Electron-impact detachment from the H⁻ and O⁻ negative ions

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The electron-impact detachment from the H⁻ and O⁻ negative ions is calculated in lowest-order distorted-wave theory. The cross sections are found to be quite sensitive to the choice of polarization potential. Reasonable agreement between the distorted-wave theory and recent ion storage ring experiments for both H⁻ and O⁻ is obtained. [S1050-2947(96)10310-3]

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Recently electron-impact cross sections for detachment from H⁻ and O⁻ have been measured near threshold using a ion storage ring [1,2]. Both cross sections were found to rise rapidly from threshold to obtain peak values in the range from 500 to 3000 Mbarns. The experimental measurements were compared with theories based on a classical reaction model and a semiclassical tunneling model. In this Brief Report, we calculate the detachment cross sections using a standard quantum mechanical treatment based on lowest-order distorted-wave theory [3,4]. The method has been applied previously to calculate direct ionization cross sections for many atoms and their positive ions, with varying degrees of success. Of crucial importance for detachment from negative ions will be the choice of polarization potential for the continuum distorted waves.

The negative ion detachment cross sections were calculated using a recently developed configuration-resolved distorted-wave computer program [5]. The method may include multiconfiguration approximations for the target atom or ion, with orbitals calculated using Fischer's MCHF program [6]. The LS term-specific angular algebra is obtained from a modified version of the WEIGHTS program of Scott and Hibbert [7]. A triple partial wave expansion of the lowest-order scattering amplitude forms the basis of the cross section code. The many distorted waves needed to evaluate the various direct and exchange matrix elements are obtained as solutions to a radial differential equation of the form

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{Z}{r} + \frac{\ell(\ell+1)}{2r^2} + V_H(r) + V_X(r) + V_{pol}(r) - \frac{k^2}{2} \right)$$
$$\times P_{k\ell}(r) = 0, \tag{1}$$

where k is the linear momentum, ℓ is the angular momentum, Z is the atomic number, and atomic units are used. The direct Hartree potential $V_H(r)$ is constructed from the target orbitals, the semiclassical exchange potential [8] is given by

$$V_X(r) = \frac{1}{2}\left(\frac{k^2}{2} + \frac{Z}{r} - V_H(r) \right)$$
$$- \frac{1}{2}\sqrt{\left(\frac{k^2}{2} + \frac{Z}{r} - V_H(r) \right)^2 + 4\pi\rho}, \tag{2}$$

where ρ is the radial probability density for the target, and the polarization potential [9] is given by

$$V_{pol}(r) = -\frac{\alpha}{2}\frac{r^2}{(r^2+r_c^2)^3}, \tag{3}$$

where α is the dipole polarizability of the target and r_c is a cutoff radius generally taken to be the mean radius of the outermost orbital.

There are several choices for the number of target electrons, N, used to construct the scattering potentials found in Eq. (1) for the distorted waves. A long-time choice [3,4] has been what may be called a mixed V^N/V^{N-1} potential method. The scattering amplitude in the mixed potential approach requires the incident and scattered electrons to be calculated in a V^N potential, while the bound and detached electrons are calculated in a V^{N-1} potential. A recent choice [10,11] may be called a strict V^{N-1} potential method, where all the bound and continuum electrons are calculated in a V^{N-1} potential. For incident energies near threshold, where only the lowest angular momentum states contribute, the strict V^{N-1} potential method is in better agreement with a more exact time-dependent close-coupling treatment [12] for electron ionization of the neutral hydrogen atom than the mixed V^N/V^{N-1} potential method. The strict V^{N-1} potential
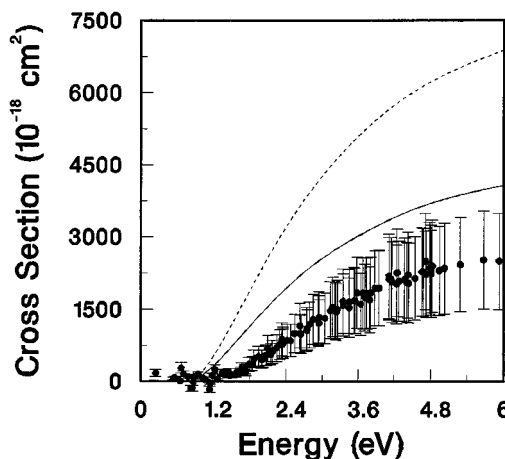

FIG. 1. Electron-impact detachment cross section for H⁻. Solid curve: distorted-wave method with polarization; dashed curve: distorted-wave method without polarization; solid circles: experimental measurements [1].
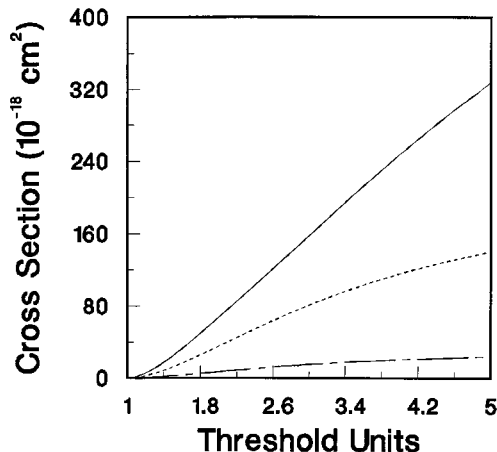

FIG. 2. Electron-impact detachment cross sections for O^-. Distorted-wave method with polarization for the $2p^5\ ^2P \rightarrow 2p^4\ ^3P$ transition is the solid curve, for the $2p^5\ ^2P \rightarrow 2p^4\ ^1D$ transition is the dashed curve, and for the $2p^5\ ^2P \rightarrow 2p^4\ ^1S$ transition is the dot-dashed curve. Threshold units are incident energy divided by the threshold energy for detachment.

distorted-wave method is the choice made here for the calculation of electron-impact detachment of negative ions in the threshold region.

Finally, due to the small threshold energies found in the detachment from negative ions (e.g., 0.75 eV for H^-), it is important to treat the long-range part of the Coulomb radial matrix elements using an analytical method. Integrals of the type

$$I = \int_R^\infty \frac{F_1(r)F_2(r)}{r^{\lambda+1}}dr, \tag{4}$$

where $\lambda \geq 0$ and $F_1(r)$ and $F_2(r)$ are continuum wave functions, are handled using the amplitude-phase method [13]. Numerical quadrature is used to obtain the full Coulomb radial integrals for 0 to R.

Electron-impact detachment cross sections for the $1s^2\ ^1S \rightarrow 1s^2S$ transition from H^-, calculated in the distorted-wave approximation, are shown in Fig. 1. The recent ion storage ring measurements [1] are also shown for comparison. The solid curve uses a polarization potential with $\alpha = 4.5$ and $r_c = 1.5$, the standard values for the polarizability and orbital mean radius of neutral hydrogen corresponding to the choice of V^{N-1} scattering potentials. The dashed curve uses just the static-exchange potential, ignoring polarization effects. The effects of distorted-wave polarization on the detachment cross section is quite large, reducing the static-exchange results and improving the agreement between theory and experiment. We note that a small reduction in the cutoff radius would move the distorted-wave theory into even better agreement with experiment.
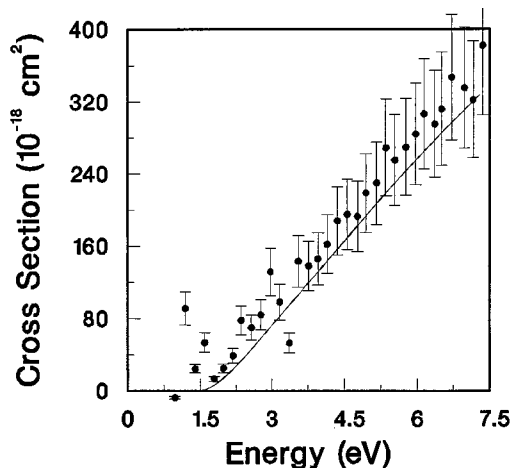

FIG. 3. Electron-impact detachment cross section for O^-. Solid curve: distorted-wave method with polarization summed over final states; solid circles: experimental measurements [2].

Electron-impact detachment cross sections for the $2p^5\ ^2P \rightarrow 2p^4\ ^3P$, ^1D, and ^1S transitions from O^-, calculated in the distorted-wave approximation, are shown in Fig. 2. The threshold energies are taken to be 1.46 eV, 3.43 eV, and 5.65 eV for the ^3P, ^1D, and ^1S final LS terms, respectively [14]. All the curves use a polarization potential with $\alpha = 4.9$ and $r_c = 1.2$, corresponding to the polarizability and outer orbital mean radius of neutral oxygen. In Fig. 3 the total detachment cross section from O^-, summed over all final LS terms, is compared with recent ion storage ring measurements [2]. The agreement between theory and experiment in the threshold region is excellent.

We regard the reasonable agreement found between the distorted-wave theory and the ion storage ring experiments for the detachment cross section from both H^- and O^- to be somewhat fortuitous. The size of the polarization effects indicate a strong correlation between the incident electron and the target, indicating that higher-order perturbation theory terms for the scattering amplitude could be important. In the future we hope to extend a recently developed nonperturbative approach [12] to electron-atom scattering so that we can make a more rigorous calculation of the electron-impact detachment process from negative ions.

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