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Electron excitation of Auger transitions in atoms

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It has been observed experimentally that total ionization cross sections for neutral atoms exhibit abrupt increases near thresholds for exciting inner-shell electrons to autoionizing states. This feature of the ionization cross section is not predicted by most of the standard first-order theories. While a recent R-matrix calculation produced cross sections of the type observed experimentally, the physical effects contributing to the structure were not apparent. We have studied this effect in the distorted-wave approximation and have found that the rapid increase in the ionization cross section near autoionization thresholds results from exchange effects. Calculated angular distributions for Li, where this mechanism operates, are dominated at backward-scattering angles, a feature amenable to experimental observation.

Cross sections for ionization of positive atomic ions by collisions with electrons show sudden jumps when new ionization channels corresponding to the excitation of autoionizing states[1] are opened. The sudden increase in ionization cross sections for positively charged ions is well understood in terms of standard threshold laws.[2] More surprising is the rapid rise of ionization cross sections for neutral species near the threshold for exciting an inner electron to an autoionizing state.[3] The rise is quite abrupt in many instances, occurring over a range of a few eV for incident electrons with 50–100 eV energy. This feature of experimental cross sections is absent in most theories, such as the first Born, Glauber, Vainshtein, and asymptotic Green's-function approximations[4] and the distorted-wave Born approximation without exchange, but has recently been seen in R-matrix calculations for the prototypical system

$$e^- + \mathrm{Li}(1s^2 2s) \rightarrow e^- + \mathrm{Li}(1s2s^2) \quad . \tag{1}$$

While the R-matrix calculations predict[5] the rapid rise in the integral cross sections near the threshold for excitation of inner-shell electrons which leads to autoionization, an interpretation of the physical effects leading to this phenomena is lacking. The purpose of the present study was to determine the physical origins which cause this sudden increase in the cross section near the threshold.

A convenient approach for isolating and examining various physical effects is through the standard perturbation series methods. Since the distorted-wave approximation has been very successful in predicting electron-excitation cross sections for other processes[6] and typically gives results qualitatively similar to the R-matrix approach, the distorted-wave approximation was chosen for this study.

We have calculated cross sections in the distorted-wave Born approximation[7] with exchange (DWBE) and without exchange (DWB) for the scattering reaction (1). The atomic wave functions used in these calculations were chosen to be identical to the ones used in the R-matrix calculations, so that comparisons will reflect differences in dynamics only. In particular, the initial ground-state $1s$ wave function was taken to be the $1s$ wave function of the $1s^2 2s$ configuration obtained by Clementi and Roetti[8] and the final-state $2s$ wave function was taken to be the $2s$ wave function of the above $1s^2 2s$ configuration. Apart from keeping the wave functions identical to those used in the previous R-matrix calculation, it may seem undesirable to use a ground-state $2s$ wave function for the excited state. However, it should be noted that a more realistic $2s$ wave function would not necessarily be orthogonal to the ground-state $1s$ wave function in spite of the fact that this orthogonality is always assumed in the evaluation of first-order amplitudes using single-particle wave functions. For this case, use of more realistic but nonorthogonal Hartree-Fock ground- and excited-state wave functions would cause a large increase in the resulting cross sections. It would be inappropriate to use wave functions of this type without evaluating the additional first-order amplitudes which result from the nonorthogonality.[9] To be consistent with the choice of wave functions, the ground-state potential was used in both channels with no additional distorting terms.

Figure 1 compares the distorted-wave Born integral cross sections with the R-matrix and plane-wave Born predictions.[10] Several features of importance emerge from this figure. First, the DWBE result is qualitatively as well as quantitatively in good agreement with the R-matrix results over the entire energy region of our consideration. In the vicinity of threshold, the agreement is excellent. The lowest energy which we could calculate without numerical difficulties was 60 eV (0.5 eV above threshold). Since the cross section is still rising at this energy, we have a situation similar to the experimental observation, where the cross section must jump from zero to some fairly large value over an energy range of 0.5 eV or less. When the DWB and DWBE results are compared, it is seen that the large increase in the cross sections near threshold for inner-shell excitation processes results from exchange effects.

An understanding of the mechanism which causes the exchange amplitude to produce the increase in the total cross sections near threshold may be found by examining the differential cross sections. In the distorted-wave approximation, the direct, exchange, singlet, and triplet amplitudes can all be written in the following general form for transitions

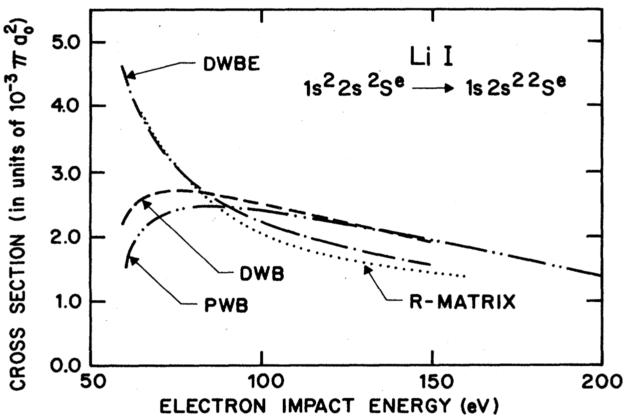

FIG. 1. Electron impact excitation cross section for the $1s2s^2$ autoionizing level in lithium; — · — ·, distorted-wave Born approximation with exchange; — — —, distorted-wave Born approximation without exchange; — · · —, plane-wave Born (PWB) approximation; · · · ·, R-matrix results.

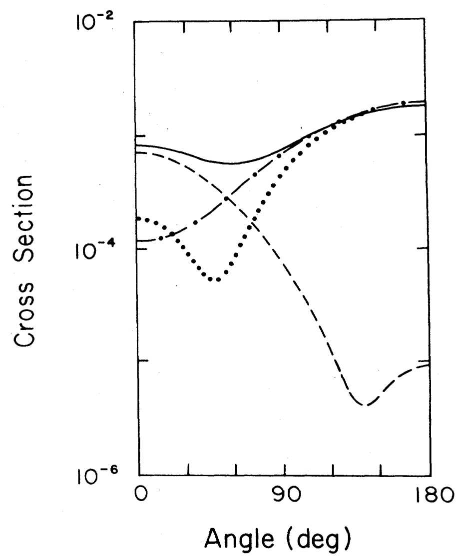

FIG. 2. Differential cross section in units of a_0^2/sr for 65-eV electron impact excitation of the $1s2s^2$ state of lithium. The curves are · · · ·, direct; — · — ·, singlet; — — —, triplet; and ——, total.

from initial s states to final s states

$$T_{fi} = \sum_{l_f} A_{l_f} Y^*_{l_f 0}(\theta, \phi) \ , \qquad (2)$$

where T_{fi} is one of the above amplitudes, Y_{lm} is a spherical harmonic, and A_{l_f} is the appropriate partial-wave amplitude. The differential cross section without exchange is given by

$$d\sigma^d = \frac{1}{16\pi^2} \frac{k_f}{k_i} |T^d_{fi}|^2 \ , \qquad (3)$$

where T^d_{fi} is the direct scattering amplitude, and $k_{f\,(i)}$ is the final- (initial-) state wave number for the projectile electron. With exchange, the differential cross section is given by

$$d\sigma^e = \frac{1}{16\pi^2} \frac{k_f}{k_i} (|T^s_{fi}|^2 + |T^t_{fi}|^2) \ , \qquad (4)$$

where T^s is the singlet amplitude

$$T^s_{fi} = \tfrac{1}{2}(T^d_{fi} + T^e_{fi}) \ , \qquad (5)$$

and T^t is the triplet amplitude

$$T^t_{fi} = (\sqrt{3}/2)(T^d_{fi} - T^e_{fi}) \ . \qquad (6)$$

The direct, singlet, triplet, and total differential cross sections are shown in Fig. 2 for 65-eV incident electrons. Examination of Fig. 2 reveals several interesting features. First, the total cross section peaks in the backward direction. The behavior seen here results from the phase difference between the s and p amplitudes which will be discussed later. As the energy of the incident electron increases, the dominance of the large angles decreases. For 100-eV incident electrons, this behavior has reversed and the largest cross section is at 0°. The total differential cross section exhibits a minimum for all incident electron energies in the 65–100-eV range. It is interesting to note that this minimum occurs at $\theta \approx 60°$ independent of the bombarding energy. A similar pattern has been observed by Crooks, DuBois, Golden, and Rudd[11] for the electron excitation of the 2^3S state of helium.

The second feature to be noticed from Fig. 2 is that the net effect of exchange is to increase significantly the small-angle cross section and to decrease slightly the large-angle cross section. It is the large increase in the small-angle differential cross section that causes the total cross section near threshold to rise. Further examination of Fig. 2 reveals that the small-angle cross section arises primarily from triplet scattering while the large-angle cross section results primarily from singlet scattering.

As the energy of the incident electron approaches threshold, the number of partial waves required for convergence of the cross section decreases. At 60 eV, the cross section is completely dominated by s-wave scattering and the differential cross sections are essentially flat. At 65 eV, over 99% of the final results were obtained for partial waves whose l values were less than or equal to three. The effect of exchange and expected shapes for differential cross sections can be easily understood by looking at this particular case. Since the appropriate Y_{l0} values contain only $\cos\theta$ dependences, the direct, exchange, singlet, and triplet amplitudes (2) for this scattering process can all be expressed as a series of powers of $\cos\theta$. Consequently, for 65-eV incident electrons we have

$$T_{fi} = \sum_{n=0}^{3} b_n \cos^n\theta \ , \qquad (7)$$

and the square of the amplitude, which is directly proportional to the differential cross section, can be expressed as

$$|T_{fi}|^2 = \sum_{n=0}^{6} c_n \cos^n\theta \ . \qquad (8)$$

Table I contains the c_n values for the direct, singlet, and triplet amplitudes for 65-eV incident electrons.

Examination of Table I reveals that the constant, $\cos\theta$, and $\cos^2\theta$ terms dominate the differential cross section and, further, that the $\cos\theta$ term is negative for the direct and singlet cross sections and positive for the triplet cross section. It is this latter sign for the $\cos\theta$ term which determines the different shapes for the singlet and triplet cross

TABLE I. Coefficients of $\cos^n\theta$ term for the square of the scattering amplitude for 65-eV incident electrons.

N	Direct	Singlet	Triplet
0	0.240	0.365	0.042
1	−0.576	−0.476	0.118
2	0.311	0.158	0.115
3	0.088	0.016	0.059
4	0.030	0.002	0.037
5	0.007		0.015
6	0.001		0.002

sections. If the s and p amplitudes dominate, cross sections of form $c_0+c_1\cos\theta$ will be peaked in the forward direction for positive c_1 and in the backward direction for negative c_1.

Assuming the dominance of the s and p amplitudes, the c_1 coefficient is proportional to the real part of $A_0^*A_1$. Consequently, the sign of this coefficient is determined by the cosine of the phase difference between the s and p amplitudes. If the phase difference between the p and s amplitudes lies in the second or third quadrant, the coefficient of the $\cos\theta$ term will be negative and the angular distributions will be peaked at large angles. If, on the other hand, this phase difference lies in the first or fourth quadrants, this coefficient will be positive and the angular distributions will be peaked at small angles. For 65-eV incident electrons, the phase difference between the p and s amplitudes is 161° for direct and singlet scattering and 19° for triplet scattering. Consequently, the direct and singlet scattering results are peaked at large angles, while the triplet scattering results are peaked at 0°. The additional structure, particularly in the direct and triplet cross sections, results from the higher-order terms.

The above phases for the singlet and triplet amplitudes are determined by the direct and exchange amplitudes. The direct and exchange amplitudes for a particular partial wave will always either have the same phase or the same phase $\pm\pi$. In the energy range considered here, the direct and exchange s and p amplitudes have the same phase. Consequently, the singlet (direct plus exchange) amplitudes will have the same phase as the direct amplitudes. The phase of the triplet amplitude (direct minus exchange) for a particular partial wave will be determined by the relative magnitudes of the direct and exchange amplitudes. If exchange is smaller than direct, the triplet amplitude would have the same phase as the direct. If, on the other hand, the exchange amplitude is larger than the direct, the triplet amplitude would have a phase of π different from the direct. For the case being considered here (65-eV incident electrons), the exchange s amplitude is greater than the direct s amplitude while the exchange p is smaller. The net result is a π change in the phase difference between the p and s amplitudes for triplet scattering. This π phase change produces the sign difference for the $\cos\theta$ term and the shape of the differential cross section which is peaked in the forward direction instead of the backward direction. As a result, the enhanced cross sections result directly from the exchange s amplitude being greater than the direct while the exchange p amplitude remains smaller.

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