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EVEN PARITY QUARTET AUTODETACHING STATES OF He^-

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Recently two groups have measured[1,2] the total photodetachment cross section of the metastable, (1s2s2p) $^4P^o$ state of He^- at several wavelengths between 10μ and 308 nm. Hazi and Reed[3] have obtained theoretical cross sections for the processes:

$$\begin{aligned} He^-(^4P^o) + h\nu \rightarrow & He(2^3S) + e(ks,kd) \\ & He(2^3P^o) + e(kp) \end{aligned}$$

from threshold (0.076 eV) to 3.0 eV photon energy. As part of these calculations, we have also studied the even parity, quartet, autodetaching states of He^- which are optically connected to the metastable $^4P^o$ state and which are associated with the n = 2 and n = 3 states of He.

In both the photodetachment and electron scattering calculations, we used extensive configuration interaction (CI) wavefunctions to describe the He target states, the He^- resonance states and the photodetachment continua. The Stieltjes moment-theory technique[4] was used to extract the partial photodetachment cross sections from the discrete representations of the electron scattering continua. The use of the Stieltjes technique allowed us to include both channel-channel coupling and fully correlated He ^3S and $^3P^o$ wavefunctions in the calculations.

The many-electron wave functions were built from orthonormal atomic orbitals which were linear combinations of Slater-type orbitals(STO). To construct the basis, we started with the (4s, 4p, 2d) "critical" basis of Bunge and Bunge,[5] which was adequate to describe He(2^3S), He(2^3P^o) and $He^-(^4P^o)$, and we augmented it with 9s, 7p and 9d diffuse STO's to approximate the scattering electron. The exponents of the augmenting functions were chosen in decreasing geometric sequences, i.e., 2s: $0.244\times2^{-n/2}$ n = 0, ...8; 2p: $0.106\times2^{-n/2}$ n = 0 ...6; and 3d: $0.2687\times2^{-n/2}$ n = 0, ...8. Complete CI calculations with the (4s, 4p, 2d) core basis gave -2.1746 and -2.1325 hartree for the energies of He(2^3S) and He(2^3P^o), respectively. The calculated ^3S - $^3P^o$ separation is 1.147 eV, in good accord with the exact value of 1.145 eV. To describe $He^-(^4P^o)$, we used all the configurations which could be constructed from the (4s, 4p, 2d) basis plus 20 additional configurations which contained one diffuse s and three diffuse p STO's. Our 120 term wave function gave -2.1774 hartree for the energy of $He^-(^4P^o)$, compared to the accurate value of -2.17807 hartree.[5] Our calculated electron affinity of He(2^3S) is 0.077 meV, which is identical to that obtained previously.[5]

Figure 1 shows the ^4P partial cross section representing the detachment of the 2s electron from $He^-(^4P^o)$ into the p-wave continuum. This channel exhibits an extremely large (~24×10^{-16} cm^2) and quite narrow peak about 10 meV above the 2^3P^o threshold. To identify the physical mechanism underlying this prominent feature of the $^4P^o \rightarrow {}^4P$ spectrum, we calculated independently the ^4P scattering phase shift using the close-coupling code IMPACT.[6] We used the same orbitals and the same 24-term He(2^3P^o) wave function as in the photodetachment calculations. Two

(1snd) ^3D pseudostates were included as closed channels. Figure 2 shows that, starting from the 2^3P^o threshold, the calculated phase shift rises rapidly over a narrow energy region to 2.5 radians, a behavior which indicates a resonance. Inspection of the corresponding wave function shows that this enhancement should be assigned to a $(1s2p^2)\ ^4P$ shape-resonance. A Breit-Wigner analysis placed the resonance at 10.6 meV above He(2^3P^o) and gave 7.0 meV for the width. These values are consistent with the shape of the detachment cross section shown in Fig. 1.

Previously, Holøein and Geltman[7] calculated the $(1s2p^2)\ ^4P$ state of He^- to be 0.2 eV below He(2^3P^o), contrary to the present results. With extensive CI wave functions containing 466 terms, we were not able to obtain a ^4P eigenvalue below He(2^3P^o), and the wave function associated with the lowest eigenvalue always represented a very low energy, 0.001 eV, scattering solution (see Fig. 2). Unpublished calculations by Bunge and Bunge also place the $(1s2p^2)\ ^4P$ state in the electron scattering continuum of He(2^3P^o).

In the energy region near the n = 3 states of He, we found only one even parity, quartet, Feshbach resonance: $(1s3p^2)\ ^4P$, which lies 0.18 eV below He($3\ ^3P^o$). For this state, our calculated binding energy of the resonant 3p electron is almost the same as that found by Oberoi and Nesbet[8] for the $(1s3s3p)\ ^4P^o$ Feshbach resonance. We did not find the $(1s3s3d)\ ^4D$ resonance which appeared in Oberoi and Nesbet's calculations[8] at 0.16 eV below He (3^3S). A possible reason for this discrepancy is the lack of f-type orbitals in our basis set. Additional calculations, using accurate wavefunctions for the n = 3 states of He, will be required to clarify this energy region.

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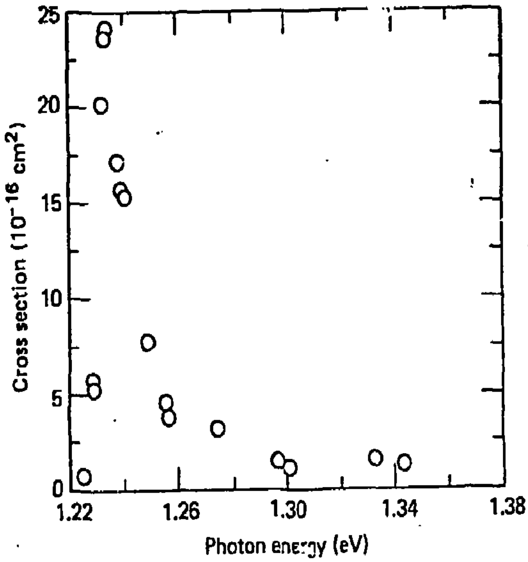

Fig. 1 ^4P partial cross section for $h\nu + He^-(^4P^o) \rightarrow He(2^3P^o) + e(kp)$. Energy relative to $He^-(^4P^o)$.

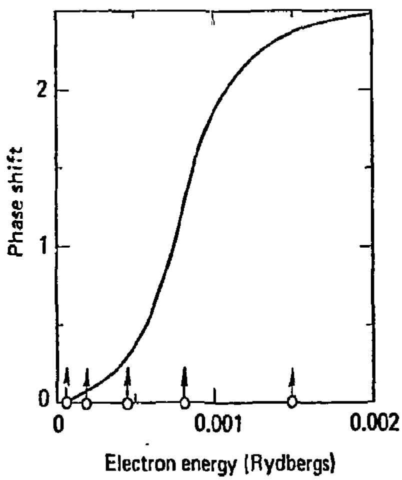

Fig. 2 ^4P phaseshift for the $He(2^3P^o) + e(kp)$ channel. The arrows indicate the energies of the discrete wave functions approximating the ^4P continuum in the Stieltjes calculations.