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Resonance states in Li⁻ and B⁻

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We have observed resonance structures in detached electron spectra arising from fast collisions of Li⁻ and B⁻ ions with gas targets. The structures are associated with the autodetaching decay of shape resonance states. Using Shore parametrization, we obtain resonance energies and widths of 50(6) and 64(25) meV, respectively, for the Li⁻($2s2p^{3}P$) state and 104(8) and 68(25) meV, respectively, for the tentatively identified B⁻($2p^{2}^{1}D$) state. Other resonances in B⁻ remain unidentified.

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Resonance structure has been detected in the detached electron spectra produced when 100-keV Li⁻ and B⁻ projectiles collide with He and Ar gas targets. This structure is associated with the transient formation and subsequent autodetaching decay of low-lying excited states of the negativeion projectiles. The resonance in Li⁻ is a shape resonance identified with the $2s2p^{3}P$ state. Although this state has received considerable theoretical attention, particularly in the context of electron-atom scattering, it has never previously been observed experimentally. The newly observed resonances in B⁻ cannot be positively identified at this time due to lack of supporting theoretical information. It is suspected, however, that they are also shape resonances the parent states of which are the $2s^2 2p^2 P$ ground state of the B atom and possibly low-lying excited states such as the core excited $2s2p^{24}P$ state. In some cases, the collisional production of these resonance states involves spin exchange.

Negative ions differ intrinsically in their structure from isoelectronic atoms and positive ions. This difference can be traced to the manner in which the outermost electron interacts with the rest of the atomic system. In the case of negative ions, the short-range binding potential typically supports a single bound state, in contrast to the infinite spectrum characteristic of atoms and positive ions where the long-range Coulomb force dominates. Although very few bound states of negative ions exist, many unstable excited states have been found embedded in continua associated with an atom

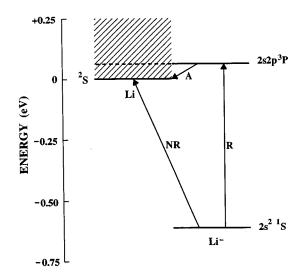


FIG. 1. Partial energy-level diagram for the Li and Li⁻ system. Resonant (*R*) and nonresonant (NR) detachment is shown. The ³*P* shape resonance decays via autodetachment (*A*) leaving the residual atom in the ground state.

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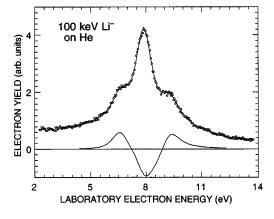


FIG. 2. Zero-degree electron-energy spectrum for 100-keV Li⁻ ions incident on a He gas target showing the central cusp peak and the kinematically doubled resonance structure. The solid curve through the data points represents the best fit obtained using Eq. (1), and the bottom curve indicates the contribution of the shape resonance including interference (see text).

and a free electron. Such states are subject to rapid decay by the spontaneous process of autodetachment. The decay of the resonance state is manifested by a structure in the detachment cross section arising from an interference between the nonresonant and resonant pathways to the same continuum state. Figure 1 shows a partial energy-level diagram for the Li and Li⁻ system in which the interfering resonant (*R*) and direct or nonresonant (NR) pathways are indicated.

Shape resonances lie energetically just above their parent atom state (see Fig. 1) and occur when an electron is temporarily trapped in a potential well arising from a combination of the repulsive centrifugal force and the attractive shortrange force due to the polarization of the parent atom. Buckman and Clark [1] have recently published a review of negative-ion resonances, further information on excited states of negative ions can be found in the monograph of Massey [2] and the reviews of Andersen [3] and Esaulov [4].

The pioneering experiments on negative-ion resonances involved electron-atom collisions where structure was observed in the elastic scattering cross sections whenever an electron was temporarily captured by the atom. An authoritative review of this field has been presented by Schulz [5]. These highly unstable states can also be observed when a beam of negative ions is passed through either a laser field or a gaseous target. In photodetachment studies, negative ions are selectively photoexcited by the use of a laser beam mated to the ion beam in either a crossed or collinear geometry. Shape and Feshbach resonances were, for example, observed in the cross section for photodetachment of the H⁻ ion by Bryant and his collaborators [6] using a crossed beam arrangement. The $1s2p^{24}P$ shape resonance in He⁻ has been studied by Peterson et al. [7] using a collinear beam geometry. The ions of a fast beam can also be excited to resonance states by collisions with atoms in a gas target. Early reviews of this nonselective, heavy-particle impact technique have been presented by Edwards [8] and Risley [9]. More recent work includes investigations of shape resonances in H⁻ by Andersen *et al.* [10] and Penent *et al.* [11] and He⁻ by Závodszky et al. [12].

In the present work, the low-lying shape resonance states

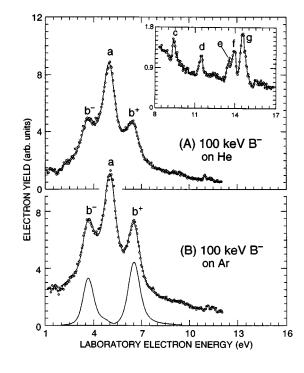


FIG. 3. Zero-degree electron-energy spectra for 100-keV B⁻ ions incident on the (A) He and (B) Ar gas targets showing the cusp (a) and the kinematically doubled resonance peaks (b^{\pm}) . The solid curve through the data points represents the best fit obtained using Eq. (1) and the bottom curve in (B) is the contribution of the shape resonance including interference (see text). Weaker and higher-lying resonances are displayed in the inset of (A).

were nonselectively populated in negative-ion-atom collisions. The apparatus used in the present experiment was a variation of a crossed laser-ion beam apparatus previously utilized in photodetachment studies [13]. Positive ions were produced in an ion source, extracted to form a beam, and finally accelerated to an energy of 100 keV. Negative ions were created by sequential double electron capture collisions when the beam of positive ions traversed a Li vapor charge exchange cell. Upon charge-state analysis, the negative-ion beam component was deflected by 10° into a beam line containing a gas target cell and a spherical-sector electron spectrometer. The spectrometer was operated in a constant transmission energy mode with an energy resolution of about 0.3 eV. Data were taken under single collision conditions. In the present 0° detached electron spectroscopy, electrons produced in negative-ion-atom collisions in the target cell were collected in the forward direction (direction of motion of the ions) and energy analyzed. The major source of background in the present experiment was due to electrons produced in collisions of the beam ions with residual gas molecules and beam-defining apertures. This background contribution was determined by accumulating spectra without gas in the target cell. The remaining spectrum consisted of two parts: a continuum associated with direct or nonresonant collisional detachment of the beam ions by the target gas and discrete structure arising from electron detachment via intermediate resonance states.

A background-corrected electron spectrum, produced in 100-keV collisions of Li⁻ projectiles with a He gas target, is

shown in Fig. 2. Similarly, in Fig. 3 we show spectra resulting from 100-keV collisions of B⁻ with both He and Ar gas targets. All spectra exhibit a cusplike peak situated at the reduced ion beam energy (corresponding to electrons traveling with the same velocity as the ions) and a kinematically doubled pair of resonance peaks that are almost symmetrically disposed about the central cusp. The cusp arises in the ion-to-laboratory-frame transformation of the direct threshold cross section. In principle, both resonant and direct single detachment cross sections should be zero at threshold for negative-ion projectiles. In practice, however, the finite energy and angle acceptances of the electron spectrometer can contribute to the cusp, since post-threshold electrons are unavoidably collected. In addition, in noncoincident measurements such as these, a small contribution (estimated to be less than 10%) to the cusp arises from one- or two-step double detachment processes.

The objective of the data analysis is to extract information on the parameters (energies and widths) of the resonances from the detached electron spectra. In the present work the spectra were analyzed by use of a parametrization method first introduced by Shore [14] and later developed by Balashov *et al.* [15] and McDonald and Crowe [16]. The Shore parametrization process is equivalent to the more commonly used Fano parametrization method [17], but is easier to apply in cases of nonselective excitation. This method of analysis has been successfully applied by Andersen *et al.* [10] and by Závodszky *et al.* [12] in their investigations of detached electron spectra arising from negative-ion-atom collisions using H⁻ and He⁻ projectiles, respectively.

The first step in the procedure is to model, in the rest frame of the ion, the expected double differential cross section (DDCS) for electron production. In this model, the non-resonant contribution is typically presented in terms of partial wave expansion with Legendre polynomials, where the contribution from each partial wave with angular momentum l is determined by the emission angle (θ) and velocity (v) of the ejected electron in the projectile ion frame. The ion-frame DDCS is then parametrically written as

$$\frac{d^2\sigma}{dE \ d\Omega} = \sum_{l=0, n=0} a_{ln} \left(\frac{v}{v_p}\right)^n P_l(\cos\theta) + \frac{\alpha\epsilon + \beta}{1+\epsilon^2}, \quad (1)$$

where v_p is the projectile ion velocity and $\epsilon = 2(E - E_r)/\Gamma$ is the reduced energy variable for the electron energy *E* in the ion frame. E_r and Γ , respectively, represent the energy and width of the resonance and α and β are the Shore parameters that describe the shape of the resonance (determined by interference). The parameters α and β are, in general, functions of v and θ , but in the present analysis the angular dependence was assumed to vary linearly with θ from a forward value to a backward one while the velocity dependence was assumed to be constant in fast collisions such as these. In the expression for the direct detachment contribution only *s* and *p* waves were retained and terms of $n \ge 2$ were neglected.

The procedure used to calculate the predicted electron yield was to first transform the ion-frame DDCS into the laboratory-frame integrating over the finite range of spectrometer acceptance angles [18] and then convolute the results using the spectrometer response function (found to be Gaussian). The resulting calculation of the predicted electron yield was then used to extract the resonance energy and width as well as the other parameters $(a_{ln}$'s, α 's, and β 's) using a least-squares fit. As a test of the procedure we first analyzed a detached electron spectrum obtained in collisions of 100-keV He⁻ ions with a He gas target. Our measured energy and width of the $1s2p^{24}P$ shape resonance in He⁻ are in good agreement with those obtained by Závodszky et al. [12], who used a similar experimental method and data analysis approach [Eq. (1)]. Our measured values also agreed well with the more accurate results obtained by Walter et al. [19], who employed photoabsorption to selectively excite this resonance state. The agreements with the results of Refs. [12] and [19] thus gave us confidence in our ability to extract meaningful resonance parameters from detached electron spectra using the Shore parametrization method.

The solid curve through the data points shown in Fig. 2 represents the best fit obtained by using Eq. (1). This fit yields a resonance energy of $E_r = 50(6)$ meV and a width of Γ =64(25) meV. The larger error quoted on the resonance width reflects the sensitivity of this parameter to the uncertainty in our knowledge of the spectrometer energy resolution. The contribution from the resonance is shown in the bottom curve in the figure. It can be seen that there exists appreciable destructive interference in the region of the cusp corresponding to the threshold region in the ion frame. This could possibly be due to the presence of a virtual state such as the theoretically predicted ${}^{3}S$ state [20]. The extracted values of the resonance parameters allow us to identify the observed structure with the $2s2p^{3}P$ shape resonance state in Li⁻, which, until now, has defied experimental investigation even though it has been the subject of numerous calculations over the past few decades. The reason for this inbalance can be traced to the experimental difficulty of detecting the verylow-energy electrons ejected in the autodetaching decay of the low-lying resonance state and the fact that the state is not efficiently optically coupled to the ${}^{1}S$ ground state of Li⁻, thereby prohibiting photodetachment studies. To overcome these problems we have collisionally populated the state and have used a beam source in order to exploit the kinematic amplification of electron energies inherent in emission from fast moving ions. For example, in the present measurements at 100 keV, the ratio of the energies of the detached electrons in the laboratory frame to those in the ion frame was more than two orders of magnitude. Table I shows the present results compared with some theoretical predictions. It can be seen that the agreement is good for both the resonance energy and the width. The calculation of Fabrikant [21] employed an effective range theory while the calculation of Sinfailam and Nesbet [20] used a variational approach.

As shown in Fig. 3, we have also observed resonances corresponding to the autodetaching decay of excited states of B^- produced in collisions of 100-keV B^- ions with He and Ar gas targets. The inset represents a more detailed study of the higher-energy resonances (peaks c-g). Our analysis of the detached electron spectra, using the Shore parametrization method, has yielded an energy of 104(8) meV and a width of 68(25) meV for the resonance associated with the lowest-lying peaks (b^{\pm}). These peaks, and all the other peaks, are kinematically doubled and shifted in the spectra. We are unable to positively identify the newly observed reso-

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TABLE I. Theoretical $(E_r^{\text{theor}} \text{ and } \Gamma^{\text{theor}})$ and experimental $(E_r^{\text{expt}} \text{ and } \Gamma^{\text{expt}})$ energies and widths (both in the units of meV) of shape resonance states in Li⁻ and B⁻.

E_r^{theor}	$\Gamma^{ ext{theor}}$	E_r^{expt}	Γ^{expt}
$\frac{1}{\text{Li}^{-}(2s2p^{3}P)} = \frac{59^{a}}{60^{b}}$	77 ^a	50±6 ^e	64±25 ^e
	57 ^b		
120 ^c	24 ^c		
115 ^d		104 ± 8^{e}	68±25 ^e
450 ^c	110 ^c		
	59 ^a 60 ^b 120 ^c 115 ^d	$ \begin{array}{cccc} 59^{a} & 77^{a} \\ 60^{b} & 57^{b} \\ 120^{c} & 24^{c} \\ 115^{d} \end{array} $	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$

^bReference [20].

^cReference [22].

^dReference [23].

^eThis work.

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nances in B⁻ due to the current lack of theoretical information. We suspect, however, that the peaks are, as in the case of Li⁻, associated with the decay of shape resonances. For the B⁻ resonances, the parent states are either the $2s^22p^2P$ ground state or low-lying excited states such as the core excited $2s2p^{24}P$ state. For example, in the former case the $2s^22p^{21}P$ and ¹S states would be candidates, while in the latter case the $2s2p^{35}S$, ³S, ³P, and ³D states are possibilities. We tentatively propose, based on the measured energy, that the lowest-energy pair of peaks (b^{\pm}) is associated with the autodetaching decay of the $2p^{2} D$ shape resonance state. In a simple model potential calculation, Hunt and Moiseiwitsch [22] estimated this state to lie 450 meV above the parent B atom ground state. Froese Fischer [23] has recently demonstrated, however, that the inclusion of electron correlation reduces the calculated value to 115 meV; a value in closer agreement with the present results (see Table I).

In summary, we have used a fast beam technique involving negative-ion-atom collisions to populate several lowlying shape resonance states. The resonances, which appear as structure in the 0° detached electron spectra, are associated with the autodetaching decay of the $2s2p^{3}P$ excited state of Li⁻ and, as yet unknown, excited states of B⁻. The lowest-energy structure in the case of B⁻ is tentatively identified with the $2p^{2}D$ state. An appeal for further calculations in the case of B⁻ is made.

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