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CLOSE-COUPLING CALCULATIONS OF ELECTRON-IMPACT EXCITATION OF THE 2s STATE AND AUTOIONIZATION BELOW THE $n=3$ LEVEL IN He^+ †

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Autoionizing states in He below the $n=3$ threshold of He^+ have been recently detected in photon-absorption and ion-bombardment experiments.[1,2] In addition, a measurement of excitation cross section of the 2s state of He^+ by means of the crossed-beam technique seemed to indicate the existence of a peak in the 1s-2s excitation cross section at about 48 eV above the first ionization threshold of He—i.e., just below the $n=3$ threshold of He^+.[3] More recently Daly and Powell,[4] using an entirely different experimental approach, have shown that the 1s-2s excitation cross section in He^+ peaked near the $n=2$ threshold. The first experiment contradicts the results of past calculations of this process[5,6] as well as the general theoretical prediction that the electron-impact excitation cross section in positive ions should decrease monotonically from onset with increasing incident electron energy above threshold.[7] Because the behavior of the excitation cross section between the $n=2$ and $n=3$ thresholds in atomic hydrogen has been recently clarified by calculations with a six-state (1s-3d) close-coupling eigenfunction expansion,[8,9] and, moreover, because close-coupling calculations correctly predict the characteristics of autoionizing states below the $n=2$ thresholds,[10,12] we have used this method to calculate the scattering of electrons by He^+ for incident energies between 42 and 52 eV.

The main results reported here are (a) the first calculations and classifications of autoionizing levels in helium between the $n=2$ and $n=3$ thresholds of He^+ which agree with the experimental observations[1,2]; (b) a possible explanation of the peak in $Q(1s\text{-}2s)$ observed in the first experiment; and (c) a prediction of the detailed shape of $Q(1s\text{-}2s)$ between the $n=2$ and $n=3$ thresholds observed in the second experiment.

Figure 1 shows the ^1S, ^1P, and ^1D partial-wave cross-section contributions to $Q(1s\text{-}2s)$. The resonances in the ^1S contribution correspond to the three series of autoionizing levels expected in this total spin and angular-momentum state of the electron–helium-positive-ion system.[10] To obtain a possible spectroscop-

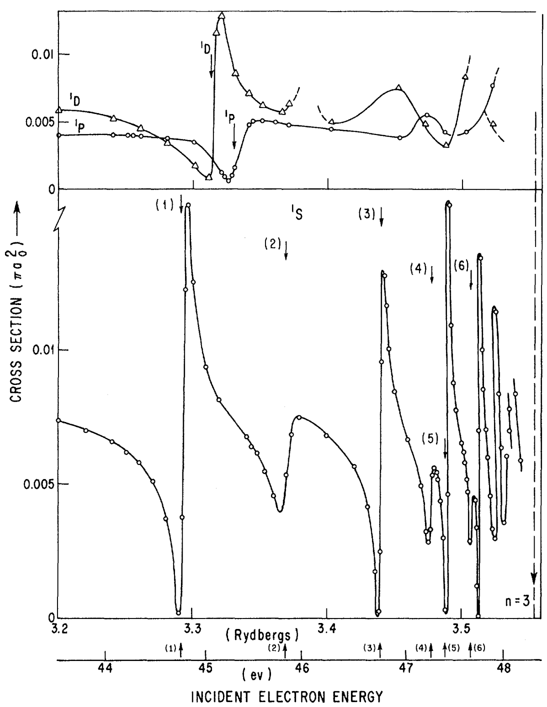

FIG. 1. ^1S, ^1P, and ^1D partial-wave contributions to $Q(1s\text{-}2s)$. The calculations were carried out at the points indicated. The calculated positions of the resonances are indicated and identified as described in the text.

ic classification of these levels, we calculated the positions of these resonances using the truncated diagonalization method (TDM),[13] as well as by making a least-squares fit to the close-coupling phase shifts.[11] The latter calculations also yielded the widths and quantum defects for the resonances. The results are summarized in Table I. Before discussing these, we recall that Cooper, Fano, and Prats[14] explained the different widths of autoionizing states in ^1P helium below the $n=2$ threshold by showing that the $2snp$ and $2pns$ series, being almost degenerate, interacted to form the now well-known (+) and (−) series $2snp \pm 2pns$. Lipsky and Russek[13] showed that this configuration mixing was true not only for ^1P, but for ^3P and ^1S states as well; and from the coefficients listed in Ref. 13 for ^1S autoionization, it is seen that the states $(2sns \pm 2pnp)$ correctly describe the levels below the $n=2$ threshold. Turning now to the ^1S case below the $n=3$ threshold, there are three series to be expected, namely, $(3sns)$, $(3pnp)$, and $(3dnd)$; but because of the high configuration mixing, a straightforward classification according to $3lnl$ $(l=0, 1, 2)$ is impossible. Instead we find that the $3sns$ and $3pnp$ series interact to form $3n\pm = 3sns \pm 3pnp$ in analogy with $n=2$. But the $3n-$ states then interact strongly with the $3dmd$ states to form the states which we designate as $3nm_d\pm = 3dmd \pm 3n-$. As can be seen from Table I, the first five states are well described by these classifications, the lowest being 96 % of the $3n+$ type, the second 96 % of the $3nm_d-$ type, and so on. The agreement for the positions calculated by the two methods is very good. However, for the fifth level, although the calculated positions agree, the TDM results imply that it should be classified as a 333_d+, while the close-coupling results for the width and quantum defect suggest that it is the third member of the $3n+$ series, i.e., 35+. This suggests that another level may exist at this energy, of width too narrow to have been found in the present calculation. Because the number of basis sets in our TDM calculations is too small to predict the location of the sixth level, additional calculations with both methods are needed to find this narrow resonance.

We have also carried out calculations for ^1P- and ^1D-wave scattering over the same energy range. From the ^1P results, shown in Fig. 1(b), we obtain for the lowest optically observable state the energy of 69.85 eV,[15] in reasonable agreement with the position of 69.94 eV quoted by Cooper and Ederer.[16] The peak seen in the bombardment experiment[2] is, however, fairly wide and hence the experimental observation of the lower levels given in Table I must await further improvements in resolution.[17] Evidence of additional (expected) structures in the ^1P and ^1D partial waves is also shown in Fig. 1(b). However, because of the great length of the scattering calculations, we feel that further attempts to isolate these resonances need not be carried out at the present time.

An explanation of the experimentally observed peak in the total $Q(1s\text{-}2s)$ can now be obtained by considering the net effect of the resonances in the partial-wave contributions, just as in the case of the same excitation process in atomic hydrogen.[9,18] The total theoretical $1s$-$2s$ excitation cross section, shown in Fig. 2, is seen to be full of structures, and the single peak observed in the experiment of Dance, Harrison, and Smith[3] represents a smearing of this. The position of such an average peak is in reasonable agreement with experiment,

Table I. Eigenvector components and the parameters of the first five autoionizing ^1S levels converging on the $n=3$ threshold of He^+. Note the rather large width of the second level and the large $(4f)^2$ component of the fifth level. The assignment of the fifth level is questioned because of the possible existence of a nearby narrow level as discussed in the text.

Hydrogen Configuration	Coefficients for Each Component, a_n (1)	(2)	(3)	(4)	(5)	(6)
33+	.94725	-.06493	.17676	.03999	-.08502	
34+	-.24414	.08304	.81296	.05016	.12376	
35+	-.06988	.01725	-.49524	-.10336	-.13279	
44+	-.00673	-.00957	-.09116	-.03002	.01397	
45+	-.00618	-.00407	-.01975	-.00083	.00778	
55+	-.00257	-.00110	-.00182	.00302	.00218	
$\Sigma\|a_n\|^2$	.96186	.01152	.94611	.01571	.04044	
333_d+	.16409	-.02051	.02744	-.24397	.53249	
344_d+	-.04271	-.13808	.15315	.23521	.59755	
355_d+	-.01033	-.03869	-.08912	.04264	.37989	
444_d+	.00196	.03534	-.01923	.06729	-.08806	
455_d+	-.00062	.01876	-.00066	-.00606	-.02915	
555_d+	.00001	.00634	.00141	.00950	-.00560	
$\Sigma\|a_n\|^2$	.02886	.02262	.03252	.12132	.79356	
333_d-	-.05093	-.87628	.00337	.20749	.11471	
344_d-	.07638	.43193	-.07753	.60415	.08179	
355_d-	.02775	.06757	.11633	-.66213	-.29169	
444_d-	-.00712	-.00641	.03878	-.07586	.04463	
555_d-	-.00054	+.00012	-.00381	.00000	.00205	
$\Sigma\|a_n\|^2$	.00926	.95904	.02107	.85229	.10711	
$(4f)^2$	.00353	.07505	-.01043	-.07467	.24153	
Type	33+	333_d-	34+	344_d-	333_d+(?)	355_d-
Position TDM (eV)	69.370	70.415	71.258	71.841	72.003	--
Position c.c (eV)	69.370	70.373	71.370	71.568	72.039	72.288
Width (eV)	0.0860	0.2246	0.0478	0.0688	0.0249	0.0297
Quantum Defect (eV)	1.0461	1.6865	1.0506	1.4383	1.1022	1.4131

but, because of the structures, the concept of a single value for the peak cross section loses its meaning. Further, a close examination of the data of Ref. 3 shows that one of the structures at 47 V, may, in fact, have been observed.

A detailed comparison of our results with the latest experiment is given in Ref. 4.[19] We note that the agreement in shape with the present calculation is very good in all details up to energies just above the $n=3$ threshold. Unfortunately, because the experiment consists of a relative measurement, the absolute value of $Q(1s\text{-}2s)$ remains unknown. Because of numerical difficulties we could not carry out the scattering calculations over a fine energy grid very close to the $n=2$ threshold, but our extrapolated value of $0.028\pi a_0^2$ is lower than that given by the three-state $(1s\text{-}2s\text{-}2p)$ eigenfunction expansion,[5] but somewhat higher than that obtained with the three-state expansion augmented by correlation terms.[20] The good agreement with experiment for the detailed shape of the excitation function encourages us to suggest that present results be used for normalization of the experimental data at these low energies.

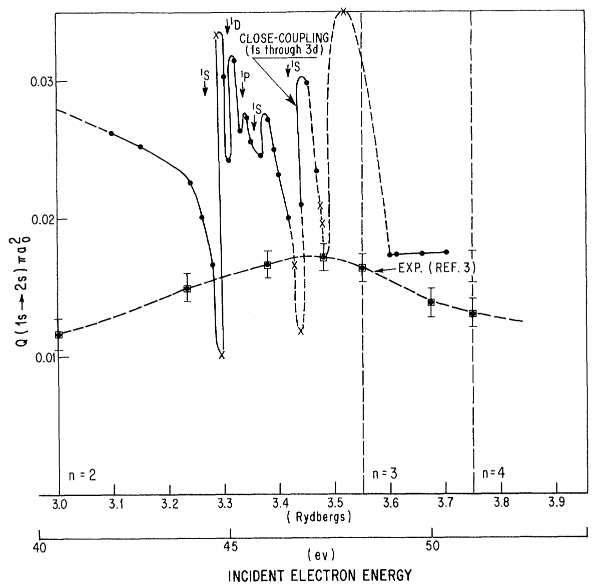

FIG. 2. The total cross section for the transition $1s$-$2s$. The experimental points are taken from Ref. 3. The points in the curve indicate the energy values where complete calculations were carried out (i.e., all the contributing singlet and triplet partial-wave cross sections were obtained by close coupling). The crosses indicate the energy values where the dominant contributing partial-wave results (i.e., ^1S, ^1P, ^1D) were combined with interpolated values for the other partial waves. Because of the infinite number of the expected resonances below the $n=3$ threshold, we have indicated by dashes the energy regions where, we feel, the shape of the total cross-section curve may be affected by future detailed calculations of the resonances.

The close-coupling calculations were carried out on the CDC 6600 at the Air Force Weapons Laboratory using the noniterative ten-channel scattering code described elsewhere[18] and derived from the code originally developed by Dr. P. G. Burke. The TDM calculations were carried out on the IBM 7094 while one of us (L.L) was a Postdoctoral Research Fellow at the National Bureau of Standards, Washington, D. C. The authors would like to thank Dr. P. G. Burke and Dr. J. Macek for their interest in this work, and Colonel R. H. Pennington for permission to use the Air Force Weapons Laboratory computer facilities. The careful and patient work of Mr. Walter Huebner at various stages of these calculations is also gratefully acknowledged.

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[17]An example of such improved resolution is the recently obtained separation of the ^1P and ^1D autoionizing states below the $n=2$ threshold of He^+ (M. E. Rudd, private communication).

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[20]P. G. Burke, private communication.

ELECTRON-IMPACT EXCITATION OF THE 2S STATE AND AUTOIONIZATION BELOW THE $n=3$ LEVEL OF He^+ (EXPERIMENTAL)

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Madden and Codling[1] have reported observing autoionizing neutral-atom energy states in helium. Cooper, Fano, and Prats[2] have interpreted the energy states theoretically. These high-energy states require the simultaneous excitation of two electrons and the states interact with the adjacent continuum and decay by autoionization in times of 10^{-13}-10^{-14} sec. The interaction leads to resonances in the photoionization continuum of helium.

Madden and Codling[3] have recently shown that autoionizing states, excited by photon absorption, exist below the $n=3$ threshold of He^+. Numerous theoretical studies have been made of the electron-impact excitation of He^+. The excitation cross section for He^+ $1S \to 2S$ has been calculated by Burgess,[4] Hummer,[5] and Burke, McVicar, and Smith.[6] Ormonde, Whitaker, and Lipsky,[7] using close-coupling calculations, have shown the effect of autoionizing levels in helium below the $n=3$ level on the cross section for He^+ $1S \to 2S$. An experimental measurement has been made by Dance, Harrison, and Smith[8] of this cross section, using the crossed-beam technique. Ormonde, Whitaker, and Lipsky[7] and Burke and Taylor[9] predict that this cross section should peak at threshold and decrease at higher energies. The experimental work showed that the cross section reached a maximum just below the $n=3$ threshold at about 48 eV. Ormonde, Whitaker, and Lipsky[7] suggest that the position of this peak can be explained in terms of autoionizing levels below the $n=3$ level of He^+.

The object of this work was to study (1) the shape of the excitation function for

$$He^+ + e \to He^+(2S)$$

very close to threshold; (2) to look for resonant effects in excitation in the preceding reaction.

An experimental technique different from the crossed-beam method used by Dance, Harrison, and Smith[8] has been used in this work to observe the excitation function for the He^+ 2S state. Also, in contrast to the crossed-beam method, the signal-to-noise ratio is very good. The method described by Baker and Hasted,[10] in which ions are trapped for considerable times by the space charge of a magnetically confined electron beam, has been used. The ion source used is based on the design described by Redhead.[11] Ions formed in the source were magnetically analyzed by a 12-in. radius, 90°-sector mass spectrometer. Ions were detected by the ion detector shown in Fig. 1. The reason for the use of this type of ion detector can be explained if we consider the reactions that can take place in the ion source. These, with their appearance potentials, are as follows:

$$He + e \to He^+(1S) + 2e, \quad 24.6\ V; \tag{1}$$

$$He^+(1S) + e \to He^+(2S) + e, \quad 40.8\ V; \tag{2}$$

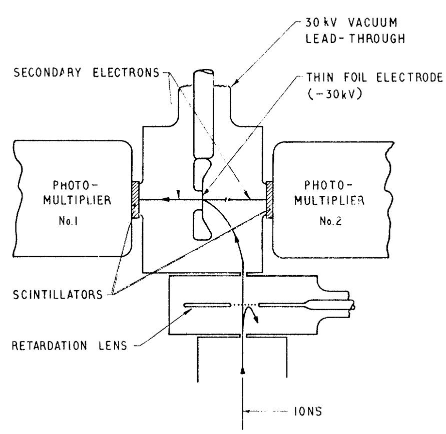

FIG. 1. Ion detector showing retardation lens and thin-foil arrangement.