comparison of our results with those of Pipin and Bishop [21] for frequencies below the $2s \to 2p$ transition shows an agreement within 0.4% and 0.6% for the $\alpha(\omega)$ and $C(\omega)$ values, respectively. Up to the excitation threshold, our results are new for the 2 ^{2}S state of lithium.

TABLE II. Dynamic dipole and quadrupole polarizability of the 2 ^2S state of Li. Comparison with the theoretical results of Pipin and Bishop. All results are in a.u.

ω	α		C	
	Our results	[21]	Our results	[21]
0.0	164.8	164.1	1430	1423
0.005	165.7	165.0	1432	1425
0.010	168.4	167.7	1437	1430
0.015	173.1	172.4	1445	1438
0.020	180.2	179.5	1456	1449
0.025	190.2	189.6	1472	1464
0.030	204.0	203.4	1490	1482
0.035	223.3	222.8	1513	1505
0.040	250.6	250.3	1540	1532
0.045	291.0	291.0	1573	1564
0.050	355.2	356.1	1611	1601
0.055	470.2		1655	
0.060	729.2		1706	
0.070	-2895.3		1835	
0.075	-764.5		1917	
0.080	-427.1		2012	
0.085	-290.1		2126	
0.090	-216.2		2263	
0.095	-170.1		2429	
0.100	-0.819			

TABLE III. Scalar $\alpha_0(\omega)$ and tensor $\alpha_2(\omega)$ polarizabilities for the $1s2s2p$ $^4P^o$ state of Li. In parentheses TDGI results obtained with the first transition energy value calculated by Chung. All results are in a.u.

ω	α_0		α_2	
	Our results	[22]	Our results	[22]
0.0	45.83	45.64	6.76	6.86
0.01	46.03	45.85	6.82	6.92
0.02	46.65	46.49	7.01	7.12
0.03	47.72	47.60	7.35	7.47
0.04	49.34	49.29	7.87	8.02
0.05	51.65	51.69	8.62	8.81
0.06	54.87	55.07	9.72	9.97
0.07	59.44	59.90	11.34	11.71
0.08	66.15	67.07	13.85	14.41
0.09	76.70	78.56	18.03	19.02
0.10	95.55 (99.76)	99.78	26.01 (28.19)	28.13
0.11	139.37 (153.54)	153.14	45.93 (53.14)	52.76
0.115	195.09 (233.41)	230.95	72.49 (91.81)	90.32
0.120	375.04 (641.54)	604.40	160.8 (294.3)	275.4

The dynamic scalar $\alpha_0(\omega)$ and tensor $\alpha_2(\omega)$ values are reported for the 2 $^4P^o$ state in Table III. The static results ($\alpha_0 = 45.83$ a.u. and $\alpha_2 = 6.76$ a.u.) are in excellent agreement with those recently obtained by Chung [22] ($\alpha_0 = 45.64$ a.u. and $\alpha_2 = 6.86$ a.u.). Within the range 0.0–0.08 a.u., it should be noted the parallel behaviour of $\alpha_0(\omega)$ and $\alpha_2(\omega)$ as functions of frequency. The main differences appear near the first resonance in the energy range $\omega = 0.10$–0.12 a.u.. These differences can be essentially explained by the calculated first transition energy value (2 $^4P^o \to$ 2 ^4P), our result being 0.0013 a.u. greater than Chung's. Indeed, when we introduce Chung's energy value in our TDGI method, we find similar $\alpha_0(\omega)$ and $\alpha_2(\omega)$ polarizabilities (see Table III).

C. Dispersion coefficients

C_6 and C_8 dispersion coefficients for the interaction between the ground 2 ^2S and the excited 2 $^4P^o$ states of Li with the ground 1 ^1S and the excited (2 ^1S, 2 ^3S) states of He were calculated by combining our $\alpha(i\omega)$ and $C(i\omega)$ TDGI values via a simple numerical integration using formula given by Langhoff, Gorden, and Karplus [46]: $C_6 = \frac{3\hbar}{\pi}\int_0^\infty \alpha^A(i\omega)\alpha^B(i\omega)d\omega$ and $C_8 = \frac{15\hbar}{\pi}\int_0^\infty [C^A(i\omega)\alpha^B(i\omega) + \alpha^A(i\omega)C^B(i\omega)]d\omega$.

Results are given in Table IV. For comparison, our best estimate of C_6 for Li(2 ^2S)–He(1 ^1S) is different by 0.5% from accurate result obtained by Thakkar *et al.* [47] through a nearly exact *ab initio* pseudodipole oscillator strength distributions (DOSD) method. As expected, the results obtained for Li(2 ^2S or 2 $^4P^o$)-He(2 ^1S or 2 ^3S) are fairly large since excited rare gas atoms lose their

TABLE IV. Calculated C_6 and C_8 dispersion coefficients for Li(2 ^2S) and Li(2 $^4P^o$) with He(1 ^1S), He(2 ^1S), and He(2 ^3S). All results are in a.u.

	C_6	C_8
Li(2 ^2S)-Li(2 ^2S)	1407.8	84316.5
Li(2 ^2S)-He(1 ^1S)	22.62 (22.49)[a]	1089.2
Li(2 ^2S)-He(2 ^1S)	3539.8	262432
Li(2 ^2S)-He(2 ^3S)	2105.1	132654
Li(2 $^4P^o$)-Li(2 $^4P^o$)	269	
Li(2 $^4P^o$)-Li(2 ^2S)	555	
Li(2 $^4P^o$)-He(1 ^1S)	14.6	
Li(2 $^4P^o$)-He(2 ^1S)	1163	
Li(2 $^4P^o$)-He(2 ^3S)	768	

[a] Reference [47].

TABLE V. Calculated C_6^0 dispersion coefficients for Li(2 ^2S)–H_2 and Li(2 $^4P^o$)–H_2 as a function of the interhydrogen distance R. DOSD result calculated at R_{HH}=1.4 a.u. All results are in a.u.

R	1.401	2.4	3.0	3.4	3.8	4.4	6.0
Li(2^2S)–H_2							
$C_6^{\parallel}$	98.54	206.9	252.2	257.1	242.6	207.6	149.3
$C_6^{\perp}$	71.31	115.3	131.7	136.9	137.9	136.7	132.9
C_6^0	80.39	145.9	171.9	176.9	172.8	160.3	138.4
DOSD	79.43	144.6	170.4	175.3	171.6		
Li(2^4P^o)–H_2							
$C_6^{\parallel}$	58.7	116	137	139	131	114	84.8
$C_6^{\perp}$	43.1	67.3	76.0	78.7	79.2	78.6	76.6
C_6^0	48.3	83.5	96.3	98.8	96.5	90.4	79.3

"closed-shell" character.

Table V presents TDGI calculations of the isotrope C_6^0 coefficients for the systems Li(2 ^2S)–H_2 and Li(2 $^4P^o$)–H_2 as functions of the interhydrogen R_{HH} distance. When possible for the ground state, our values are compared with the DOSD results obtained by Thakkar *et al.* [47]. For the Li(2 $^4P^o$)–H_2 system, our results are original. For both systems, C_6^0 dispersion coefficients are obtained using the accurate TDGI dipole polarizabilities of H_2 calculated in [17] at seven R_{HH} distances ranging from 1.401 to 6.0 a.u. Very good agreement with the DOSD calculations of Thakkar *et al.* [47] is obtained, the maximum difference being 0.8%. A C_6^0 maximum value occurs for both systems at the R_{HH} distance corresponding to the maximum polarizability of H_2. C_6^0 (Li 2 ^{2}S–H_2) coefficients are roughly 75% at 80% higher than the C_6^0 (Li 2 $^4P^o$–H_2) value for all R_{HH} distances.

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