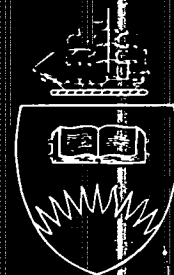*The Flinders University of South Australia*

ELECTRONIC STRUCTURE OF MATERIALS CENTRE

Convergent J-matrix calculation of electron-lithium resonances
Short title : Calculation of electron-lithium resonances

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Short title: *Calculation of electron-lithium resonances*

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Abstract. The recently developed Convergent J-matrix method is used to calculate resonances in the electron-lithium scattering cross sections (elastic, total, 2^2P, 3^2S, 3^2P and 3^2D). The positions and widths of the resonances are calculated using the poles of the S-matrix.

1. Introduction

Recent review of atomic negative-ion resonances by (Buckman and Clark 1994) revealed that little progress has been made in the study of resonances in electron-lithium scattering since the classic review article by Schulz (1973). This compares to the progress made on electron-hydrogen resonances where a number of high accuracy experimental measurements and theoretical calculations exist, e.g. see the J-matrix calculations of Konovalov and McCarthy (1994a) and references therein.

The electronic structure of lithium is comparatively simple: the atom can be well described as an inert core containing two electrons in $1s$ orbitals plus one valence electron above the core. The excited states of Li and Li$^-$ are expected to be very similar to those of H and H$^-$. Therefore it is possible that there are a large number of Rydberg type excited Li$^-$ states (resonances) associated with most of the excited states of lithium. Lin (1983) and Stewart *et al* (1974) showed that there are, in fact, some doubly-excited states of Li$^-$ which could manifest themselves as resonances in electron-lithium scattering below 5.39 eV (auto-ionisation resonances are not dealt with in this work). Buckman and Clark (1994) summarised recommended energies (in eV) and classifications of resonances in Li$^-$ as: $2s2p\,^3P$ at 0.06; $2p3p\,^1P + 2p^2\,^1D$ at 1.85; ^1S, ^3P, ^3S at 3.11-3.34; and ^1D, ^1S, ^3P, ^1P at 3.70-3.78.

The close-coupling (CC) calculations below 5.39 eV, the five-state $(2s-2p-3s-3p-3d)$ CC calculation of Moores (1986) and two-state $(2s-2p)$ CC calculations of Burke and Taylor (1969) and Walters (1976), fail to discover any resonant structures in elastic (2^2S), 3^2S and 2^2P cross sections. A possible reason for this lack of resonances is that the energy mesh was not fine enough to resolve sharp resonance behaviour. Another possibility is that the small size close-coupling expansion is not

enough to describe the resonances.

In order to verify the existence of Li$^-$ resonances, the Convergent J-matrix calculation is performed at the range of energies from 1.6 eV to 4 eV. The method is essentially a close-coupling method where a complete set of square-integrable (L^2) Laguerre functions are used to describe the target and the scattering electron bound and continuum states. The successful usage of the method relies on the non-trivial fact that it is possible to achieve convergence in physical observables (e.g. cross sections) when the number of L^2 functions is increasing. This assumption has been verified by a large number of publications, some examples are: calculations of electron-hydrogen (Bray et al 1991) and electron-lithium (Bray et al 1993) scattering using the coupled-channels optical potential method; the Convergent J-matrix calculations of resonances in the electron-helium (Konovalov and McCarthy 1995) and electron-hydrogen (Konovalov and McCarthy 1994a, Konovalov and McCarthy 1994b) scatterings; and Convergent Close-Coupling (CCC) method of Bray and Stelbovics (1992).

2. Theory

The formulation of the J-matrix method could be found in the paper of Broad and Reinhardt (1976) and references therein (this combined reference will be referred to as BR76 hereafter). The following formulas for the J-matrix method are for electron-atom scattering. Generalization of the method for electron-ion scattering together with its derivation can be found in BR76.

2.1 Multichannel equations for electron-atom scattering

This subsection is basically a summary of BR76 which is presented here for completeness. The notation of Broad and Reinhardt (1976) is changed slightly to make it more convenient for computer programming. While the LS-coupling expansion is used, modifications for the jj-coupling expansion naturally follow from the formulas below. The following notations are used:

- $l, \frac{1}{2}, L^t, S^t, L$ and S are the orbital and spin angular momentum of the projectile electron, the target atom (denoted by t) and negative ion (total system of the scattering electron and atom), respectively. The corresponding Z-axis projections are denoted by m, m_s, M^t, M^t_S, M and M_S.

- μ is a set of other quantum numbers needed to distinguish excited states of the atom. Quantum numbers are grouped into $\gamma = \{\mu, L^t, S^t\}$ and $i = \{\mu, L^t, S^t, l, L, S\} = \{\gamma, l, L, S\}$.

- E, E_0 and E_{γ_0} are total energy of the system (negative ion), the incident electron energy and the initial target state, respectively. i_0 denotes the incident channel (the state of the atom before the collision with the electron).

The set of target internal coordinates is denoted by ρ with the set of the target states, $R_\gamma(\rho)$, obtained by diagonalising the target Hamiltonian, H_t, on a set of square-integrable configurations,

$$\langle R_{\gamma',M^{t'},M_S^{t'}}|H_t|R_{\gamma,M^t,M_S^t}\rangle = \delta_{\gamma'\gamma}\delta_{M^{t'}M^t}\delta_{M_S^{t'}M_S^t}E_\gamma. \tag{1}$$

It is assumed that the nonrelativistic Hamiltonian is used, hence γ's are good quantum numbers. If the relativistic terms are included, γ will need to be modified to $\gamma = \{\mu, L^t, S^t, J^t\}$, where J^t is the total momentum of the atom.

The projectile electron is described differently for the *outer* and *inner* function spaces. The outer radial functions are taken to be,

$$\phi_{pl}(r) = (\lambda_l r)^{l+1} e^{-\lambda_l r/2} L_p^{2l+1}(\lambda_l r), \quad p = N_l, N_l + 1, ...\infty. \tag{2}$$

The inner radial functions are built as a linear combination of the ϕ_{pl} with $p < N_l$,

$$\psi_{pl}(r) = \sum_{p'=0}^{N_l-1} \phi_{p'l}(r)\, D_{p'p}^l, \quad p = 0, 1, ..., N_l - 1 \tag{3}$$

The ϕ_{pl} functions play a fundamental role in the J-matrix method as they form the overlap matrix,

$$J_{p'p}^i = \langle \phi_{p'l}| - \frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{1}{2}k_\gamma^2|\phi_{pl}\rangle, \tag{4}$$

which is of the tridiagonal, or Jacobi, form. The channel momentum, k_γ, is defined by $\frac{1}{2}k_\gamma^2 = E_0 + E_{\gamma_0} - E_\gamma$. The J-matrix defines s_p^i and c_p^i coefficients by

$$\sum_{p'=0}^\infty J_{pp'}^i s_{p'}^i = 0, \quad \sum_{p'=0}^\infty J_{pp'}^i c_{p'}^i = \beta\delta_{p0}, \quad \beta = k_\gamma/(2s_0^i), \quad p = 0, 1, ..., \infty. \tag{5}$$

Equations (4) and (5) are solved analytically (explicit formulas can be found in BR76).

The total wave function is expanded into two sets of functions,

$$\Psi_{i_0}(\rho, \mathbf{r}) = \sum_{i'} \sum_{p'=0}^{N_{l'}-1} \Phi_{p'}^{i'}(\rho, \mathbf{r})a_{p'}^{i'i_0} + \sum_{i'} \sum_{p'=N_{l'}}^\infty \Phi_{p'}^{i'}(\rho, \mathbf{r})f_{p'}^{i'i_0}, \tag{6}$$

where

$$\Phi_p^i(\rho, \mathbf{r}) = A\chi_i(\rho, \hat{\mathbf{r}})\psi_{pl}(r), \quad p = 0, 1, ..., N_l - 1 \tag{7}$$

$$= A\chi_i(\rho, \hat{\mathbf{r}})\phi_{pl}(r), \quad p = N_l, N_l + 1, ..., \infty, \tag{8}$$

and where: A is the antisymmetrization operator; i denotes the channel quantum numbers $\{\gamma, l, L, S\}$; $\chi_i(\rho, \hat{\mathbf{r}})$ is made from the function $R_{\gamma, M^t, M_S^t}(\rho)$, the spherical harmonic $Y_{lm}(\hat{\mathbf{r}})$ and a Pauli spinor $\chi_{m_s}^{1/2}$ to have the total angular momentum L and total spin S.

The total Hamiltonian H is diagonalized on a set of Φ functions (7) providing eigenvectors $U_{pp'}^{ii'}$ and eigenvalues E_p^i. The Schrödinger equation is solved using c^i, s^i and J^i from Eq.(5),

$$\langle \Phi_{p''}^{i''}|(H - E)^{N_l}|\Psi_i\rangle = 0, \tag{9}$$

where the superscript N_l indicates that all potentials and symmetrization operators are omitted in matrix elements with $p \geq N_l$.

The scattering matrix $S_{i'i}$ is defined using the reactance matrix $R_{i'i}$,

$$S = (1 + iR)(1 - iR)^{-1}, \quad R_{i'i} = -\left[B^{-1}A\right]_{i'i}, \tag{10}$$

$$A_{i'i} = \left(W_{i'i}J_{N_l-1,N_l}^i s_{N_l}^i + \delta_{i'i}s_{N_l-1}^i\right)(\pi k_\gamma/2)^{-1/2}, \tag{11}$$

$$B_{i'i} = \left(W_{i'i}J_{N_l-1,N_l}^i c_{N_l}^i + \delta_{i'i}c_{N_l-1}^i\right)(\pi k_\gamma/2)^{-1/2}, \tag{12}$$

$$W_{i'i} = \sum_{p'=0}^{N_{l'}-1}\sum_{p=0}^{N_l-1} D_{N_{l'}-1,p'}^{l'}[(H - E)^{-1}]_{p'p}^{i'i}D_{N_l-1,p}^l, \tag{13}$$

where i and i' in the calculation of the S-matrix (10), i in the R-matrix (10) and the A-matrix (11) are defined only for open channels ($E_0 + E_{\gamma_0} - E_\gamma > 0$), and where $c_p^i + is_p^i$ are used instead of c_p^i for closed channels in equation (12).

The cross section for the transition from γ to γ' states of the atom, $\sigma_{\gamma'\gamma}$, is defined by

$$\sigma_{\gamma'\gamma} = g \sum_{l'l''LS} \sigma_{i'i}, \quad \sigma_{i'i} = \frac{\pi}{k_\gamma^2}(2L + 1)(2S + 1)|\delta_{i'i} - S_{i'i}|^2, \tag{14}$$

$$g = [2(2L^t + 1)(2S^t + 1)]^{-1}. \tag{15}$$

The differential cross section is defined by

$$\frac{d\sigma_{\gamma'\gamma}}{d\Omega} = g(2\pi)^4\frac{k_{\gamma'}}{k_\gamma}\sum_{M^{t'}M^t}\sum_S(2S + 1)|T(\gamma'M^{t'}Sk' \leftarrow \gamma M^t Sk)|^2, \tag{16}$$

$$T(\gamma'M^{t'}Sk' \leftarrow \gamma M^t Sk) = \sum_{l'l}\left(\frac{(2l + 1)}{4\pi}\right)^{1/2}Y_{l'm'}(\hat{k}')T_{i'i} \tag{17}$$

$$\times C(L^{t'}, l', L; M^{t'}, m', M^t)C(L^t, l, L; M^t, 0, M^t), \tag{18}$$

where the C's are Clebsch-Gordan coefficients and where the T-matrix is defined from $S_{i'i} = \delta_{i'i} - 2\pi i(k_{\gamma'}k_\gamma)^{1/2} T_{i'i}$.

2.2 Convergent J-matrix formalism

The success of the L^2 expansion is based on the ability to increase the size of the basis until convergence is achieved in the required physical observables. The set of non-orthogonal radial functions ϕ_{pl} of Eq.(2) used in the J-matrix is a *complete* basis in the L^2 space if all p are included. In order to achieve such completeness the ϕ_{pl} functions or their linear combinations must be used with $0 \leq p < N_l$ to create one-electron orbitals. The following basis functions are used

4

$$\psi_{pl}(r) = \sum_{p'=0}^{N_l-1} \hat{\psi}_{p'l}(r) \ C_{p'p}^l, \qquad p = 0, 1, ..., N_l - 2, \tag{19}$$

$$\psi_{N_l-1,l}(r) = \hat{\psi}_{N_l-1,l}(r), \tag{20}$$

$$\hat{\phi}_{pl}(r) = P_p^l \ (\lambda_l r)^{l+1} e^{-\lambda_l r/2} L_p^{2l+2}(\lambda_l r), \qquad p = 0, 1, .., N_l - 1. \tag{21}$$

The $\hat{\psi}_{pl}$ function is orthonormal (P_p^l - normalisation coefficient) and can be expressed as a linear combination of the ϕ functions of Eq.(2) via

$$L_p^{\alpha+1}(x) = \sum_{p'=0}^{p} L_{p'}^{\alpha}(x). \tag{22}$$

The set of $\hat{\psi}$ functions provides a convenient basis not only for the scattering part of the problem but also for the multi-configuration calculations of the target atom and negative ion system. Also, the special form of ψ_{pl} for $p = N_l - 1$ (20) leads to $D_{N_l-1,p}^l = \delta_{N_l-1,p} P_{N_l-1}^l$ and, as a result, to some considerable simplification for the $W_{i'i}$ matrix (13),

$$W_{i'i} = P_{N_{l'}-1}^{l''}[(H - E)^{-1}]_{N_{l'}-1,N_l-1}^{i'i} P_{N_l-1}^l. \tag{23}$$

Any reasonable set of λ_l is allowed as the calculated physical observables are independent of the internal parameters of the J-matrix method, this is providing that convergence is achieved. The only difference between various sets of λ's is how large N_l are required and how many i's need to be coupled to reach the convergent results. The following $\lambda_l = \lambda_0(N_l + l + 1)/(N_0 + 1)$ are used, insuring that roughly the same size of the coordinate space is covered for all l considered.

2.3 Resonances as the poles of the S-matrix

Resonances can be defined as the poles of the S-matrix in the complex energy plane. A particular resonance will have its position ($E_\nu + \Delta_\nu$) and width ($\Gamma_\nu \equiv \Gamma_{p_r}^{i_r}$), where $\nu \equiv (p_r, i_r)$. If Γ_ν is small compared to the distance between excited states (E_ν) of the negative ion, the corresponding state becomes metastable and it will manifest itself as a resonance in cross sections. For a particular resonance E_ν with a small Γ_ν, Eq.(23) can be approximated by

$$W_{i'i} = \frac{Z^{i'\nu} Z^{i\nu}}{(E_\nu - E)}, \tag{24}$$

$$Z^{i\nu} = U_{N_l-1,p_r}^{ii_r} \ P_{N_l-1}^l, \quad [(H-E)^{-1}]_{p'p}^{i'i} = \sum_{i''} \sum_{p''}^{N_{l''}-1} \frac{U_{p'p''}^{i'i''}(U^T)_{p''p}^{i''i}}{(E_{p''}^{i''} - E)}. \tag{25}$$

Using the fact that $R = R^T$ (Broad and Reinhardt 1976), Eq.(10) can be rewritten as

$$S_{i'i}\hat{c}_i^{(+)} + \sum_{i''} S_{i'i''}W_{i''i}C_{i''}^{(+)} = \delta_{ii'}\hat{c}_i^{(-)} + W_{i'i}C_{i'}^{(-)}, \tag{26}$$

$$\hat{c}_i^{(\pm)} = (c_{N_l-1}^i \pm is_{N_l-1}^i)(\pi k_\gamma/2)^{-1/2}, \quad c_i^{(\pm)} = (c_{N_l}^i \pm is_{N_l}^i)(\pi k_\gamma/2)^{-1/2} \tag{27}$$

$$C_i^{(\pm)} = c_i^{(\pm)} J_{N_l-1,N_l}^i. \tag{28}$$

Due to the separability of W in (24), the equation for the S-matrix (26) can be solved exactly (Smirnov et al 1990) giving

$$S_{i'i} = \frac{1}{\hat{c}_i^{(+)}} \left(\delta_{i'i} \hat{c}_i^{(-)} + \frac{Z^{i\nu} Q_{i'}}{E_\nu - E} \right), \quad Q_i = Z^{i\nu} C_i^{(-)} - \sum_{i''} S_{ii''} Z^{i''\nu} C_{i''}^{(+)}. \quad (29)$$

Substituting S in the equation for Q (29), Q_i can be determined and the S-matrix (29) becomes

$$S_{i'i} = \frac{\hat{c}_{i'}^{(-)}}{\hat{c}_i^{(+)}} \left(\delta_{ii'} + \frac{Z^{i\nu} Z^{i'\nu} (L_i^{(-)} - L_i^{(+)})}{E_\nu + \Delta_\nu - i\Gamma_\nu/2 - E} \right) \quad (30)$$

$$L_i^{(\pm)} = C_i^{(\pm)}/\hat{c}_i^{(\pm)}, \quad (31)$$

$$\Delta_\nu = \text{Re} \sum_i (Z^{i\nu})^2 L_i^{(+)}, \quad \Gamma_\nu = -2\text{Im} \sum_i (Z^{i\nu})^2 L_i^{(+)}. \quad (32)$$

3. Li and Li$^-$ states

The lithium atom is described as an inert (frozen) core of two $1s$ electrons with a valence electron above the core. Bray et al (1993) showed that this model is sufficient to reach complete agreement with experimental data for such sensitive physical observables as spin asymmetries and differential cross sections for the range of incident electron energies from 5.4 to 200 eV. This work is concerned with Li$^-$ resonances below the ionisation threshold of lithium (5.39eV). This together with the results of Bray et al (1993) indicates that core-excited configurations can be omitted from the calculation without loss of accuracy for the cross sections considered (elastic (2^2S), 2^2P, 3^2S, 3^2P and 3^2D).

The core $1s$ orbital is created by diagonalizing the one electron Hamiltonian,

$$\langle \psi_{q0} | - \frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{Z_{1s}}{r} | \psi_{q'0} \rangle = \epsilon_q \delta_{qq'} \quad Z_{1s} = 2.6875, \quad q, q' = 0, .., N_l - 2 \quad (33)$$

The value of Z_{1s} is optimized to minimize the ground state energy of Li$^+$, $E(\text{Li}^+) = \langle (1s)^2 | H(\text{Li}^+) | (1s)^2 \rangle$, within one configuration, $(1s)^2$ ^1S.

The ground and excited states of Li and Li$^-$ are created by diagonalizing the corresponding Hamiltonians on the following configurations

$$\text{Li}: \ |\psi_{10}, \psi_{10}, \psi_{qL^t}; \ q \ ^{2S^t+1}L^t) \quad q = 0, ..., N_{L^t} - 1, \quad (34)$$

$$\text{Li}^-: \ |\psi_{10}, \psi_{10}, \psi_{qL^t}, \psi_{q'l}; L^t, S^t, l, \frac{1}{2}, LS; \ ^{2S+1}L), \quad q < N_{L^t}, \quad q' < N_l, \quad (35)$$

where $L^t \leq 7$ and $l, L \leq 13$. General formulas of Fano (1965) were used for the calculation of many electron (three for Li and four for Li$^-$) Hamiltonian matrix elements. The resulting eigenvalues of Li are presented in Table 1. The ionisation threshold of Li and the electron affinity of Li$^-$ are calculated to be 5.35 eV and 0.6206 eV respectively. That compares well with the corresponding experimental values of 5.39 eV (Moore 1949,1971) and 0.618 eV (Smirnov 1982).

4. Results and Conclusions

In the present calculation more than 1000 Li^- states were generated for some values of LS. Not every eigenvector for Li^- is an autodetaching metastable state in the sense of Buckman and Clark (1994) or doubly-excited state of Lin (1983), some of them are L^2 representations of the Li^- continuum. Only the metastable excited states of Li^- lead to the resonances in the cross sections, provided that a large number of L^2 states are coupled and convergent results are achieved. Pseudo-resonances appear only when a small number of L^2 states are used, e.g. Heller and Yamani (1974), and disappear with an increase in the basis size (Konovalov and McCarthy 1994b).

Not every Li^- state leads to a resonance in the sense of Eq. (30). The main assumption in the derivation of the Eq.(30) was that Γ for a single pole of the S-matrix is small. The position and width for each of the Li^- state is calculated using the formulas for the poles of S-matrix (32). Pathak *et al* (1988) showed that most of the H^- resonances have widths less than about 40 meV. This value is used to select the resonances which are expected to be described accurately by the Eq.(32). The resulting values are presented in table 2 for resonances which have Γ's less than 40 meV and $L \leq 2$.

It is found that the cross sections are converged to an accuracy of better than 2% when the following set of N_l is used ($\lambda_0 = 1.2$)

$$\{\lambda_0; N_0, N_1, ... N_{13}\} = \{1.2; 21, 16, 13, 11, 9, 7, 5, 4, ...4\}. \tag{36}$$

All open channels (i's) at each energy E_0 are coupled together with a few closed channels. A number of closed channels is increased until the cross sections become insensitive to a further increase. That resulted in more than 100 channels being close-coupled for some LS. The resulting cross sections are presented in figures 1 and 2. The 0.01 eV step is used for the incident electron energy, E_0. The cross sections can be obtained in tabular form from the author on request. Some values of E_0 are presented in Table 3.

The present J-matrix calculation reveals a great number of resonances. That is in line with the expectation that the highly excited (Rydberg) states of Li^- must be very similar to those of H^-.

Table 1 shows that present energy levels are calculated to an accuracy of about 0.01-0.04 eV. That indicated that the positions of resonances are expected to be correct to at least the same level of accuracy.
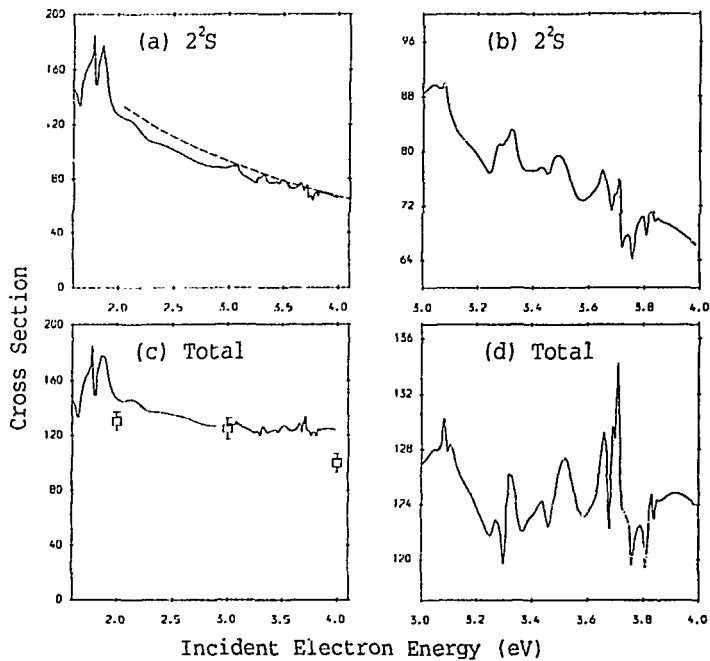
Figure 1.

Elastic (2^2S) and total cross sections (πa_0^2). The solid line is the present J-matrix calculation. The broken line denotes the five-state close-coupling calculations of Moores (1986). Squares denote experimental results of Jaduszliwer *et al* (1981).

Figure 2.

3^2D (dotted line in (a)), 3^2P, 3^2S and 2^2P excitation cross sections (πa_0^2). Squares denote experimental results of Leep and Gallagher (1974). The broken line in (c) and circle in (b) denote the five-state CC calculations of Moores (1986).

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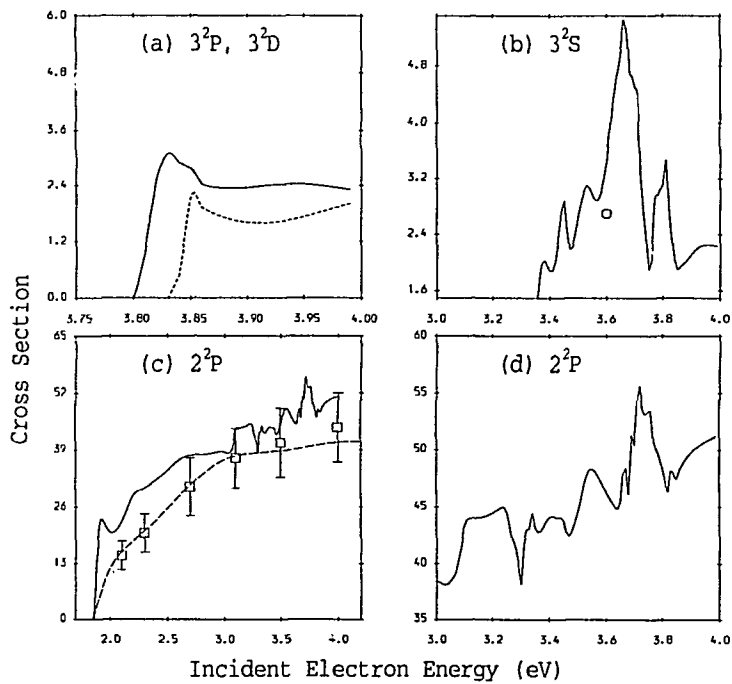
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TABLES

Table 1. The excitation thresholds (eV) of $n=2,3,4$ states of the lithium atom relative to its ground state (^2S). Experimental values (Exp.) derived from the analysis of optical spectra are by (Moore 1949,1971).

	$2p\,^2P$	$3s\,^2S$	$3p\,^2P$	$3d\,^2D$	$4s\,^2S$	$4p\,^2P$	$4d\,^2D$	$4f\,^2F$
Li(Present)	1.863	3.341	3.810	3.838	4.303	4.487	4.4997	4.4998
Li(Exp.)	1.8473	3.3721	3.8330	3.8774	4.3396	4.5202	4.5393	4.5401

Table 2. Energies (E(eV)) and widths (Γ(meV)) of resonances in electron-lithium scattering calculated using the poles of the S-matrix for $L=0$, 1 and 2.

$^{(2S+1)}L^\pi$	E	Γ	E	Γ	E	Γ
^1S	-0.6206	0.00	0.027	1.00	0.114	8.17
	0.265	27.91	1.913	3.96	2.008	17.34
	3.076	33.92	3.362	17.31	3.846	7.36
	3.957	36.64	3.9825	30.04	4.083	32.47
	4.3715	14.14	4.603	23.92	4.757	34.45
^3S	0.017	0.42	0.083	4.82	0.207	18.72
	3.415	23.53	3.573	18.43	3.679	20.56
	4.065	11.68	4.318	21.19	4.450	22.78
	4.580	32.68	4.619	27.425	4.675	27.66
$^1P^o$	0.044	2.48	0.133	12.97	0.2755	37.57
	1.887	22.94	1.940	7.79	2.0635	33.87
	3.353	11.57	3.419	32.915	3.847	21.93
	3.927	13.26	3.944	20.83	3.986	26.35
	4.038	34.40	4.330	9.61	4.469	27.275
$^3P^o$	0.038	1.32	0.087	4.91	0.1845	20.45
	1.885	0.76	1.940	7.30	1.961	6.50
	2.064	30.43	2.0965	23.21	3.389	27.45
	3.751	14.48	3.825	4.80	3.864	9.70
	3.904	13.49	3.930	8.57	3.986	22.11
	4.406	31.72	4.445	20.77		
$^1D^e$	0.075	6.91	0.195	28.54	1.905	12.17
	1.978	15.66	3.750	15.66	3.826	23.795
	3.890	6.46	3.9225	23.105	3.941	12.67
	3.990	36.21	4.027	37.26	4.358	33.38
$^3D^e$	0.075	6.86	0.194	27.21	1.810	13.085
	1.977	14.68	1.964	39.99	3.4125	15.92
	3.464	33.385	3.8565	15.64	3.897	9.63
	3.9685	25.30	4.018	36.55	4.2885	19.37

Table 3. Elastic (2s) and excitation cross sections (πa_0^2) from the ground state to $n = 2$ and $n = 3$ states for electron-lithium scattering.

$E_0(eV)$	total	2s	2p	3s	3p	3d
3.80	121.83	70.29	48.43	3.11	0.00	0.00
3.81	119.40	67.54	47.42	3.46	0.98	0.00
3.82	122.58	70.91	46.33	2.81	2.51	0.00
3.83	124.69	71.07	48.20	2.34	3.08	0.00
3.84	122.92	69.61	47.90	2.04	2.89	0.48
3.85	124.31	70.05	47.43	1.90	2.77	2.16
3.86	124.23	69.68	48.26	1.94	2.43	1.92
3.87	124.33	69.49	48.70	1.98	2.36	1.80
3.88	124.50	69.32	49.10	2.02	2.34	1.71
3.89	124.65	69.15	49.45	2.07	2.34	1.65
3.90	124.77	68.94	49.73	2.13	2.36	1.61
3.91	124.82	68.68	49.98	2.17	2.38	1.60
3.92	124.82	68.40	50.20	2.21	2.41	1.60
3.93	124.77	68.10	50.39	2.23	2.42	1.63
3.94	124.68	67.78	50.56	2.24	2.43	1.67
3.95	124.57	67.45	50.71	2.25	2.43	1.73
3.96	124.43	67.12	50.85	2.25	2.41	1.80
3.97	124.28	66.80	50.98	2.25	2.38	1.87
3.98	124.11	66.48	51.10	2.24	2.35	1.94
3.99	123.94	66.17	51.21	2.24	2.31	2.02

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