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Resonant Structure of Lithium Between the 2^3S and 2^1P Thresholds

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Close coupling calculations of the optically allowed states in the 60-70 eV range above the ground state of atomic lithium have been performed. An interpretation of the resonant structure in this region is given based upon these calculations and recent experimental evidence.

The previous Letter[1] provides a preliminary report of a detailed resonant structure in atomic lithium observed in absorption in the region 60-70 eV above the ground state. Bound-state calculations[2] have served to identify the two lowest lying observed states as $1s(2s2p\,{}^3P)^2P$ and $1s(2s2p\,{}^1P)^2P$ and to identify the states immediately above this as a $1s2s({}^3S)np$ series converging to the $1s2s\,{}^3S$ limit of Li^+. In order to clarify the resonant structure above the $1s2s\,{}^3S$ limit, close-coupling calculations involving the expansion of the total wave function in terms of the four $n=2$ states of Li^+, $1s2s\,{}^{1,3}S$, $1s2p\,{}^{1,3}P$, have been performed for the region immediately above the 2^3S threshold. This Letter presents the initial results of these computations and provides a comparison between the calculated resonant structure and that observed in absorption. Specifically these results include (a) identification of the first five resonances above the 2^3S threshold; (b) calculation of the quantum defects for all six series converging on the four series limits; (c) tentative identification of the resonance observed at 193.58 Å[1] which perturbs the $1s2s({}^3S)np$ series.

The method of calculation is based on the procedure outlined by Smith and Morgan.[3] The total wave function is expanded as an antisymmetrized sum of products of bound-state wave functions corresponding to the $1s2s\,{}^{1,3}S$ and $1s2p\,{}^{1,3}P$ terms of Li^+ and functions representing a bound or free electron. The close-coupling expansion is similar to that used to describe electron scattering on helium[4] with the following differences:

(1) Here the expansion is in terms of ionic rather than neutral core functions and thus asymptotically the coupled electron will move in a Coulomb field. The presence of the Coulomb field means that in this case there will be six well defined Rydberg series converging on the four $n=2$ thresholds of Li^+.

(2) The wave functions describing the coupled electron are in this approximation constrained to be orthogonal to the core orbitals. This constraint eliminates some of the exchange terms which arise in the treatment in Ref. 4. The effect of these terms is compensated for by including "virtual" bound states in the close-coupling expansion.[3]

In the calculations reported here a single virtual bound state $1s2s(^3S)2p\ ^2P$, composed of the same orbitals as the ion core terms, was included in the expansion.

The bound-state wave functions used were those of Morse, Young, and Haurwitz.[5] The experimental values of the energies[6] corresponding to the $1s2s\ ^{1,3}S$ and $1s2p\ ^{1,3}P$ thresholds rather than the eigenvalues of the bound-state wave functions were used in the computations. Since the ground state of lithium is ^2S (even), only $^2P^\circ$ (odd) states can be reached by optical absorption. Thus the calculations reported here are limited to such states. The solution of the close-coupling equations was performed by using a general purpose close-coupling program[7] based on the formalism of Ref. 3.

The output of the computations consists of an S matrix which characterizes the asymptotic form of the wave functions of free electrons coupled to the ion core states and has dimensions corresponding to the number of open channels. In the case of $^2P^\circ$ when all channels are open (above the 2^1P threshold), there are six open channels corresponding to free electron states $(1s2s\ ^{1,3}S)\epsilon p$, $(1s2p\ ^{1,3}P)\epsilon s$, and $(1s2p\ ^{1,3}P)\epsilon d$, respectively. As in the work on helium[4] we define eigenphases (δ) via the matrix equation $e^{2i\delta}=S$, where S is the diagonalized S matrix. The eigenphases above the 2^1P threshold as calculated are shown at the right of Fig. 1. These eigenphases provide estimates of the quantum defects for states converging on the four series limits via the relation $\pi\sigma_j=\delta_j$, where σ_j is the quantum defect and δ_j the eigenphase. Estimates of resonant positions have been obtained by extrapolating the calculated eigenphases below each threshold. The energy of each extrapolated resonance below the appropriate threshold is given by the relation $E_j^{(n)}=-1/[n-\pi\delta_j(E_j^{(n)})]^2$, where $E_j^{(n)}$ is the energy below the threshold and $\delta_j(E_j^{(n)})$ the extrapolated eigenphase at that energy. These estimated resonances are shown as triangles in Fig. 1. Experimental positions of observed resonances including the first few members of the two observed series $1s2s(^3S)np$ and $1s2p(^1P)ns$ and "effective" eigenphases, i.e., $\pi\sigma_{\text{obs}}$, are shown as circles. The estimated experimental uncertainties are indicated for the higher series members.[1]

Direct calculations of the first five resonances above the 2^3S threshold have been obtained by calculating the single eigenphase between the 2^3S and 2^1S thresholds and obtaining the resonance position and width via the relation $\cot(\delta_j-\delta_0)=[E-E_j^{(n)}]/\frac{1}{2}\Gamma$ graphically. These data are shown in Table I along with the observed resonant positions of corresponding absorption peaks.[8] The directly calculated resonances are also shown on the eigenphase plot of Fig. 1 as squares. These data are preliminary since the energy grid used in the calculations (~3 or 4 points for each resonance) was relatively coarse. The width of the first resonance is uncertain since the background phase shift (δ_0) rises from ~0.4 to ~0.8 rad at higher energies. However, the energies of the four higher resonances are probably correct to 0.01 eV and their widths to the number of significant figures given in the table.

The eigenphase plot in Fig. 1 shows good agreement between the extrapolated eigenphases for the $2(^1P)ns$ series and the observed "effective" eigenphases, the calculated eigenphases being ~0.1 higher than those observed. The calculations also predict that the $2(^1P)nd$ series may be observable above the 2^3P limit and that it will have a small (~−0.06) and negative quantum defect.

The resonant structure immediately above the 2^3S limit is further complicated since for lower series members the appropriate zero order coupling is $1s(2s\,np\ ^{1,3}P)^2P$ or $1s(2p\,ns\ ^{1,3}P)^2P$ rather than $(1s2s\ ^{1,3}S)np\ ^2P$ or $(1s2p\ ^{1,3}P)ns\ ^2P$. The effect is to shift the energy levels for $n=3$ states. This is confirmed by the direct calculations above the 2^3S threshold. The lowest calculated resonance lies above the expected positions of $1s2s(^1S)3p$ obtained by extrapolating the $2(^1S)\epsilon p$ eigenphase. The resonance position is shown in Fig. 1 with an "effective" phase shift of ~0.2. Similarly the $2^1P\ 3s$ and $2^3P\ 3d$ levels obtained from the extrapolation lie below the next two calculated levels. These levels agree closely with the narrowly spaced doublet observed in absorption.

The agreement of the experimental and calculated positions for this doublet suggests that the broad region of absorption immediately above the 2^3S threshold is due to the first calculated resonance above threshold and that the doublet consists of $2(^1P)3s$ and $2(^3P)3d$ states which have been shifted to higher energies than those obtained by extrapolation. It also implies that the perturbing level observed between the $n=6$ and 7 levels of the $2(^3S)np$ series is the level $2(^3P)3s$ which has been pushed below the 2^3S threshold by the strong interaction between the $n=3$ states. The "effective" phase shifts for the $2(^3S)np$ series and for the perturbing level (assuming it is bound to the 2^3P threshold) shown at the left of

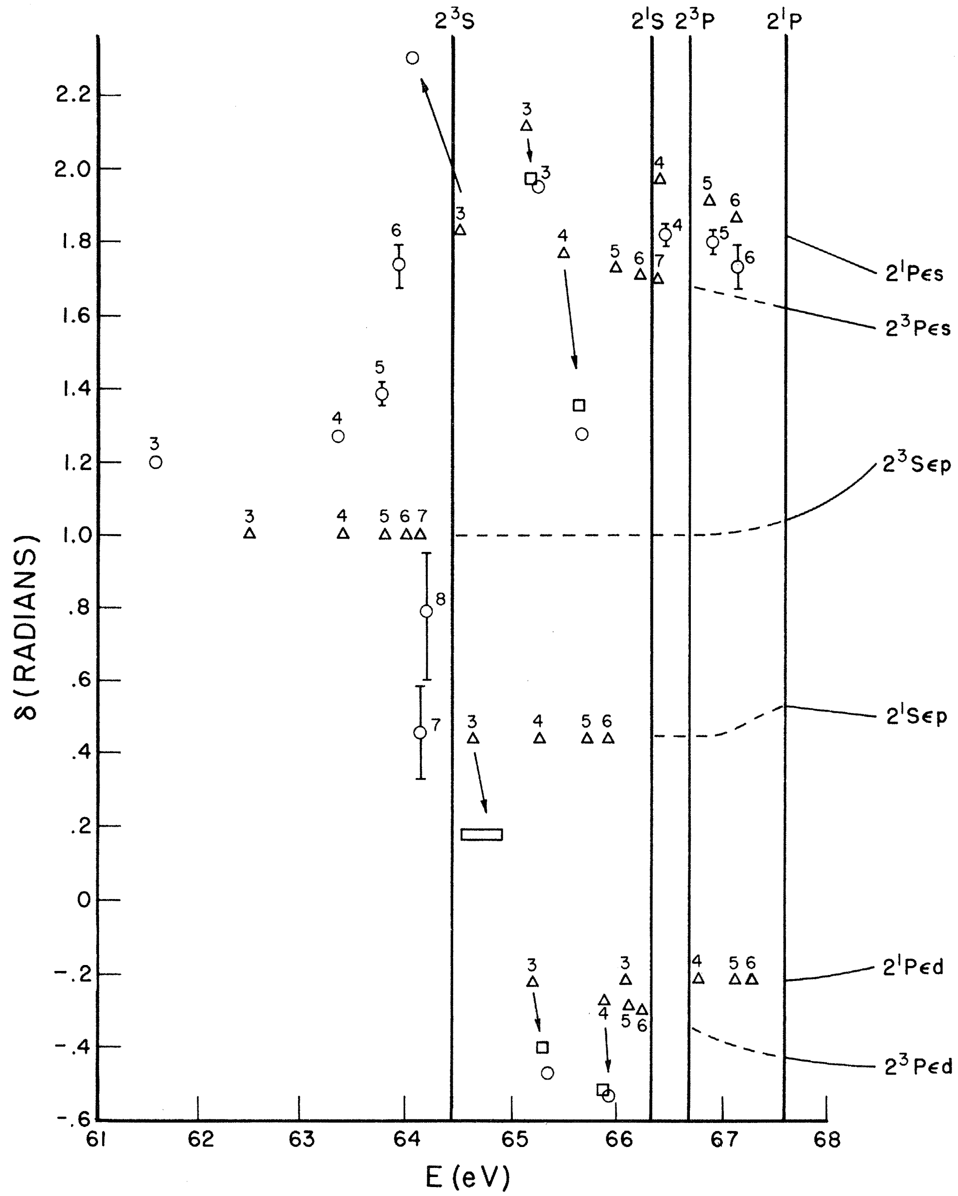

FIG. 1. Eigenphases and "effective" eigenphases for resonances versus energy. Circles correspond to observed resonances, triangles to extrapolated eigenphases, and squares to directly computed resonances. Energy is shown as electron volts above the lithium ground state. The arrows indicate the shifts in resonance positions from the extrapolated eigenphases.

Fig. 1 confirm this suggestion.

The two highest resonances shown in Table I, while they agree closely with observed peaks in absorption, require further investigation. A tentative identification of these resonances as $2(^3P)4s$ and $2(^3P)4d$ is indicated by the "effective" phase shifts shown in Fig. 1. Further analysis of the structure immediately below the 2^1S threshold will be difficult since, due to the narrow spacing between the 2^1S and 2^3P thresholds, all three series converging to those limits will contribute to the resonant structure in that region.

The work presented here provides information on the widths and positions of the observed resonant structure. Further calculations similar to those performed for beryllium[9] are desirable in order to predict the detailed shape of the observed absorption spectrum reported in Ref. 1.

We would like to thank the authors of Ref. 1 and Dr. A. W. Weiss both for prior communication of unpublished results and for lively discussions on the interpretation of the resonant structure

Table I. Resonances above the 2^3S threshold. Experimental energies represent peaks in absorption (Ref. 8). The theoretical positions were obtained by fitting the phase shift to the expression $\cot(\delta-\delta_0)=[E-E_j^{(n)}]\frac{1}{2}\Gamma$. Approximate widths obtained using the indicated background phase shifts (δ_0) appear in the third column. Resonant energies are expressed as energies above the ground state of lithium.

Theory	Experiment	Γ (eV)	δ_0	Classification
64.7	64.6-65.1	0.4	0.4	$(1s2s\,^3S)3p$
65.17	65.25	0.01	0.8	$(1s2p\,^3P)3s$
65.28	65.30	0.004	0.8	$(1s2p\,^3P)3d$
66.59	65.66	0.12	0.8	$(1s2p\,^3P)4s$
65.87	65.89	0.004	0.8	$(1s2p\,^3P)4d$

reported here. We also are indebted to Dr. Aaron Temkin of the Goddard Space Flight Center for arranging for the computations upon which this Letter is based to be performed at Goddard.

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Can a Solid Be "Superfluid"?

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It is suggested that the property of nonclassical rotational inertia possessed by superfluid liquid helium may be shared by some solids. In particular, nonclassical rotational inertia very probably occurs if the solid is Bose-condensed as recently proposed by Chester. Anomalous macroscopic effects are then predicted. However, the associated superfluid fraction is shown to be very small (probably $\lesssim 10^{-4}$) even at $T=0$, so that these effects could well have been missed. Direct tests are proposed.

Most of the striking macroscopic properties of superfluid liquid helium can be explained if we make the following assumption, which we shall call the assumption of nonclassical rotational inertia (NCRI): Suppose that we enclose a number N of helium atoms in a cylindrical annulus of internal radius R and thickness d, and rotate the enclosing surfaces about the axis of the cylinders at constant angular velocity ω. Then the free energy $F(\omega)$ measured in the rest frame is assumed to be of the form

$$F(\omega)=F_0+\tfrac{1}{2}I_0\omega^2+\Delta F(\omega), \tag{1}$$

where F_0 is the free energy for $\omega=0$ and I_0 is the classical moment of inertia NmR^2 (here, as everywhere, we neglect terms in d/R and also the effect of density redistribution due to the centrifugal forces, which is proportional to ω^4 and negligible at low velocities). The term $\Delta F(\omega)$ by which $F(\omega)$ departs from the classical result is assumed to be even and periodic in ω with period ω_0:

$$\omega_0=\hbar/\alpha mR^2, \tag{2}$$

where α is a number of order 1 (not order N); for $\omega<\omega_0/2$ the function $\Delta F(\omega)$ is of the form

$$\Delta F(\omega)=-\tfrac{1}{2}(\rho_s/\rho)I_0\omega^2, \tag{3}$$

which defines the superfluid fraction ρ_s/ρ. For a normal system $\Delta F(\omega)$ is either identically zero