He photoionization to the doubly excited $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ series

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We present an application of a configuration-interaction method for the *continuum spectrum* to He photoionization from the ground state to the doubly excited $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ series, using a finite L^2-basis set constructed from a nearly complete set of spline-based one-particle hydrogenic orbitals. Our calculated resonance structures are in good agreement with the recent high-resolution synchrotron-radiation spectra [M. Domke, G. Remmers, and G. Kaindl, Phys. Rev. Lett. **69**, 1171 (1992)]. Our calculated widths, resonance energies, and peak photoionization cross sections are also in close agreement with the most accurate existing theoretical results.

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With an energy resolution of $\cong 4$ meV, Domke, Remmers, and Kaindl [1] have recently observed the double-excitation Rydberg series of He below the He^+ $N=2$ threshold in a photoionization experiment using synchrotron radiation. In particular, they have resolved the $(sp,2n^-)$ and $(2pnd)$ $^1P^o$ series, which are separated by energy differences ranging from a maximum of 16.4 ± 0.4 meV for the 4^--$3d$ pair to an estimated 4 ± 2 meV for the 7^--$6d$ pair. The reported energy seperations between the neighboring $2pnd$ and $sp,2(n+1)^-$ resonances are determined by fitting the measured photoionization spectra to a standard Fano-type profile [2] for the $sp,2(n+1)^-$ lines and a near-symmetric monochromator function corresponding to a weighted sum of a Gaussian and a Lorentzian profile for the $2pnd$ lines.

Theoretically, the $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ series have been studied extensively in recent years following the early work by Burke and McVicar [3] using a four-channel close-coupling calculation over two decades ago. Specifically, Salomonson, Carter, and Kelly [4] have derived the resonance widths and the q values of the $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ series from the calculated photoionization spectra based on a nine-channel coupled-equation calculation within the framework of many-body perturbation theory (MBPT). Gersbacher and Broad [5] have calculated in detail the profile parameters for the $(sp,23^-)\,{}^1P^o$ resonance using a L^2-based R-matrix method [5]. Sánchez and Martín [6] have examined quantitatively the $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ resonance structures using a Slater-type-orbital- (STO) based L^2-basis method. These two relatively narrow $^1P^o$ series have also been studied qualitatively in other recent theoretical works, including (i) the L^2-basis calculation by Moccia and Spizzo [7], (ii) the variational R-matrix calculation by Hamacher and Hinze [8], and (iii) the spline-based multiconfiguration-Hartree-Fock (MCHF) calculation by Froese Fischer and Idrees [9].

Except for minor quantitative details, the calculations by Salomonson, Carter, and Kelly [4] and Sánchez and Martín [6] have both suggested an asymmetric resonance profile for the $2pnd$ series with a significantly larger negative q value than the one for the $sp,2n^-$ series. As a result, contrary to the observed spectra, a higher peak photoionization cross section σ_{max} is expected for the $2pnd$ resonances than that for the $sp,2n^-$ resonances. A direct comparison between the observed spectrum and the theoretical resonance structure derived from the calculated profile parameters corresponding to an *isolated single* resonance is also difficult due to the close proximity between $2pnd$ and $sp,2(n+1)^-$ resonances.

In this paper we present a quantitative comparison for a few selected $sp,2n^-$ and $2pnd$ resonances between the observed resonance structures and the calculated photoionization spectra based on a configuration-interaction method for the *continuum spectrum* (CIC) [10]. The effectiveness of this CIC procedure has been demonstrated by its recent applications to the photoionization of a two-electron atom and the single and multiphoton ionization of a divalent atom [10]. In Table I we compare the observed resonance energies and the energy separations for the He $(2pnd)$ and $(sp,2n^-)\,{}^1P^o$ series with the results from the present calculation and several other recent theoretical results which are not referred to in Ref. [1]. The most recent theoretical values by Ho [11] using the complex rotational method are also included for comparison. Some of the calculated resonance energies are modified to account for the use of different energy-conversion factors. The overall agreement between experiment and theory is excellent.

Our calculated photoionization cross sections in the vicinity of the $(sp,23^-)$, $(2p3d)$, and $(sp,24^-)\,{}^1P^o$ resonances are shown in Fig. 1. To compare directly with the observed spectra, the theoretical energies have been shifted to lower energy by 3 meV for all three resonances. To normalize the observed spectra, it is necessary to match two values of the *photoionization yield* to the calculated cross sections since no unit is given in Fig. 2 of Ref. [1]. For a specific photoionization yield ϕ, we first measure the energy difference Δ between its corresponding photon energies on the opposite side of the observed resonance structure. Second, we determine the photoionization cross section σ corresponding to the photoionization yield ϕ by matching the experimental energy difference Δ to the theoretical energy difference between two photon

TABLE I. The resonance energies E_r of selected He $(sp,2n^-)$ and $(2pnd)$ $^1P^o$ resonances and their energy separations below the $N=2$ threshold. The numbers in parentheses are experimental errors in units of the last digits. The energy separation given by $a[-b]=a\times10^{-b}$ eV. The energy in eV is converted using the factor employed in Ref. [1], i.e., 1 Ry=13.6503 eV and the ionization potential is 79.0078 eV.

	Observed	Theory					
State	(Ref. [1])	Present	Ref. [12]	Ref. [11]	Ref. [6]	Ref. [8]	Ref. [4]
				Resonance energy E_r (eV)			
3^-	62.7580(2)	62.7611	62.7611	62.7611	62.757	62.766	62.761
$3d$	64.1189(2)	64.1217		64.1211	64.118		64.127
4^-	64.1353(2)	64.1377	64.1379	64.1374	64.134	64.109	64.142
$4d$	64.6485(4)	64.6514		64.6512	64.648		64.654
5^-	64.6574(2)	64.6598	64.6599	64.6598	64.656	64.629	64.662
				Energy separation (eV)			
3^--4^-	1.3773(4)	1.3766	1.3768	1.3763	1.377	1.343	1.381
4^--5^-	0.5221(4)	0.5221	0.5220	0.5224	0.522	0.520	0.520
$3d$-$4d$	0.5296(6)	0.5297		0.5301	0.530		0.527
4^--$3d$	16.4(4)[−3]	16.0[−3]		16.3[−3]	16.0[−3]		16.0[−3]
5^--$4d$	8.9(6)[−3]	8.4[−3]		8.6[−3]	8.0[−3]		8.0[−3]

energies, which correspond to σ. Following this procedure, the photoionization yields corresponding to $\Delta=5$ and 7.5 meV for the $sp,23^-$ resonance are normalized to theoretical cross sections of 1.37 and 1.32 Mb, respectively. The same normalization procedure has also been applied to the observed $2p3d$ and $sp,24^-$ spectra shown in Fig. 1. The calculated and the observed structure profiles appear to agree well. A hint of a sharp drop to a minimum in cross section is seen on the high-energy side of the $sp,2n^-$ resonances. With an energy resolution of 4 meV, it is not unexpected that the sharp dip in cross section (with a "width" less than 2 meV) next to the $2p3d$ resonance is not observed experimentally. Similarly, the top portions of the resonance structures are also absent in the observed profiles when their widths become less than 2 meV.

In Table II we list our calculated widths of all three doubly excited $^1P^o$ series, i.e., $sp,2n^+$, $sp,2n^-$, and $2pnd$, below the He^+ $N=2$ threshold based on a more elaborate configuration-interaction (CI) procedure presented elsewhere [13,14]. Our results compare well with the results from some of the most accurate theoretical calculations. For the higher members of the $sp,2n^-$ series, when the CI calculation includes only bound-continuum types of configuration series, our theoretical widths (not shown in Table II but very close to the results of Ref. [4]) generally agree well with other calculations. However, as we include continuum-continuum types of configuration series in our CI calculation, the theoretical widths (i.e., those listed in Table II) become slightly narrower than the ones from other earlier calculations. In addition, we also compare the peak photoionization cross sections

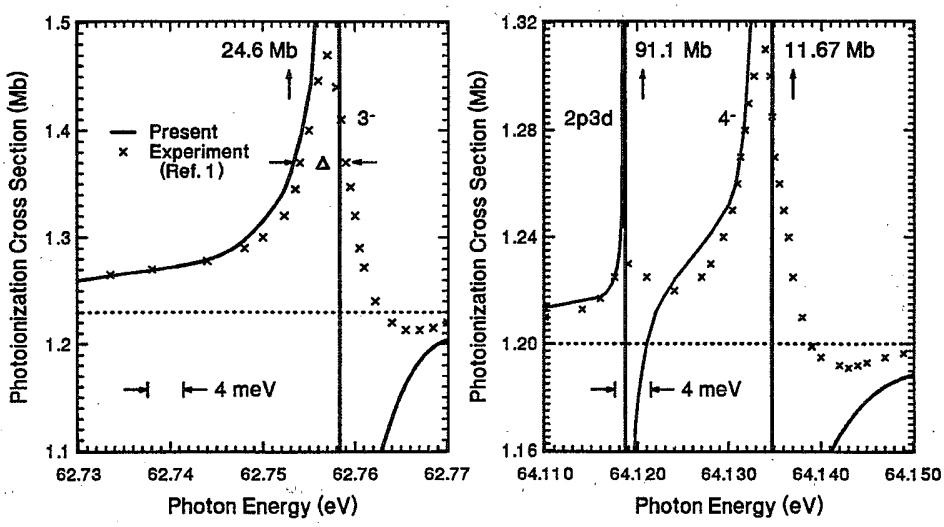

FIG. 1. Comparison of the calculated and the observed photoionization cross sections near the doubly excited $(sp,23^-)$, $(2p3d)$, and $(sp,24^-)$ $^1P^o$ resonances of the He atom below the $N=2$ threshold.

TABLE II. The widths Γ (upper entry in $a[-b]=a\times10^{-b}$ Ry) and the peak photoionization cross sections σ_{max} (lower entry in Mb) for selected He $(sp,2n^+)$, $(sp,2n^-)$, and $(2pnd)\,{}^1P^o$ resonances below the $N=2$ threshold.

State	Present	Ref. [12]	Ref. [11]	Ref. [6]	Ref. [4]	Ref. [8]	Ref. [5]	Ref. [15]
2^+	2.78[−3] 12.50	2.66[−3]	2.75[−3]	2.82[−3] 12.38	2.96[−3] 11.18	2.95[−3] 11.56	2.75[−3] 12.10	2.70[−3]
3^+	6.08[−4] 9.66	6.20[−4]	6.02[−4]	6.17[−4] 9.90	6.59[−4] 8.62	6.57[−4] 9.20	5.60[−4] 9.60	5.94[−4]
4^+	2.21[−4] 9.04	2.48[−4]	2.58[−4]	2.63[−4] 9.44	2.82[−4] 8.24	2.83[−4] 8.78		
5^+	1.34[−4] 9.10	1.32[−4]	1.29[−4]	1.37[−4] 9.15	1.45[−4] 8.07	8.82[−5] 8.19		
3^-	7.67[−6] 26.40	7.78[−6]	7.70[−6]	8.23[−6] 18.92	8.31[−6] 21.78	8.82[−6] 14.54	8.60[−6] 22.96	8.53[−6]
4^-	4.00[−6] 11.67	4.16[−6]	4.10[−3]	4.18[−6] 11.48	5.03[−6] 7.71	3.82[−6] 1.89		
5^-	1.95[−6] 11.29	2.04[−6]		2.04[−6] 11.00	2.46[−6] 7.33	4.04[−6] 17.09		
$3d$	∼2.4[−7] 91.1		3.2[−8]	1.15[−7] 133.4	2.43[−7]			
$4d$	∼7.1[−8] 208.7			2.76[−8] 254.3	7.11[−8] 199.4			

σ_{max}, which is proportional to $(1+q^2)$, with other existing calculations. The agreement is in general satisfactory except for the $sp,23^-$ resonance, where σ_{max} from the present calculation is higher than the results from all other calculations. This discrepancy can be partially attributed to the difference in the calculated widths since σ_{max} is inversely proportional to the resonance width [see, e.g., Eq. (46) of Ref. [16]].

To summarize, the observed high-resolution He photoionization spectra near the $(sp,2n^-)$ and $(2pnd)\,{}^1P^o$ doubly excited resonances appear to agree qualitatively with the more elaborate theoretical results. An improved energy resolution is required for a more detailed quantitative comparison between theory and experiment for the resonance structures, especially at energies near the sharp dip in cross section on the high-energy side of the individual resonance.

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