Comments and Addenda

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Autoionization and quasibound states of Li^+

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The positions $E = \mathcal{E} + \Delta$ of the $^{1,3}(S^e, P^o, D^e)$ autoionizing states of Li^+ below the $n = 2$ threshold of Li^{++} have been calculated using the Feshbach projection-operator technique. The trial wave function is of Hylleraas type. Widths Γ and shifts Δ of these states have been calculated using the exchange approximation for the continuum functions. The calculated positions are generally lower than those obtained in previous calculations. Widths of most of the states have not previously been calculated. The positions are also compared with experimental results of Ziem, Bruch, and Stolterfoht and Bruch *et al.* Positions of the nonautoionizing (quasibound) $^3P^e$, $^{1,3}D^o$ states have also been calculated. The positions in all cases are lower than those obtained in previous calculations.

AUTOIONIZATION STATES

During the last few years, the autoionization states of He and H^- have been studied extensively both theoretically and experimentally. Recently, Bruch *et al.*[1] determined the positions of the lowest $^{1,3}P$ autoionization states in Li^+ by beam-foil experiments, and Ziem *et al.*[2] determined the lowest ^1S and $^{1,3}P$ resonance positions by He^+ and H^+ impact on Li^+. Bruch *et al.*[1] also calculated the positions of a large number of resonances using hydrogenic functions, but did not calculate widths.

In this paper we present the positions and widths of these resonances obtained by the Feshback projection-operator technique. In this method which is now well-known,[3] we define the projection operators P and Q such that $P+Q=1$. P does not affect the asymptotic form of the wave function, and Q is such that QHQ has a discrete spectrum whose eigenvalues are very close to the autoionization energies of the system. The details of the calculations have been given in previous papers.[4] Here we give the necessary formulas for the positions and the widths.

The position of the resonance is given by

$$E = \mathcal{E} + \Delta , \tag{1}$$

where $\mathcal{E}$ is determined variationally by minimizing the functional

$$\mathcal{E} = \langle \Phi Q H Q \Phi \rangle / \langle \Phi Q \Phi \rangle . \tag{2}$$

The total Hamiltonian of the system is given by

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2z}{r_1} - \frac{2z}{r_2} + \frac{2}{r_{12}} . \tag{3}$$

(Rydberg units are used throughout.) The projection operator is given by

$$Q = 1 - P_1 - P_2 + P_1 P_2 \tag{4}$$

$$= 1 - P , \tag{5}$$

$$P_i = |\varphi_0(\vec{\mathbf{r}}_i)\rangle\langle\varphi_0(\vec{\mathbf{r}}_i)| , \tag{6}$$

where $\varphi_0(\vec{\mathbf{r}}_i)$ is the ground state of the ith particle in the nuclear field of charge z:

$$\varphi_0(\vec{\mathbf{r}}) = (z^3/\pi)^{1/2} e^{-zr} . \tag{7}$$

Φ is a trial function of angular momentum, spin, and parity appropriate to the state.[4] In this case, Φ is a Hylleraas-type function. The width of the resonance is calculated from

$$\Gamma = 2k\,|\langle P\Psi H Q \Phi\rangle|^2 , \tag{8}$$

where k^2, the energy of the scattered electron, is related to the resonance position by

$$k^2 - z^2 = E . \tag{9}$$

The nonresonance continuum function, $P\Psi$, is here calculated in the exchange approximation[5] in which

TABLE I. Autoionization states of Li^+.

				Present results [a]					Perrott and Stewart [b]			Experiment			
												Bruch *et al.* [c]	Ziem *et al.* [d]		Bruch *et al.* [c]
	λ	N	$-\mathcal{E}_\lambda$	$\mathcal{E}$	Γ	Δ_c	Δ_b	Δ	E	$\mathcal{E}$	Γ	$\mathcal{E}$	E	Γ	E
$^1S^e$	1	70	3.814 705	70.5502	0.157	0.0121	0.0215	0.0335	70.5837	70.6129	0.173	70.6930	70.62 ± 0.030	0.05 ± 0.03	
	2	84	3.263 796	78.0458	0.0111	0.00993	0.0284	0.0384	78.0842	78.1451	0.65×10^{-2}	78.5396			
	3	84	2.831 983	83.9210	0.0776	0.0119	0.00694	0.0189	83.9398			84.0379			
$^3S^e$	1	56	2.880 446	83.2616	0.277×10^{-3}	0.149×10^{-3}	0.790×10^{-3}	0.939×10^{-3}	83.2625			83.2655			
	2	56	2.720 668	85.4355	0.153×10^{-4}	0.388×10^{-4}	0.116×10^{-2}	0.120×10^{-2}	85.4367			85.4803			
	3	56	2.572 896	87.4461	0.189×10^{-3}	0.933×10^{-4}	0.283×10^{-3}	0.376×10^{-3}	87.4464			87.4645			
$^1P^o$	1	84	3.514 487	74.6349	0.0593	-0.767×10^{-2}	0.392×10^{-2}	-0.728×10^{-2}	74.6277			74.9049	74.67 ± 0.030		74.67 ± 0.5
	2	84	2.861 075	83.5251	0.163×10^{-3}	0.134×10^{-3}	0.710×10^{-3}	0.844×10^{-3}	83.5260			83.5526			
	3	84	2.722 121	85.4157	0.0195	-0.259×10^{-2}	0.249×10^{-3}	-0.234×10^{-2}	85.4134			85.5387			
$^3P^o$	1	84	3.758 790	71.3110	0.892×10^{-2}	0.0115	0.0225	0.0339	71.3449			71.4403	71.38 ± 0.030		71.27 ± 0.5
	2	84	2.813 074	84.1782	0.317×10^{-2}	0.502×10^{-2}	0.579×10^{-2}	0.0108	84.1891			84.2759			
	3	84	2.797 014	84.3968	0.951×10^{-4}	-0.628×10^{-5}	0.208×10^{-3}	0.202×10^{-3}	84.3970			84.4328			
$^1D^e$	1	112	3.543 926	74.2344	0.111	0.0387	0.551×10^{-2}	0.0443	74.2787	74.3545	0.113	74.5394			
	2	112	2.747 702	85.0677	0.0218	0.0135	0.241×10^{-3}	0.0137	85.0814			85.2190			
	3	112	2.689 481	85.8598	0.0133	0.480×10^{-3}	0.108×10^{-3}	0.588×10^{-3}	85.8604			85.8763			
$^3D^e$	1	112	2.810 487	84.2134	0.538×10^{-5}	0.150×10^{-3}	0.913×10^{-3}	0.106×10^{-2}	84.2145			84.2472			
	2	112	2.722 625	85.4089	0.258×10^{-3}	0.160×10^{-3}	0.144×10^{-4}	0.171×10^{-3}	85.4090			85.4051			
	3	112	2.539 484	87.9007	0.187×10^{-3}	0.357×10^{-5}	0.344×10^{-3}	0.348×10^{-3}	87.9010			87.8676			

[a] λ represents the sequential order of the resonances. N is the total number of terms in the trial wave function Φ. All results, except $\mathcal{E}_\lambda$ which are in Rydberg units, are in eV computed by using $\mathcal{R}_\infty = 13.605\,826$ eV (see Appendix of Ref. 4). The positions in all cases are with respect to the ground state of Li^{++}.

[b] Reference 7.

[c] Reference 1.

[d] Reference 2.

the wave function is approximated by

$$\Psi = P\Psi = (1/\sqrt{2})[u(\vec{r}_1)\varphi_0(\vec{r}_2) \pm (1 \rightleftharpoons 2)], \quad (10)$$

where $u(\vec{r})$ is the scattering function. The upper sign corresponds to the singlet states, and the lower sign corresponds to the triplet states. Widths of autoionization states in He were found to be insensitive to different approximations.[4] And since the polarizability of Li^{++} is even smaller than that of He^+, the exchange approximation should be more than sufficient in this case. This is because the polarization is the main additional contribution to the nonresonant equation[6] beyond the exchange approximation itself; this correction can confidently be omitted in this application. The shift is given by

$$\Delta = \frac{1}{2\pi}\left(\sum_\nu \frac{\Gamma_\nu}{E - E'_\nu} + \mathcal{P}\int \frac{\Gamma(E')\,dE'}{E - E'}\right)$$

$$= \Delta_b + \Delta_c, \quad (11)$$

where the first term represents the contribution from the bound states and the second term represents the contribution from the continuum.[4]

Table I gives the quantities $\mathcal{E}$, Δ_b, Δ_c, Δ, the positions E with respect to the ground state of Li^{++}, and the widths Γ of the $^{1,3}S^e$, $^{1,3}P^o$, and $^{1,3}D^e$ autoionization states of Li^+. The results of the calculations of Perrott and Stewart[7] and of Bruch *et al.* are also given. Perrott and Stewart carried out their calculation in Q space using a restricted Hylleraas-type wave function. It should be noted that Bruch *et al.* constructed the wave functions for these states to be explicitly in Q space by using hydrogenic functions. Therefore the positions calculated by them as well as those of Perrott and Stewart correspond to the unshifted positions $\mathcal{E}$; in both calculations shifts were not computed. The present results are seen to be lower than their results except in the case of the second and third $^3D^e$ states. The widths of the lowest $^1S^e$ and $^1D^e$ states of Perrott and Stewart are the only available results, and the agreement of the two sets of results is good.

Table I also gives the positions of the lowest $^1S^e$, $^{1,3}P^o$ states determined experimentally by Ziem *et al.*[2] and the positions of the lowest $^{1,3}P^o$ states determined by Bruch *et al.*[1] The experimental results are seen to be higher than the calculated positions. The only experimental determination of the widths is for the $^1S^e$ state as reported by Ziem *et al.*, but the error in this state is rather large. It would be desirable to have an experimental determination of the positions of other states and widths of all states.

TABLE II. Positions of $^3P^e$ and $^{1,3}D^o$ states of Li^+.

State	λ	N	E (Ry)	E [a]	Bruch *et al.* [b]
$^3P^e$	1	84	−3.593 296	73.5627	73.7251
	2	84	−2.747 178	85.0748	85.1713
	3	84	−2.521 086	88.1510	88.2070
	4	84	−2.420 559	89.5187	89.5521
$^1D^o$	1	112	−2.743 196	85.1290	85.1564
	2	112	−2.518 775	88.1824	88.2003
	3	112	−2.419 012	89.5398	89.5493
$^3D^o$	1	112	−2.714 228	85.5231	85.5668
	2	112	−2.507 804	88.3317	88.3596
	3	113	−2.413 457	89.6154	89.6290

[a] λ represents the sequential order of the states. N is the total number of the terms in the trial wave function Φ. The positions in eV are with respect to the ground state of Li^{++} obtained by using $\mathcal{R}_\infty = 13.6056826$ eV.
[b] Reference 1.

QUASIBOUND STATES

The $^3P^e$ and $^{1,3}D^o$ states cannot undergo autoionization because the parity and angular momentum of these states cannot be conserved relative to the ground state of Li^{++} and a scattered electron. Therefore these states can be calculated as bound states.[8] Their positions are calculated variationally by minimizing the functional

$$E = \langle \Phi H \Phi \rangle / \langle \Phi \Phi \rangle . \quad (12)$$

The wave function for $^3P^e$ states, which was misprinted in the previous paper,[9] is given by

$$\Phi(\vec{r}_1, \vec{r}_2) = [f(r_1, r_2, r_{12}) + f(r_2, r_1, r_{12})]\mathfrak{D}_1^{0+}, \quad (13)$$

where $\mathfrak{D}_1^{0+}$ is the rotational harmonic depending on the symmetric Euler angles[10] θ, ϕ, ψ. The trial radial function f is given by

$$f(r_1, r_2, r_{12}) = e^{-(\gamma r_1 + \delta r_2)} r_1 r_2 \sin\theta_{12}$$

$$\times \sum_{l\geq 0}\sum_{m\geq 0}\sum_{n\geq 0} r_1^l r_2^m r_{12}^n, \quad (14)$$

where γ and δ are the nonlinear parameters. The wave function for $^{1,3}D^o$ states is given in Ref. 11. The positions of some of these states converging to the $n = 2$ threshold of Li^{++} are given in Table II, and the results are compared with those of Bruch *et al.* The present positions are lower than their results.

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[1]R. Bruch, G. Paul, J. Andrä, and L. Lipsky, Phys. Rev. A 12, 1808 (1975).
[2]P. Ziem, R. Bruch, and N. Stolterfoht, J. Phys. B 8, L480 (1975).
[3]T. F. O'Malley and S. Geltman, Phys. Rev. 5, A1344 (1965).
[4]A. K. Bhatia and A. Temkin, Phys. Rev. A 11, 2018 (1975), and the references cited in this paper.
[5]P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933).
[6]A. K. Bhatia and A. Temkin, Phys. Rev. 182, 15 (1969).
[7]R. H. Perrott and A. L. Stewart, J. Phys. B 1, 381 (1968); 1, 1226 (1968).
[8]A. Temkin, in *Autoionization,* edited by A. Temkin (Mono. Book Corp., Baltimore, 1966).
[9]A. K. Bhatia, Phys. Rev. A 2, 1667 (1970).
[10]A. K. Bhatia and A. Temkin, Rev. Mod. Phys. 36, 1050 (1964).
[11]A. K. Bhatia, Phys. Rev. A 6, 2498 (1972).