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Time-dependent Hartree-Fock calculations for the excited 'S' states of Lithium isoelectronic sequence

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Time-dependent HF (RPA) calculations have been performed to estimate the transition energies and excited state wavefunctions of Li, Be^+, B^{2+} and C^{3+} for the transitions $1s^22s:{}^2S \rightarrow 1s^2ns:{}^2S$ $(n=3,4,\ldots 8)$. The excitation energies and excited state wavefunctions are extracted from the position of the poles of a linearised variational functional. The excitation energies are in excellent agreement with those obtained spectroscopically. The excited state wavefunctions are utilised to find the matrix elements of different operators and the cusp values.

Key words: RPA calculations—excited states—atomic wavefunctions

1. Introduction

Investigation of excitation energies and excited states are necessary to interpret the observed spectra of many electron systems which are nowadays available through various experimental observations [1]. Such spectra, particularly spectra of multiply charged ions are of spectral interest for astrophysical observations [2]. The work of Burkhalter et al [3] and Mansfield et al. [4] with laser produced plasmas and the beam foil measurements of Dietrich et al. [5] yield substantial data in this matter.

Excitation energies and excited state wavefunctions are usually obtained theoretically using multiterm functions within variational framework [6–13]. In this respect time-dependent Hartree–Fock theory (TDHF) provides an alternative but reasonably accurate method and has, in a number of cases, been applied successfully in the past [14], for transitions involving different symmetries from that of the ground state. The accuracy is mainly due to the inclusion of substantial amount of correlation effects. It has been shown explicitly [15–17] that TDHF is equivalent to RPA and in RPA, correlation effects are incorporated chiefly through the inclusion of doubly excited configurations in the ground state. It was shown earlier by Bhattacharya et al. [18] that for two electron isoelectronic sequence, excellent results are obtained for transitions involving the same symmetry as that of the ground state.

In this paper, we applied TDHF theory within variational framework to calculate the excitation energies and excited state wavefunctions of three electron isoelectronic system for the first few transitions $2^2S \rightarrow n^2S (n=3, \ldots 8)$. Perturbative calculations involving inverse powers of Z have been performed earlier [19–21] for such systems.

The present method is nonrelativistic and ignores core relaxation effect, which however, is very small for the present case.

2. Methods

A detailed discussion of the theory was given earlier [14, 18]. We shall briefly outline here the essential features. We construct a variational functional (atomic units are used)

$$J(\Phi) = \frac{1}{T} \int_0^T \frac{\langle \Phi(\boldsymbol{r}, t) | H - i(\partial/\partial t) | \Phi(\boldsymbol{r}, t) \rangle \, dt}{\langle \Phi(\boldsymbol{r}, t) | \Phi(\boldsymbol{r}, t) \rangle} \tag{1}$$

subject to

$$\delta J(\Phi) = 0 \tag{2}$$

where H is the total Hamiltonian including interaction with the external time-dependent field and Φ is the total wavefunction represented by

$$\Phi(\boldsymbol{r}, t) = e^{-iE_0 t} A \Pi_i (\psi_i + \delta\psi_i^- \, e^{-i\omega t} + \delta\psi_i^+ \, e^{i\omega t}) \tag{3}$$

Here E_0 is the HF ground state energy, A is a normalised antisymmetriser, $\delta\psi_i^\pm$ represent the admixtures to the ground orbital ψ_i because of the two components of the perturbing Hamiltonian,

$$h_i'(\boldsymbol{r}, t) = h_i'(\boldsymbol{r}) \, e^{-i\omega t} + h_i'^+(\boldsymbol{r}) \, e^{i\omega t} \tag{4}$$

ω is the external frequency.
For the present case excitations corresponding to $\Delta l = 0$ occur and we choose

$$h'(\boldsymbol{r}) \sim f(r) \, Y_{00}(\theta, \varphi) \tag{5}$$

such that

$$\delta\psi_i^-(\boldsymbol{r}) \sim h_i'(\boldsymbol{r}) \psi_i(\boldsymbol{r}). \tag{6}$$

We expand the radial part of $\delta\psi(r)$ as

$$\delta\psi_i^\pm(r) = \sum_q C_{iq}^\pm \chi_{iq}(r) \tag{7}$$

where C_{iq}'s are variation parameters and χ_{iq}'s are appropriate preassigned basis functions. Applying linear response theory we get a set of matrix equations from Eq. (2)

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix}\begin{pmatrix} C^- \\ C^+ \end{pmatrix} = \omega \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}\begin{pmatrix} C^- \\ C^+ \end{pmatrix} + \begin{pmatrix} -\Lambda^- \\ \Lambda^+ \end{pmatrix} \tag{8}$$

where A and B involve matrix elements of the Hamiltonian in the perturbing basis $\{\chi\}$, S is the associated overlap matrix and Λ denotes a column matrix involving perturbing term. It follows from the linear response theory that the excitation spectrum for the ground state corresponds to the eigenvalues of the associated homogenous problem of Eq. (8). Thus one can diagonalize the non-hermitian matrix eigenvalue Eq. from (8) to generate the excitation energies and excited state vectors. Alternatively, one can seek poles of the vector $\begin{pmatrix} C^- \\ C^+ \end{pmatrix}$ at different frequencies by solving Eq. (8) and the position of the poles gives the excitation energies and corresponding functions. The results are equivalent. Since for many cases we are interested in the value of the functional at different frequencies (e.g. in frequency dependent optical susceptibility calculations), we follow here the second method. As the position of the poles does not depend on the choice of $f(r)$, only the symmetry matters, we choose here $f(r) \sim 1/r$ for convenience.

3. Results and discussion

The first four members of Lithium isoelectronic sequence Li, Be^+, B^{2+} and C^{3+} have been chosen for our study. We consider excitations $2^2S \rightarrow n^2S(n=3, 4, \ldots 8)$ for all the systems. The ground state functions are those of Clementi [22]. For the radial part of all the excited states we choose a 12 parameter representation of the form (see Eq. (7))

$$\chi_q(r) = r^{n_q} e^{-\rho_q r}. \tag{9}$$

Normally with a given basis set we tried to obtain as many resonances as possible. Whenever that is not possible, we choose a different basis set. This is very prominent for Li, the transition energies of which are listed in Table 1.

Here four different basis sets are used to get complete information for all the transitions. Since the higher excited state wavefunctions are highly diffuse, it is quite difficult to choose a proper basis initially which is equally effective for all the transitions. Table 1 also shows the spectroscopic values [23] and the elaborate theoretical values of Knight and Sanders [21]. Agreement within 1% is observed for all the transitions. The transition energies for Be^+, B^{2+} and C^{3+} are listed in Table 2, along with those of Moore [23–24] and Knight and Sanders [21]. Here agreement within 0.5% is achieved for all transitions wherever experimental values are available. We have to choose two different basis sets for each ion to obtain all the transitions $2s \rightarrow 3s, 4s, \ldots 8s$. However, with the second basis set all the resonance points have not been scanned since it requires extra computation

Table 1. Transition energies for Li as observed from frequency dependent calculations

Transition	Observed[a] (a.u.)	Calculated[b] (a.u.)	Present (a.u.) Basis 1	Basis 2	Basis 3	Basis 4	% Dev.[c]
$2s \to 3s$	0.1240	0.1239	0.1225	0.1225	0.1225	0.1233	0.56
$2s \to 4s$	0.1595	0.1597	0.1580	0.1578	0.1578	0.1579	1.00
$2s \to 5s$	0.1745	0.1747	0.1782	0.1727	0.1727	0.1728	0.97
$2s \to 6s$	0.1822	0.1819	—	0.1805	0.1804	0.1804	0.99
$2s \to 7s$	0.1867	0.1860	—	—	0.1848	0.1851	0.86
$2s \to 8s$	0.1895	—	—	—	—	0.1884	0.58

For Li: 1 a.u. = 219457.446 cm^{-1}.
[a] See Ref. [23].
[b] See Ref. [21].
[c] Percentage deviation is calculated with respect to the results of basis 4

Table 2. Transition energies for Be^{+}, B^{2+}, C^{3+}

Ion	Transition	Observed[a] (a.u.)	Calculated[b] (a.u.)	Present (a.u.)	% Dev.
Be^{+}	$2s \to 3s$	0.4020	0.4020	0.3998[d]	0.55
	$2s \to 4s$	0.5261	0.5263	0.5232[d]	0.55
	$2s \to 5s$	0.5802	0.5803	0.5774[d]	0.48
	$2s \to 6s$	0.6086	0.6083	0.6057[d]	0.48
	$2s \to 7s$	0.6253	0.6246	0.6227[e]	0.42
	$2s \to 8s$	—	—	0.6336[e]	
B^{2+}	$2s \to 3s$	0.8211	0.8211	0.8200[d]	0.13
	$2s \to 4s$	1.0831	1.0831	1.0797[d]	0.31
	$2s \to 5s$	1.1991	1.1991	1.1960[d]	0.26
	$2s \to 6s$	—	1.2604	1.2574[d]	—
	$2s \to 7s$	—	1.2966	1.2936[e]	—
	$2s \to 8s$	—	—	1.3197[e]	—
C^{3+}	$2s \to 3s$	1.3799	1.3800	1.3767[d]	0.23
	$2s \to 4s$	1.8288	1.8287	1.8244[d]	0.24
	$2s \to 5s$	2.0293	2.0293	2.0245[d]	0.24
	$2s \to 6s$	2.1360	2.1360	2.1310[d]	0.23
	$2s \to 7s$	2.1993	2.1994	2.1955[e]	0.17
	$2s \to 8s$	2.2402[c]	—	2.2414[e]	0.05

For Be^{+}: 1 a.u. = 219461.246 cm^{-1}, B^{2+}: 1 a.u. = 219463.67 cm^{-1}, C^{3+}: 1 a.u. = 219464.572 cm^{-1}.
[a] See Ref. [23].
[b] See Ref. [21].
[c] See Ref. [24].
[d] Refers to basis 1 for each ion.
[e] Refers to basis 2 for each ion

time without affecting the results much. This is also clear from the results of the four different basis sets for Li.

In Table 3 the matrix elements of the different operators for the different excited states are listed. For Li, the results for all the four basis sets are given. As far as

Table 3. Matrix elements of different operators and cusp values

Ion	Configuration	Basis	$\langle 1/r \rangle$ (a.u.)	$\langle r \rangle$ (a.u.)	$\langle r^2 \rangle$ (a.u.)	Cusp Values
Li	3*s*	1	1.8356	3.7784	39.7428	−3.0504
		2	1.8355	3.7821	39.8513	−2.9714
		3	1.8356	3.7790	39.7823	−3.0267
		4	1.8362	3.7982	40.5735	−2.9024
	4*s*	1	1.8137	7.1292	156.6085	−2.5924
		2	1.8143	6.8710	142.9723	−3.0732
		3	1.8142	6.8850	143.1162	−3.0673
		4	1.8144	6.8947	143.7389	−2.9187
	5*s*	1	1.8174	7.2810	177.8483	−1.2833
		2	1.8052	10.9523	377.3133	−3.1006
		3	1.8052	10.9210	376.8787	−3.0017
		4	1.8049	11.1172	386.5719	−2.8847
	6*s*	1	—	—	—	—
		2	1.8017	14.8473	717.4791	−3.2626
		3	1.8006	15.9414	820.1159	−2.9775
		4	1.7998	16.4589	858.7398	−2.8795
	7*s*	1	—	—	—	—
		2	—	—	—	—
		3	1.7974	22.4405	1637.2731	−3.0071
		4	1.7959	25.4512	2045.7526	−2.8305
	8*s*	1	—	—	—	—
		2	—	—	—	—
		3	—	—	—	—
		4	1.7936	39.1782	4781.4418	−2.7591
Be^+	3*s*	1	2.5386	2.1591	12.2650	−4.0996
	4*s*	1	2.5003	3.7787	41.5667	−4.1683
	5*s*	1	2.4830	5.9758	109.3341	−3.9878
	6*s*	1	2.4736	8.8731	247.4613	−3.9059
	7*s*	2	2.4710	11.3532	426.1962	−4.4309
	8*s*	2	2.4644	17.3265	966.9050	−4.4147
B^{2+}	3*s*	1	3.2422	1.5334	6.0156	−5.6640
	4*s*	1	3.1868	2.6362	19.8517	−5.7169
	5*s*	1	3.1625	4.0978	51.2274	−5.3967
	6*s*	1	3.1503	5.8652	109.3662	−5.2374
	7*s*	2	3.1395	8.4596	225.5392	−5.6129
	8*s*	2	3.1323	12.8020	514.5396	−5.3905
C^{3+}	3*s*	1	3.9447	1.1922	3.5688	−6.5957
	4*s*	1	3.8733	2.0364	11.6687	−6.7742
	5*s*	1	3.8412	3.1195	29.1041	−6.7581
	6*s*	1	3.8238	4.4641	61.4653	−6.7826
	7*s*	2	3.8112	6.4332	129.3911	−6.3573
	8*s*	2	3.8009	9.8312	299.3057	−6.0199

the authors know, no other theoretical results for the expectation values of these operators are available for comparison. To have a feeling for the behaviour of the excited state wavefunctions we calculated the cusp values [25] for all the transitions and listed them in Table 3. In all cases the calculated cusp values show reasonably good agreement with the ideal value $-Z$.

Table 4. Excited state wavefunctions obtained from the frequency dependent calculation

Li

n	ρ	3s	4s	5s	6s	n	ρ	7s	8s
0	3.0	7.05501 (−1)†	4.27181 (−1)	2.89470 (−1)	2.04791 (−1)	0	3.0	1.22993 (−1)	7.84255 (−2)
1	2.0	6.88655 (−2)	3.47239 (−2)	3.33650 (−2)	2.46829 (−2)	1	2.0	2.08497 (−2)	1.88923 (−2)
2	1.2	−2.85799 (−1)	−1.72970 (−1)	−1.28898 (−1)	−9.62734 (−2)	2	1.2	−7.06076 (−2)	−4.88923 (−2)
3	1.2	4.73266 (−3)	1.67056 (−3)	7.45367 (−3)	7.99810 (−3)	3	1.2	1.19090 (−2)	9.84260 (−3)
4	0.8	−3.15408 (−3)	−1.21805 (−3)	−1.28092 (−3)	−1.00105 (−3)	4	0.8	−1.04344 (−3)	−9.48591 (−4)
5	0.8	9.31933 (−4)	5.81215 (−4)	5.19197 (−4)	4.13885 (−4)	5	0.8	3.61978 (−4)	2.79360 (−4)
5	0.4	1.30686 (−5)	7.70725 (−6)	1.95312 (−7)	−2.47265 (−6)	5	0.4	−6.53629 (−6)	−5.76123 (−6)
6	0.4	−5.19101 (−7)	−1.00870 (−6)	−5.63567 (−7)	−3.25172 (−7)	6	0.4	1.30670 (−7)	2.07977 (−7)
6	0.2	7.86065 (−10)	−8.19726 (−10)	9.63592 (−9)	1.64472 (−8)	6	0.2	1.07478 (−8)	5.79450 (−9)
7	0.2	−1.73027 (−11)	1.53258 (−11)	−1.51461 (−10)	−4.44111 (−10)	7	0.2	−3.39714 (−10)	−2.00541 (−10)
7	0.1	1.49702 (−14)	−7.45209 (−15)	5.91804 (−14)	6.80930 (−14)	7	0.1	1.01527 (−12)	1.27157 (−12)
8	0.1	−1.37240 (−16)	6.62275 (−17)	−5.27541 (−16)	−6.12216 (−16)	8	0.1	−8.04639 (−15)	−1.50243 (−14)

Be$^+$

n	ρ	3s	4s	5s	6s	n	ρ	7s	8s
0	6.0	1.61186	1.01394	7.00467 (−1)	5.11842 (−1)	0	4.5	5.23039 (−1)	3.34249 (−1)
1	4.0	3.06317	1.85725	1.40946	1.07186	1	3.0	3.61296 (−2)	2.84980 (−2)
2	3.0	−3.45869	−1.99695	−1.80454	−1.47832	2	2.0	−1.92888 (−1)	−1.48167 (−1)
3	3.0	1.13463 (−1)	−2.91155 (−1)	4.48301 (−1)	5.67603 (−1)	3	2.0	−1.07382	−6.46294 (−1)
4	2.2	−1.31221	−6.93852 (−1)	−7.45700 (−1)	−6.44907 (−1)	3	1.4	5.43642 (−1)	3.32306 (−1)
5	2.2	4.96809 (−1)	2.39119 (−1)	3.40069 (−1)	3.16819 (−1)	4	1.4	−1.74461 (−1)	−1.07966 (−1)
5	1.5	−5.02670 (−2)	−1.39580 (−2)	−3.40953 (−2)	−3.47607 (−2)	4	0.8	2.40893 (−2)	1.59387 (−2)
6	1.5	1.81502 (−2)	9.25903 (−3)	1.19517 (−2)	1.10408 (−2)	5	0.8	−4.20068 (−3)	−2.87240 (−3)
6	0.75	5.69429 (−5)	−2.78799 (−5)	−1.16069 (−4)	−1.34061 (−4)	5	0.4	7.39975 (−5)	6.03939 (−5)
7	0.75	−3.89974 (−6)	−4.28109 (−6)	6.39063 (−6)	1.01217 (−5)	6	0.4	−4.36086 (−6)	−3.87198 (−6)
7	0.4	3.97087 (−9)	−3.07929 (−9)	7.46262 (−8)	1.02923 (−7)	6	0.2	1.00443 (−8)	2.33650 (−8)
8	0.4	−1.38492 (−10)	9.54343 (−11)	−2.07728 (−9)	−5.50788 (−9)	7	0.2	−1.33171 (−10)	−5.64815 (−10)

B^{2+}

n	ρ	3s	4s	5s	6s	n	ρ	7s	8s
0	8.5	2.77678	1.75366	1.22760	9.47550 (−1)	0	7.0	6.85547 (−1)	4.59001 (−1)
1	4.5	7.87492	4.88055	3.80961	3.06118	1	4.0	9.50894 (−1)	7.38784 (−1)
2	3.5	−1.44793 (+1)	−8.89337	−7.96593	−6.85786	2	2.5	−1.92680	−1.56415
3	3.5	5.29475	2.51938	4.93939	5.07124	3	2.5	5.93854 (−1)	7.19935 (−1)
4	2.6	−4.12461	−2.16138	−3.12779	−3.05064	4	1.5	1.85098 (−2)	−3.95440 (−2)
5	2.6	2.02012	9.92619 (−1)	2.02888	2.13308	5	1.5	3.56810 (−2)	5.81497 (−2)
5	1.8	−7 26800 (−2)	5.51524 (−2)	−1.81019 (−1)	−2.37132 (−1)	5	1.0	−9.00656 (−3)	−1.34471 (−2)
6	1.8	5.26420 (−2)	1.16729 (−2)	6.61629 (−2)	7.77438 (−2)	6	1.0	6.97473 (−4)	1.66334 (−3)
6	1.0	1.32827 (−4)	−7.66755 (−4)	−2.20867 (−3)	−2.68263 (−3)	6	0.6	5.80146 (−5)	1.56832 (−5)
7	1.0	−1.01925 (−5)	1.35871 (−5)	2.46885 (−4)	3.48845 (−4)	7	0.6	−5.06567 (−6)	−2.10396 (−6)
7	0.5	2.22538 (−9)	−1.50862 (−8)	3.48831 (−7)	−1.46800 (−7)	7	0.3	1.07365 (−8)	1.48713 (−8)
8	0.5	−9.43916 (−11)	6.59259 (−10)	−1.37496 (−8)	−5.43837 (−9)	8	0.3	−2.42159 (−10)	−5.19831 (−10)

C^{3+}

n	ρ	3s	4s	5s	6s	n	ρ	7s	8s
0	10.0	3.96645	2.53920	1.79329	1.34609	0	8.5	9.58252 (−1)	5.82278 (−1)
1	6.5	1.35028 (+1)	8.19094	5.81354	4.33085	1	5.5	2.05324	1.44410
2	4.5	−1.89217 (+1)	−1.04708 (+1)	−7.60399	−5.62781	2	3.5	−4.80445	−3.64130
3	4.5	−7.65521	−9.80663	−6.83635	−5.48482	3	3.5	3.10017	4.08570
4	3.0	−7.64000	−2.32343	−1.60055	−9.88825 (−1)	3	2.2	−1.44392	−1.17105
5	3.0	5.70076	7.44237 (−1)	4.95514 (−1)	1.30587 (−1)	4	2.2	1.18138	1.17701
5	2.2	−2.91438 (−1)	8.25292 (−1)	7.00757 (−1)	6.31640 (−1)	5	1.4	−1.24414 (−2)	−2.67338 (−2)
6	2.2	2.22223 (−1)	−1.48632 (−1)	−1.48880 (−1)	−1.46055 (−1)	6	1.4	−5.15704 (−3)	1.28768 (−3)
6	1.1	1.26642 (−4)	−2.74123 (−3)	−3.96122 (−3)	−3.90544 (−3)	6	0.8	6.23255 (−4)	3.51133 (−4)
7	1.1	−1.29681 (−5)	2.40275 (−4)	6.22980 (−4)	7.42647 (−4)	7	0.8	−6.83452 (−5)	−4.25746 (−5)
7	0.65	2.59774 (−8)	−5.68548 (−7)	5.00410 (−7)	−5.53568 (−6)	7	0.4	1.25892 (−7)	1.87213 (−7)
8	0.65	−1.30203 (−9)	2.99384 (−8)	−1.97693 (−8)	1.70994 (−7)	8	0.4	−3.75960 (−9)	−8.55071 (−9)

† $(\pm n) = 10^{\pm n}$

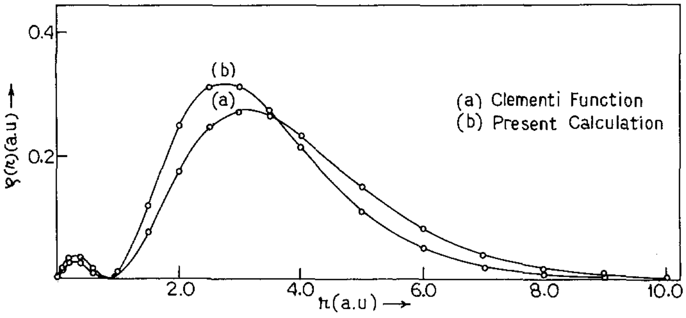

Fig. 1. Comparison of radial density of the deexcited component for Li obtained in the present calculation and that of Clementi $2s$ function

The parameters and coefficients for the wavefunctions have been displayed in Table 4.

For Li, only the results of the fourth basis are listed, while for Be^{+}, B^{2+} and C^{3+} the results for the two different basis sets are listed.

A numerical plot of the wavefunctions produce the proper no. of nodes in all cases. Extra orthogonality constraint is also not needed here [18]. As discussed earlier TDHF theory incorporates an appreciable amount of correlation through the presence of doubly excited configurations [17]. For closed shell systems the doubly excited configurations get deexcited to singly excited configurations of the original system via the external perturbation. The situation is complicated for open shell systems like Li where a deexcitation yields a three open shell system. For example, the presence of $1s3s^2:{}^2S$, doubly excited configuration yields a deexcited $1s2s3s:{}^2S$ configuration at resonance corresponding to $2s \rightarrow 3s$ transition. The presence of such a configuration is explicitly demonstrated in this calculation. In Fig. 1 we plot the density of the renormalised deexcited coefficient for the transition $2s \rightarrow 3s$ for Li. The deexcited density clearly represents the $2s$ nature of the orbital. To get a further check we also plot in Fig. 1 the density of the Clementi [22] $2s$ orbital. The close resemblance clearly demonstrates the functional similarity between the two orbitals.

The present method may be applied to study the inner-shell excitation process for three electron system. However, in this case the effect of core rearrangement is very important and must be explicitly taken care of. This is under present study and results will be reported in due course.

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