Auger decay of the photoexcited $1s^{-1}np$ Rydberg series in neon

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Photoabsorption of neon in the region of the inner shell excited $1s^{-1}np$ resonance series is treated using an optical potential *R*-matrix method. Compared to standard *R*-matrix results, an extremely broadened resonance profile is determined, due to implicit inclusion of core Auger decay states via the optical potential, remarkably reproducing recent high-precision experimental results.

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Photoionization in the vicinity of inner shell excited resonance series is difficult to treat theoretically since there usually exists an infinite number of singly excited ionic continua to which these resonances can autoionize. Particularly for methods based on a close-coupling expansion [1], such as the widely used *R*-matrix method [2], which necessarily uses a finite basis, it is impossible to include all of these channels. As a result, the computed Auger rates in any given limited calculation can be severely underestimated due to the neglect of those omitted autoionization channels. In a recent study [3] (hereafter referred to as paper I), an *R*-matrix method, which included an optical potential within multichannel quantum defect theory (MQDT), was introduced to account for these otherwise missing channels, and was applied to the $2p^{-1}$ inner shell photoexcited resonance series in argon. While the general qualitative experimental features [4] were theoretically reproduced using this method, there were noticeable differences between theory and experiment, attributed mostly to the lack of convergence of the computed relative resonance positions.

The $2p^{-1}_{3/2,1/2}ns,md$ inner shell resonances in argon are complicated by both the fine structure splitting of the $2p^{-1}$ ionic core *and* the multiple ns and md valence electrons attached to these cores, giving rise to a somewhat complex spectrum of overlapping resonances. Inaccuracies in theoretically determined relative positions can then significantly affect the overall resonance profile, as was seen especially in the case of the $2p^{-1}4s$ resonances. The $1s^{-1}np$ resonance series in neon, on the other hand, is devoid of core fine structure splitting and furthermore has just a single np valence electron coupled to the core.

The purpose of the present paper is to theoretically study inner shell photoexcitation followed by Auger decay in neon, where the absence of fine structure splitting and the singular $1s^{-1}np$ series makes this the simplest rare gas system for studying inner shell processes. The *R*-matrix MQDT optical potential method used in paper I for argon will be applied here for neon, and results will be compared to recent high-resolution experimental measurements [5] (in that study, corresponding theoretical results were given that excellently reproduced the measured ones).

The specific processes of interest are inner-shell photoexcitation of the neon ground state,

$$h\nu+1s^22s^22p^6\rightarrow 1s2s^22p^6np, \quad (1)$$

followed by two competing decay routes. First, there is *participator* Auger decay

$$\begin{aligned}1s2s^22p^6np&\rightarrow 1s^22s^22p^5+e^-\\&\rightarrow 1s^22s2p^6+e^-, \quad (2)\end{aligned}$$

where the valence electron np takes part in the autoionization process; the decay rate therefore scales as $1/n^3$. There is also the more important (yet less amenable to close-coupling studies) *spectator* Auger decay

$$\begin{aligned}1s2s^22p^6np&\rightarrow 1s^22s^22p^4np+e^-\\&\rightarrow 1s^22s2p^5np+e^-\\&\rightarrow 1s^22p^6np+e^-, \quad (3)\end{aligned}$$

where the valence electron np does not take part in the autoionization process, giving instead a decay rate that is independent of *n*. Spectator Auger decay is therefore the dominant decay route as $n\rightarrow\infty$, but as will be seen, in neon it dominates even for $1s^{-1}3p$, the lowest inner shell resonance. Similar behavior was observed experimentally and explained theoretically for autoionization of the lowest $1s2s^22p(^1P)$ inner-shell resonance in Be [6], where the spectator decay rate to the $1s^22p\epsilon s$ continuum was found to be about 20 times greater than the participator decay rate to the $1s^22s\epsilon' p$ continuum due to cancellation effects. A constant spectator width also leads to a smearing of higher-*n* resonances and a smooth transition from the below-threshold to above-threshold photoabsorption cross section, making an accurate determination of the threshold position difficult.

In the present study, the photoabsorption cross section contributions from each decay route are treated somewhat differently. The *main line* cross sections to the $1s^22s^22p^5$ and $1s^22s2p^6$ ions in Eq. (2) are accounted for by including these two as target states in the close-coupling expansion; the $1s2s^22p^6$ state is also included for describing the $1s2s^22p^6np$ resonances. Computed energies of these three ionic states, as well as the $1s^22s^22p^6$ ground state, are given in Table I. Brief computational details are that the bound and pseudo-orbitals $\{1s,2s,2p,\overline{3s},\overline{3p},\overline{3d}\}$ are used to generate a configuration-interaction (CI) basis consistent with single and double promotions out of the above three ionic configurations; for the electron-ion collision problem, twenty continuum orbitals are attached to the final three linear CI com-

TABLE I. Ne and Ne^+ energies.

		Theoretical		Experimental	
		Absolute (a.u.)	Relative (eV)	Relative (eV)	Photon energy (eV)
Ne	$1s^2 2s^2 2p^6\ ^1S_0$	−128.735	−23.40	−21.56 [a]	0.00
Ne^+	$1s^2 2s^2 2p^5\ ^2P^o$	−127.875	0.00	0.00	21.56
	$1s^2 2s 2p^6\ ^2S$	−126.960	24.91	26.91 [a]	48.47
	$1s 2s^2 2p^6\ ^2S$	−96.767	846.36	848.64	870.17 [b]

[a]Reference [7].
[b]Reference [5].

binations of these and all configurations from the bound and pseudo orbitals consistent with single, double, and triple promotions from the ground state configuration are also included. The Belfast *R*-matrix codes [8] are used for the final calculations. Results for the photoabsorption cross section are shown in Fig. 1 as the solid line, where the resonance features are seen to be extremely narrow due to the neglect of spectator Auger decay, and are indeed impossible to fully resolve with any finite mesh of energy points (the 10 000 equidistant energy points used to produce the results in Fig. 1 are insufficient for resolving more than the lowest resonances, and miss altogether those near the Rydberg limit).

Spectator Auger decay to the *satellite line* cross sections in Eq. (3) are instead accounted for by including an optical potential in the *R*-matrix calculations (see paper I for more complete details). This approach is equivalent to adding an imaginary term to the ionic core energies of the resonance, an idea first proposed for including missing radiative channels [9,10]. The ionic energy for the closed channel $1s2s^2 2p^6 np$ is modified as

$$E_{1s^{-1}} \rightarrow E_{1s^{-1}} - i\Gamma_{1s^{-1}}/2, \tag{4}$$

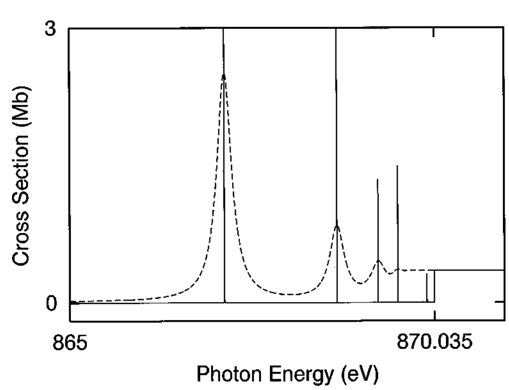

FIG. 1. Photoabsorption of neon in the region of the $1s^{-1}np$ resonances: results from the standard *R*-matrix calculation (solid line) and the present optical potential *R*-matrix results (dashed line), using a $1s^{-1}$ threshold of 870.035 eV. Results using the length and velocity forms of the dipole operator are indistinguishable on this scale.

where $\Gamma_{1s^{-1}}$ is the spectator Auger decay rate and is computed in lowest-order perturbation theory using the program AUTOSTRUCTURE [11]:

$$\Gamma_{1s^{-1}} = 2\pi \sum_{i+j=6} \sum_{\ell, S_c, L_c} \times |\langle 1s2s^2 2p^6(^2S)|V|1s^2 2s^i 2p^j(^{2S_c+1}L_c)\epsilon\ell(^2S)\rangle|^2 = 0.241 \ \text{eV}. \tag{5}$$

While this value is slightly lower than the value of 0.271 eV computed recently for the $1s^{-1}$ width [5], the overall qualitative resonance profiles determined in the present study were fairly insensitive to such small differences in core decay rates. Multichannel quantum defect theory (MQDT) facilitated the modification in Eq. (4) since an analytic expression for the energy dependence of the $1s2s^2 2p^6 np$ closed channel is thereby obtained. Photoabsorption results using this modified method are also shown in Fig. 1, where tremendous broadening of the resonance features is seen.

In comparing these theoretical results to the experimental ones [5], it was first necessary to adjust the theoretical $1s2s^2 2p^6$ threshold. While, according to Table I, this is experimentally determined as 870.17 eV [5], an enforced theoretical threshold of 870.035 eV was instead used so as to align the lower resonance members ($n=3-5$) with experimental results, in closer agreement with the theoretically determined value from that same study of 870.07 eV [5]. The experimental cross section results are only given in arbitrary units [5], so a scaling factor of 1.55 was chosen to multiply those arbitrary units in order to align the peak of the theoretical and experimental $1s^{-1}5p$ resonance. As seen in Fig. 2, the optical potential *R*-matrix results agree quite well with the high-resolution experimental results, showing only slight disagreement in the lowest $1s^{-1}3p$ resonance peak height and the nonresonant cross section, especially above the $1s^{-1}$ threshold. Since the experimental resolution is much smaller than the natural widths, the resonances are fully resolved in the experiment, ruling out any experimental broadening of the resonances. As for the discrepancy above threshold, this is probably due to the omission of higher $1s2\ell^7 n\ell'$ ionic

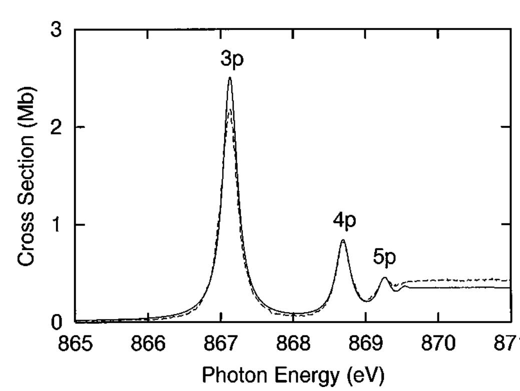

FIG. 2. Photoabsorption of neon in the region of the $1s^{-1}np$ resonances: present optical potential *R*-matrix results (solid line) and experimental results (dashed line, arbitrarily normalized to coincide with theory at the peak of the $1s^{-1}5p$ resonance).

states in the close coupling expansion, and therefore the neglect of polarization effects in the theoretical results; a many-body perturbation theory study of inner shell photoionization in argon found that polarization effects increased the near-threshold cross section considerably [12]. Nevertheless, this simple approach of performing a three-state *R*-matrix calculation, with an optical potential inclusion, remarkably reproduces the essential resonance features in the $1s^{-1}np$ inner shell photoabsorption of neon.

In conclusion, it has been demonstrated that standard close-coupling expansion methods using a limited basis, such as the present simplified three-state *R*-matrix approach, drastically underestimate inner shell excited resonance widths due to the unavoidable omission of spectator Auger decay channels. However, implicit inclusion of these missing channels can be accomplished by using an optical potential, and give computed results for the photoabsorption of neon near the $1s^{-1}$ threshold that reproduce rather well the recent high-resolution experimental results [5]. It was necessary to set the theoretical photon energy of the $1s^{-1}$ Ne^{+} ionic state to 870.035 eV in order that the lowest $1s^{-1}np$ resonances aligned with experimental ones. This may therefore suggest some additional utility in using theoretical close-coupling methods, together with experimental photoabsorption measurements, for determining the series limit, since it is not possible to determine this limit from photoabsorption measurements alone due to the smearing of constant-width high-*n* resonances with the above-threshold continuum.

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