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LETTER TO THE EDITOR

A new type of He^- resonance states in the autoionisation region

P J M van der Burgt and H G M Heideman

Fysisch Laboratorium, Rijksuniversiteit Utrecht, Princetonplein 5, 3584 CC Utrecht, The Netherlands

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Abstract. We have studied the near-threshold excitation of autoionising states in electron-helium scattering. Only a particular set of autoionising states is observed in the measurements, which has led us to formulate a selection rule for threshold excitation of autoionising states. Evidence is presented that autoionising states belonging to this particular set are strongly excited near their thresholds by hitherto unknown shape resonances.

In a recent experiment (Buckman *et al* 1983) numerous resonances were found in the yield of metastable atoms resulting from electron impact excitation of helium in the threshold region of the singly excited states. It was found that the resonances occur in distinct groups, the energies of which could be fitted to a modified Rydberg formula that takes into account the two-electron correlations in these doubly excited resonances (Read 1983).

By analogy with the threshold excitation of singly excited states in the 19–25 eV range we expect that negative-ion resonances also significantly affect the threshold excitation cross sections of autoionising states lying in the 57–66 eV range. The question arises whether (modified) Rydberg series of resonances also exist in this region.

A study of the threshold excitation of autoionising states in ejected-electron spectra is, however, hampered by the post-collision interaction (Read and Comer 1980), which causes an energy exchange between the ejected electron and the scattered electron that has excited the autoionising state. At incident energies close to the thresholds of the autoionising states this energy exchange results in the capture of the scattered electron into a singly excited state of the neutral atom (Heideman 1980). Resonance structures very close to or at the thresholds of autoionising states will therefore not appear in ejected-electron spectra but rather give rise to narrow structures in the excitation functions of singly excited states. In this paper we present the first results of new measurements performed with a better resolution of the incident electron beam than in previous measurements (Heideman 1980). A more detailed discussion and more experimental results will be given in a subsequent paper (van der Burgt *et al* 1985c).

When analysing structures observed in the excitation functions, three different mechanisms for indirect excitation of singly excited states have to be taken into account. Firstly, a negative ion resonance may decay directly to the singly excited states and give rise to a Beutler-Fano resonance lineshape in the optical excitation functions in a narrow range around a fixed incident electron energy.

A second mechanism involves the excitation of an autoionising state followed by autoionisation and post-collision interaction (PCI). This mechanism only gives rise to

structures in the optical excitation functions when the scattered electron loses so much energy during PCI that it is captured into a singly excited state. PCI structures may extend over several eV above the thresholds of the autoionising states (van der Burgt *et al* 1985c). The phase of the PCI amplitude varies strongly with the excess energy above the thresholds of the autoionising states, but also with the principal quantum number of the singly excited state with an excitation function in which the PCI structure is observed. Due to interference with the direct excitation of the singly excited states the peaks and dips in the PCI lineshape exhibit small shifts to higher energies with the increase of the principal quantum number. This energy shift distinguishes PCI structures from resonance structures due to the first mechanism.

A third mechanism, related to the second, involves excitation of an autoionising state via a negative-ion resonance. It is important to ask how many resonances are expected in the 57–66 eV range. Fano and Cooper (1965) have argued that four He^- resonances with three electrons in the $n = 2$ shell are accessible. So far, experiments have identified unambiguously only the $\text{He}^-(2s^22p)^2\text{P}$ resonance at 57.22 eV and the $\text{He}^-(2s2p^2)^2\text{D}$ resonance at 58.30 eV. Using the terminology of Nesbet (1978) these are valence-shell resonances, formed by three electrons at approximately equal distances from the nucleus. Nesbet (1978) has calculated the positions of the resonances observed near the $n = 3$ thresholds of the singly excited states in the experiment of Brunt *et al* (1977). These calculations showed that a different type of resonance exists, in which one electron is very weakly bound in the polarisation potential of a singly excited state. These so-called non-valence resonances generally lie very close to, or at the thresholds of, the singly excited states and decay very strongly (if not exclusively) to their respective parent states.

By analogy with the resonances in the 19–25 eV range, we expect that non-valence resonances may also exist near the thresholds of the doubly excited states, and that these resonances, in which one electron (at a relatively large distance) is weakly bound in the polarisation potential of a doubly excited state, (almost) exclusively decay to their parent states. Nesbet (1976) has already suggested that the electron impact excitation of autoionising states near their thresholds mainly takes place via negative-ion resonances, but he only considered the four valence-shell resonances in the $n = 2$ shell.

The existence of a non-valence resonance near an autoionisation threshold is obviously related to the polarisability of the autoionising state and thus to the correlated state of the two electrons in the doubly excited atom. In order to gain some insight in such a relationship it is sensible to use a classification scheme for doubly excited states that is based upon the analysis of electron correlations. Very recently such a classification scheme was proposed by Lin (1984). This classification scheme is unique for all states of a two-electron atom and is based upon the study of two-electron correlations in hyperspherical coordinates (Lin 1974, Fano 1983) and the supermultiplet classification of intrashell doubly excited states (Herrick and Kellman 1980). The quantum numbers $(K, T)^A$ are introduced where K and T (Sinanoglu and Herrick 1975) replace the angular momentum quantum numbers l_1 and l_2 of both electrons and are used to describe the angular correlations between the two electrons. The quantum number A is introduced (Lin 1984) to distinguish different types of radial correlations. The classification is denoted as

$${}_n(K, T)_N^A {}^{2S+1}L^\pi$$

where n is the principal number of the outer electron and N that of the inner electron; N thus indicates the He^+ dissociation limit if $n \rightarrow \infty$. States with identical $(K, T)^A$,

$A = \pm 1$, but different L , S and π (orbital angular momentum, spin and parity, respectively) have isomorphic correlation patterns (Lin 1984) and exhibit a multiplet structure which may be interpreted in terms of a collective rotational and bending vibrational motion, analogous to the rovibrational motion of linear triatomic molecules (Kellman and Herrick 1980). We have given the classification of Lin (1984) in table 1 for a number of $\pi = (-1)^L$ states of He^{**} .

Table 1. A number of autoionising states of He in the $N = 2$ channels. Only doubly excited states of parity $\pi = (-1)^L$, which can decay by autoionisation, are included in the table. Above 63 eV the table is incomplete.

$(Nl, nl')^{1,3}L$	${}_n(K, T)_N^{A1,3}L^\pi$	Energy (eV)	Width (eV)
$\text{He}^{**}(2s^2)^1S$	$\text{He}^{**}{}_2(1, 0)_2^+ {}^1S^e$	57.82 ^a	0.138 ^a
$(2s2p)^3P$	${}_2(1, 0)_2^+ {}^3P^o$	58.30 ^a	<0.015 ^a
$(2p^2)^1D$	${}_2(1, 0)_2^+ {}^1D^e$	59.90 ^a	0.072 ^a
$(2s2p)^1P$	${}_2(0, 1)_2^+ {}^1P^o$	60.130 ^b	0.038 ^b
$(2p^2)^1S$	${}_2(-1, 0)_2^+ {}^1S^e$	62.06 ^a	
$(2s3s)^3S$	${}_3(1, 0)_2^- {}^3S^e$	62.62 ^c	
$(23sp^-)^1P$	${}_3(1, 0)_2^- {}^1P^o$	62.758 ^b	
$(2s3s)^1S$	${}_3(1, 0)_2^+ {}^1S^e$	62.94 ^a	0.041 ^a
$(23sp+)^3P$	${}_3(1, 0)_2^+ {}^3P^o$	63.07 ^a	
$(2p3p)^1D$	${}_3(1, 0)_2^+ {}^1D^e$	63.50 ^a	
$(2s4s)^1S$	${}_4(1, 0)_2^+ {}^1S^e$	64.18 ^a	
$(24sp+)^3P$	${}_4(1, 0)_2^+ {}^3P^o$	64.23 ^a	
$(2p4p)^1D$	${}_4(1, 0)_2^+ {}^1D^e$	64.39 ^a	

^a Hicks and Comer (1975).

^b Madden and Codling (1965).

^c Lipsky *et al* (1977) (calculated value).

We shall now discuss our measurements, presented in figures 1 and 2. These measurements have been performed with a conventional electron spectrometer. The incident electrons are directed through a hemispherical energy selector, operated at a resolution of about 110 meV, before entering the interaction chamber containing the helium gas. In order to detect photons emitted in a large solid angle the interaction chamber was equipped with a spherical mirror at the bottom and an optical fibre at the top. At the fibre exit photons of particular wavelengths are detected using interference filters and a photomultiplier. The multiplier pulses are stored and accumulated in a multichannel analyser, the advance address of which is swept synchronously with the incident electron energy. Measuring times were typically one to three days per spectrum.

The 3S and 3P excitation curves in figures 1 and 2 show a wealth of structures in the energy range from 57 to 65 eV. At 57.22 eV the $\text{He}^-(2s^2p)^2P$ resonance causes a Beutler-Fano resonance profile, which was used for calibration of the incident energy scale. Between 57.82 and 62 eV three significant structures are observed, related to the $\text{He}^{**}(2s^2)^1S$, $\text{He}^{**}(2s2p)^3P$ and $\text{He}^{**}(2p^2)^1D$ autoionising states. The $\text{He}^{**}(2s2p)^1P$ autoionising state is clearly not present as no sharp structure is observed at the 60.13 eV threshold in the 4^3S and 5^3S excitation functions. The structures around 60 eV in the 4^3P and 5^3P excitation functions clearly have their onset at 59.90 eV and there is no

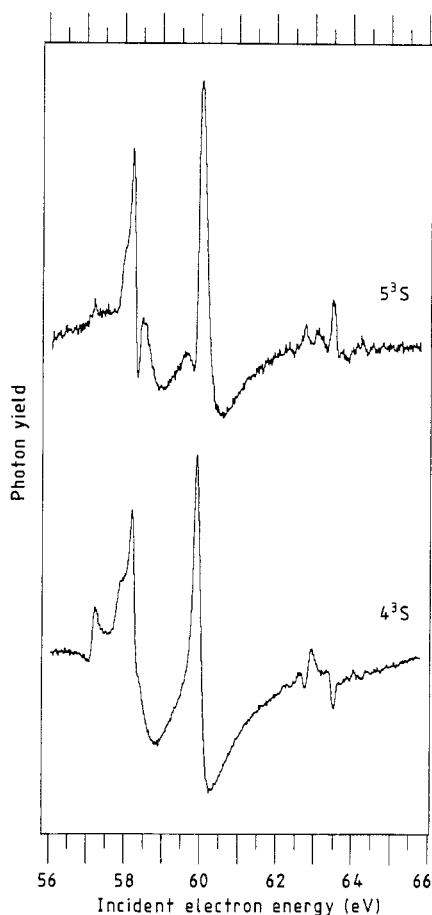


Figure 1. The excitation of the 4^3S and 5^3S singly excited states of helium as a function of the incident-electron energy. The PCI structure between 59.90 and 62 eV is due to the $\text{He}^{**}(2p^2)^1D$ autoionising state. The narrow peak at 59.90 eV shows a very strong threshold excitation of the $\text{He}^{**}(2p^2)^1D$ autoionising state caused by the presence of a negative-ion resonance.

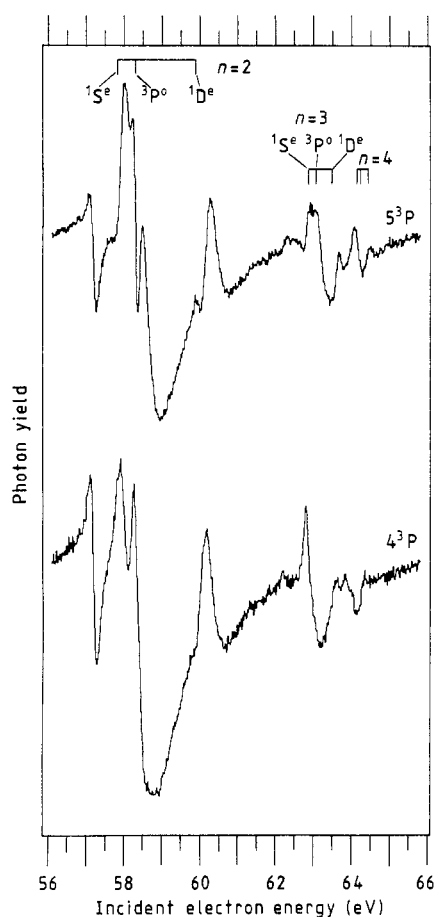


Figure 2. The excitation of the 4^3P and 5^3P singly excited states of helium as a function of the incident-electron energy. Subsequent groups of 1^1S^e , 3^1P^o and 1^1D^e autoionising states give rise to groups of structures observed in the excitation functions. The thresholds of the autoionising states in the first three groups are indicated. The 1^1S^e , 3^1P^o and 1^1D^e states in each group (indicated by the principal quantum number $n=2, 3$ and 4 of the outer electron) correspond to different rotational modes of the $K=1$, $T=0$ vibrational mode in the collective rovibrational model of the doubly excited helium atom (Kellman and Herrick 1980).

evidence for a superposition of structures. Also, the $\text{He}^{**}(2p^2)^1S$ and $\text{He}^{**}(2s3s)^3S$ autoionising states, at 62.06 and 62.62 eV respectively, are observed very weakly or not at all in our measurements. Above 62.7 eV the rapidly increasing number of autoionising states cannot be resolved in our experiment. Moreover the incident energy scale, which was calibrated on the $\text{He}^-(2s^22p)^2P$ resonance at 57.22 eV, may have shifted by some tens of meV near 63 eV. We note, however, that the $\text{He}^{**}(23sp-)^1P$ autoionising state is not observed in the ejected-electron spectra of Hicks and Comer (1975) which were

measured with a resolution of about 40 meV. We therefore attribute the structures observed around 63 eV in the 4^3P and 5^3P excitation functions to the $\text{He}^{**}(2s3s)^1\text{S}$ and $\text{He}^{**}(23sp+)^3\text{P}$ states at 62.94 and 63.07 eV. The structure having its onset near 63.50 eV is clearly to be ascribed to the $\text{He}^{**}(2p3p)^1\text{D}$ state.

Comparing the autoionising states observed in our excitation functions with the supermultiplet classification scheme of Lin (1984) in table 1, it is easily seen that only states with quantum numbers $(K, T)^A = (1, 0)^+$ are present in the excitation functions. As the ground state of helium is classified as $1(0, 0)_1^+ 1\text{S}^e$ we find a selection rule

$$\Delta K = 1 \quad \Delta T = 0 \quad \Delta A = 0$$

for the near-threshold excitation of autoionising states in e-He scattering. This selection rule is related to near-threshold electron impact excitation of autoionising states. At higher incident-electron energies a much weaker selection rule $\Delta A = 0$ holds. This can be verified by looking at the autoionising states observed in the ejected-electron spectra of Hicks and Comer (1975).

Table 1 shows that the states with $(K, T)^A = (1, 0)^+$ occur in distinct groups containing 1S^e , 3P^o and 1D^e states. The states of each group form a rotor series (Lin 1984), and may be interpreted, in terms of the collective rovibrational model of Kellman and Herrick (1980), as different rotational modes of a particular vibrational mode with the correlation quantum numbers $(1, 0)^+$. The group between 57.82 and 62 eV is the lowest vibrational member of the $(1, 0)^+$ mode. Apparently the other vibrational modes, $(-1, 0)^+$, $(0, 1)^+$ and $(1, 0)^-$, which lie in the energy range covered, are not excited in our experiment. Based on the selection rule we conclude that the autoionising states observed in the excitation functions occur in distinct groups, each group being labelled by the quantum numbers $n(1, 0)_2^+$. The appearance of the $n = 2, 3$ and 4 groups can easily be seen in the 4^3P and 5^3P excitation functions. This is in complete analogy with the measurements of Buckman *et al* (1983), where distinct groups of resonances appear in the cross section for electron impact excitation of metastable helium atoms.

We now come to the question of whether non-valence resonances exist near the thresholds of the autoionising states. It may be clarifying in this respect to compare the 59.90 eV structures in the 4^3S and 5^3S excitation functions with the structures observed in the 4^3P and 5^3P excitation functions. In the 3^3P excitation functions interference structures are observed which have their onsets (not their peaks) at 59.90 eV (note the small dip at 59.90 eV in the 5^3P excitation function) and which show a small shift to higher energies with the increase of the principal quantum number. One would normally expect to observe such structures in relationship with autoionisation and the post-collision interaction.

The structure observed above 59.90 eV in the 4^3S and 5^3S excitation functions is exceptional, not only because of the height of the peak but even more because of the position of the peak precisely at the threshold of the $\text{He}^{**}(2p^2)^1\text{D}$ autoionising state. This structure is not due to direct decay of a negative-ion resonance to the 3^3S singly excited states as only a weak structure is observed in the 3^3S excitation function (not shown in figure 1). Therefore we attribute the 59.90 eV structure in the 3^3S excitation functions to a very high threshold excitation cross section caused by the presence of a He^- non-valence resonance. As this resonance is only observed in the 3^3S excitation functions it apparently occurs only in the $l_{sc} = 0$ partial wave of the scattered electron (assuming that no angular momentum exchange between the scattered and the ejected electron occurs during PCI). Using the notation of Nesbet (1978) the (approximate) configuration of the resonance is easily seen to be $\text{He}^-(2p^2\bar{s})^2\text{D}$, i.e. an s electron

weakly bound in the polarisation potential of the $\text{He}^{**}(2p^2)^1D$ autoionising state. Some experimental evidence for the presence of a negative-ion resonance at 59.90 eV in ejected-electron spectra was already presented by van der Burgt *et al* (1985a).

We believe that the $^1S^e$ and $^3P^o$ members of the ${}_2(1, 0)_2^+$ rotor series are also excited strongly near their thresholds due to the presence of non-valence resonances. The 4^1D excitation function (van der Burgt *et al* 1985b) exhibits a structure at 58.30 eV of similar appearance to the 59.90 eV structure in the 4^3S excitation function. It must be noted in this respect that structures at 58.30 eV are difficult to interpret. We suspect the presence of both a valence shell and a non-valence resonance at this position. A discussion will be given in a subsequent paper (van der Burgt *et al* 1985c).

The strong peaks observed near 57.8 eV in the 4^3P and 5^3P excitation function show that the $\text{He}^{**}(2s^2)^1S^e$ autoionising state is also excited strongly at its threshold, probably due to a non-valence resonance of the configuration † $\text{He}^-(2s^2\bar{p})^2P^o$. The profound dip observed at 59 eV in both 3P spectra may be explained by a superposition of dips of the PCI lineshapes due to the $^1S^e$ and $^3P^o$ autoionising states.

The presence of non-valence resonances in the lowest rotor series raises the question of whether non-valence resonances also exist near the thresholds of the autoionising states in the higher rotor series. Evidence that this is indeed the case is found in the 4^3P and 5^3S excitation functions. At 62.94 eV in the 4^3P excitation function a narrow peak is observed at the threshold of the $\text{He}^{**}(2s3s)^1S^e$ autoionising state. Baxter *et al* (1979) also report the presence of a resonance at this energy. In the 5^3S excitation function a narrow peak is observed just above the $^1D^e$ threshold at 63.50 eV, analogous to the peak situated just above the $^1D^e$ threshold at 59.90 eV.

We have pointed to a relationship between the polarisability of a doubly excited state and the presence of a non-valence resonance near its threshold. To see which states have a large polarisability and which states have not, it is helpful to look at the surface charge distribution plots of Lin (1982). The polarisation of a doubly excited state may be visualised by a decrease of amplitude around the Wannier point $\alpha = \tan^{-1}(r_2/r_1) = \pi/4$ and $\vartheta_{12} = \cos^{-1}(\hat{r}_1 \cdot \hat{r}_2) = \pi$ and an increase of amplitude towards smaller ϑ_{12} . Therefore we expect that those doubly excited states which have a small amplitude outside the Wannier region have the highest polarisability. See, for instance, figure 6 of Lin (1982). This figure shows plots of the surface charge distribution for $\mu = 2A$ and $2B$ channels of $\text{H}^-^1S^e$. The $\mu = 2A$ and $2B$ channels correspond to the $\mu = (1, 0)_2^+$ and $\mu = (-1, 0)_2^+$ channels of Lin (1984). The surface charge distributions for He^1S^e have a similar appearance. It is seen that the $(1, 0)_2^+$ surface charge distribution has a large amplitude inside and a very small one outside the Wannier region and thus meets the requirements for a high polarisability posed above; indeed these states occur very prominently in our measured excitation functions. On the other hand the $(-1, 0)_2^+$ surface charge distribution is more spread out over the whole (α, ϑ_{12}) plane and doubly excited states with $(-1, 0)^+$ quantum numbers are therefore only weakly polarisable. Accordingly these states do not support non-valence resonances near their thresholds and are not observed in the excitation functions. This also explains

† It might be argued that such a configuration with one electron outside a closed-shell core cannot be stable. However, such a reasoning relies on the independent-electron model for the classification of atomic states. When electron-electron correlations are accounted for, two 1S states are found with both electrons in the $n = 2$ shell; one with a large probability to find the two electrons at opposite sides and equal distances from the nucleus and another where the two electrons occupy a much larger domain of configuration space (see figure 6 of Lin 1982). The former is expected to have a fairly large polarisability, so that a potential well may be formed deep enough to bind a third electron.

why the selection rule $\Delta K = 1$, $\Delta T = 0$, $\Delta A = 0$ mentioned earlier in this letter applies only close to the thresholds of the autoionising states.

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