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LETTER TO THE EDITOR

Formation and decay of the $_3\{1\}_4^+$ $^1P^o$ autoionizing resonance of helium

H R Sadeghpour and Michael Cavagnero†

† Harvard-Smithsonian Center for Astrophysics, 60 Garden St, Cambridge, MA 02138, USA

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Abstract. We present results of an eigenchannel R-matrix calculation of the photoabsorption spectrum of He below the $He^+(n = 3)$ threshold. The observed $_n\{v\}_m^A$ $=_3$ $\{1\}_4^+$ resonance is found to decay with an 84.4% branching ratio to the $_2\{1\}^o$ ('2pϵd') channel, in violation of a radial correlation propensity rule, $\Delta A = 0$. The $\Delta v = 0$ propensity rule is satisfied, however, indicating that angular correlation is preserved in the decay of this resonance.

The eigenchannel R-matrix method has now been successfully applied to the photoionization spectra of a number of two-electron atoms, including all of the alkaline-earth elements (Greene and Aymar 1991, Greene 1988). Application of this method to atomic helium, however, requires the use of quantum defect functions describing the motion of the photoelectron in combined Coulomb and dipole fields, and so has not been presented previously. The dipole component of the long-range interaction results from the 'permanent' dipole moment induced in the excited He^+ fragment as a consequence of the degeneracy of its hydrogen-like energy levels (Seaton 1961, Gailitis and Damburg 1963). In this Letter we present the first results of our application of the generalized quantum defect theory (Greene *et al* 1982) and of the eigenchannel R-matrix method to the He spectrum.

We analyse the formation and decay of a prominent resonance attributed to the first excited bending mode of the '+' family of doubly-excited states below the $He^+(n = 3)$ threshold. (A similar resonance belonging to a repulsive dipole photoabsorption channel is absent in H^- (Hamm *et al* 1979).) The symbol $A = +(-)$ specifies that the two-electron wavefunction has an antinode (node) in the radial degree of freedom near the line $r_1 = r_2$ (Lin 1983). Our analysis of the partial photoionization cross sections and of the eigenvectors of the delay-time matrix (Smith 1960) indicates that this resonance decays primarily to the $_2\{1\}^o$ channel associated with the $He^+(n = 2)$ threshold. This decay mode violates the A-preserving ($\Delta A = 0$) radial correlation propensity rule satisfied by all other He autoionizing resonances observed thus far (Sadeghpour 1991, Lin 1983, Tang *et al* 1992, Domke *et al* 1991, Zubek *et al* 1989). The coupling of this resonant state to the $_2\{1\}^o$ continuum is dominant since both of these channels ($_3\{1\}^+$ and $_2\{1\}^o$) include a node in the bending coordinate $\theta_{12} = \cos^{-1}(\hat{r}_1 \cdot \hat{r}_2)$; i.e. they are both classified as $v = 1$ channels in the $_n\{v\}_m^A$ classification scheme described in detail by Sadeghpour (1991). Our results also confirm a prediction by Rost and Briggs (1990), who argued—based on their molecular orbital model of doubly-excited states—that this decay mode is preferred due to rotational coupling.

† Permanent address: Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506-0055, USA.

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The eigenchannel R-matrix method which we employ determines a set of variational solutions of the full two-electron Schrödinger equation in a finite spherical volume. These solutions satisfy the boundary condition

$$\left.\frac{\partial \psi_\beta}{\partial n}\right|_{r_0} + b_\beta \psi_\beta(r_0) = 0 \tag{1}$$

on the spherical reaction surface $r = r_0$ (Fano and Lee 1973). In our application to the autoionizing resonances below the $He^+(n = 3)$ threshold we use $r_0 = 25$ au so that the exchange interaction is negligible outside the R-matrix box. For each of the nine open and weakly closed channels included in our calculation, eighteen He^+ wavefunctions that are zero on the box boundary and two He^+ wavefunctions that are non-vanishing at r_0 are used to represent the eigenchannel solutions, $\{\psi_\beta\}$, for $r \leqslant r_0$.

With the R-matrix calculation completed, the set $\{\psi_\beta\}$ is matched at the boundary of the reaction zone to a set of quantum defect functions representing the motion of the photoelectron in the long-range field of the He^+ fragment (Greene *et al* 1982, Bely 1966, Dubau 1978). This field is approximated by its dominant multipoles: a monopole term due to the charge of the ion and a dipole term resulting from the ion's induced moment. The effect of the dipole term is to produce a non-integral orbital angular momentum, ℓ, of the photoelectron, which is complex for attractive dipole moments; the incorporation of Coulomb functions with non-integral ℓ into the eigenchannel R-matrix method is the technical accomplishment of our effort.

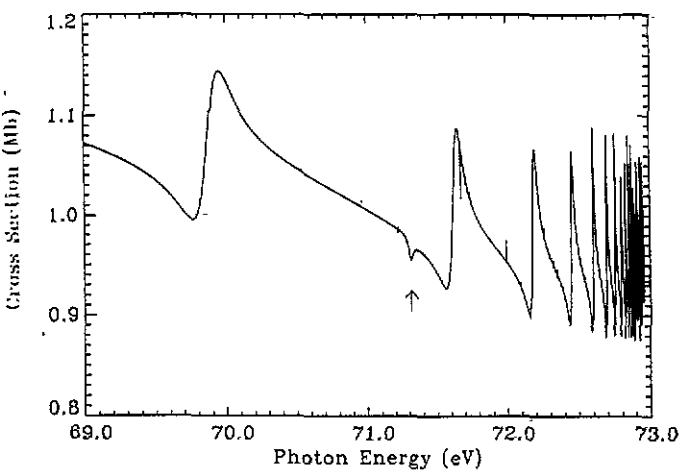

Figure 1. Total photoabsoprtion cross section of helium below $He^+(n = 3)$ as a function of photon energy in eV. The ${}_3\{1\}_4^+$ resonance, which appears as a dip near 71.3 eV, is indicated by an arrow.

Figure 1 displays our calculated total photoionization cross section for the resonance region below the $n = 3$ threshold. The ${}_3\{1\}_4^+$ resonance at 71.3 eV corresponds to the only prominent resonance with a quantum of bending excitation (Domke *et al* 1991, Zubek *et al* 1989). This 'precursor' resonance is the first of a series whose higher members are blended with the dominant ${}_3\{0\}_m^+$ resonances and so are not readily apparent in the spectrum. A complete analysis of the spectrum, including a study of the many narrow resonances, will

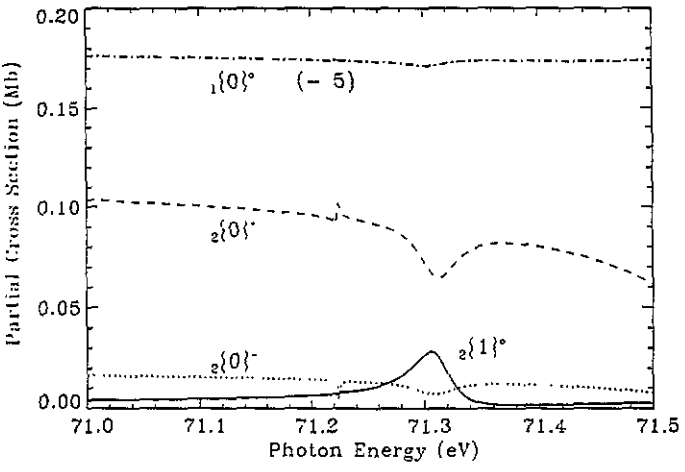

Figure 2. Partial photoabsorption cross sections of helium in the vicinity of the $_3\{1\}_4^+$ resonance. The full curve gives the cross section in the $_2\{1\}^o$ channel, the broken curve the cross section in the $_2\{0\}^+$ channel, the dotted curve the cross section in the $_2\{0\}^-$ channel and the chain curve the cross section in the $_1\{0\}^o(1s\epsilon p)$ channel, reduced by a factor of 5.

be presented separately—we focus here on the excitation and decay of the singular $_3\{1\}_4^+$ resonance feature.

Figure 2 displays the partial cross sections for ionization in each of the four available open channels in the energy region of interest. The resonance appears as a window resonance in the $_2\{0\}^+$ ionization channel, and as an asymmetric peak in the $_2\{1\}^o$ channel. The continua associated with the ionic ground state and with the $_2\{0\}^-$ channel show smaller window-type resonance features. These figures and the analysis below lead us to conclude that the resonance decays primarily to the $_2\{1\}^o$ continuum.

The resonance observables—energy position, decay width and the decay probabilities—are best extracted from the delay-time matrix $\mathbf{Q} = -i(dS/dE)S^\dagger$. Details of this proceedure were presented in our earlier application to H^- (Sadeghpour *et al* 1992). The largest eigenvalue of the delay-time matrix is a Lorentzian function of the energy; the resonance energy (E_0) is the position of the Lorentzian peak and the resonance width (Γ) is obtained from its maximum value, q_{max}, such that $\Gamma = 4/q_{max}$. For the $_3\{1\}_4^+$ resonance we obtain $E_0 = -0.28273$ au and $\Gamma = 1.49 \times 10^{-3}$ au, to be compared with Ho's results of $E_0 = -0.28283$ au and $\Gamma = 1.46 \times 10^{-3}$ (Ho 1982). The modulus squared of individual eigenvector components corresponding to the largest eigenvalue of $\mathbf{Q}$ gives the decay probability into different available open channels. For the four continua, $_1\{0\}^o(1s\epsilon p)$, $_2\{0\}^-$, $_2\{0\}^+$ and $_2\{1\}^o$, we find probabilities of 0.3%, 5.0%, 10.3%, and 84.4%, respectively.

Previous studies of the photoabsorption of helium indicated that '+' resonances decay primarily to '+' continua, and likewise for the '−' states (A-preserving propensity rule) (Greene *et al* 1992, Lin 1986). Resonant states within different '+' channels were also anticipated to have a propensity for decay to '+' continua with the same v quantum number (v-preserving propensity rule) (Sadeghpour 1991). For the $_3\{1\}_4^+$ resonant state there is no available '+' continuum with $v = 1$. The only continuum channel with one quantum of bending vibration is the $_2\{1\}^o$ continuum. This precursor resonance thus favours the $\Delta v = 0$ propensity rule more strongly than the radial correlation propensity rule, in agreement with the prediction of Rost and Briggs (1990) that this transition occurs via rotational coupling from the $n = 3$ state of $3p\pi_u$ to the $n = 2$ continuum of $3p\sigma_u$.

In conclusion, we have found that the primary mode of decay of the ${}_3\{1\}_4^+$ resonance in the photoabsorption of helium is the ${}_2\{1\}^o$ continuum channel. This result is based on *ab initio* R-matrix calculations of the partial photoionization cross sections, complemented with an analysis of the eigenvectors of the delay-time matrix.

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