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Ning-Yi Du
University of Colorado National Institute of Standards and Technology, Boulder, Colorado

Anthony F. Starace
University of Nebraska-Lincoln, astarace1@unl.edu

Min-Qi Bao
University of Nebraska - Lincoln

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Photodetachment of the $2p^2(^3P^e)$ state of H^-

Ning-Yi Du* and Anthony F. Starace†

Joint Institute for Laboratory Astrophysics, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado 80309-0440

Min-Qi Bao

Department of Physics and Astronomy, The University of Nebraska, Lincoln, Nebraska 68588-0111

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Results of semiempirical, adiabatic hyperspherical calculations are presented for the photodetachment cross section of the process $H^-\ 2p^2\ (^3P^e) + \gamma \rightarrow H(n=2) + e^-$ at photon energies in the range from threshold to 0.125 a.u. above. We find the detachment cross section to have a maximum value of 482 Mb at 25.7 meV above threshold, in good agreement with results of close-coupling calculations by Jacobs, Bhatia, and Temkin [Astrophys. J. **242**, 1278 (1980)]. In contrast to the close-coupling results, however, we find that the detachment cross section rises by a factor of more than 400 from its threshold value to its maximum.

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I. INTRODUCTION

The H^- ion has an excited state, usually designated as $2p^2(^3P^e)$, which has been shown theoretically to be bound below the $H(n=2)$ threshold [1-7]. Nearly all theoretical calculations place the electron affinity of this state between 9.53 meV [3] and 9.65 meV [4], with the latter value stemming from the lowest variational result for the energy of the state. Despite the importance of H^- as a fundamental example of an interacting three-body Coulomb system, this unique $^3P^e$ bound excited state has never been observed in the laboratory. The difficulty for experiment stems from the fact that (in LS-coupling) angular momentum and parity selection rules prohibit this state from decaying by autoionization; similarly, it cannot be produced in $e^- - H(1s)$ scattering experiments. The primary decay mode is by radiative detachment to the ground state of H [8–10]:

$$H^-\ 2p^2(^3P^e) \rightarrow H(1s) + e^- + \gamma\,. \tag{1}$$

In this process the detached electron and the emitted photon share the excess energy. The distribution of emitted photons peaks on the long-wavelength side of the Lyman-α transition in H [8–10]. The process inverse to that in Eq. (1), the radiative attachment process, has been predicted to be an efficient means of absorbing ultraviolet light in stellar atmospheres and in laboratory plasmas [9,11]. This inverse process has been observed in rocket measurements of the stellar absorption spectrum of Zeta Tauri [12]. An attempt to observe the decay process (1) under controlled laboratory conditions, however, gave negative results [13].

A much less probable decay process is photon emission to the $2s2p\ ^3P^o$ autoionizing state [4,8]:

$$H^-\ 2p^2(^3P^e) \rightarrow H^-\ 2s2p(^3P^o) + \gamma\,. \tag{2}$$

In this case, a discrete spectral line which peaks at a wavelength $\lambda = 3783\ \mathrm{cm}^{-1}$ is produced [4]. Because of the width of the autoionizing $^3P^o$ state, the spectral line has a width of 51 cm^{-1} [4]. Recently, Mercouris and Nicolaides [7] have studied the influence of resonant laser intensity and frequency on process (2) and its inverse.

Because the $H^-\ 2p^2\ (^3P^e)$ state has yet to be observed in the laboratory, it is of interest to make theoretical predictions for other processes involving this state. (For example, we note that very recently Mercouris and Nicolaides have carried out a theoretical study of two-photon, double photodetachment of the $^3P^e$ state [14].) In this paper, we present semiempirical, adiabatic hyperspherical results for photodetachment of the $^3P^e$ state in which the H atom is left in the $n=2$ state:

$$H^- 2p^2(^3P^e) + \gamma \rightarrow H(2s,2p) + e^-\,. \tag{3}$$

*Present address: Radiation Oncology Department, William Beaumont Hospital, 3601 West Thirteen Mile Road, Royal Oak, MI 48073-6769.

†Present address: Department of Physics and Astronomy, The University of Nebraska, 116 Brace Laboratory, Lincoln, NE 68588-0111.

This process has been studied by Jacobs, Bhatia, and Temkin [15], who performed a $1s$-$2s$-$2p$ close-coupling calculation that employed an 84-term Hylleraas-type bound state wave function for the $^3P^e$ state. Jacobs *et al.* [15] found an exceedingly large cross section for the photodetachment process (3). They attributed this large value to the threshold of the process, although their first calculated point was at 27.2 meV above the threshold.

Confirmation of these very interesting predictions is warranted because similar three-channel close-coupling calculations [16] for photodetachment of the ground state of H^- with excitation of $H(n = 2)$ did not give good agreement with experimental cross sections or with cross sections obtained by other more elaborate calculational methods (including adiabatic hyperspherical calculations) [17]. On the other hand, the use of semiempirical means to include correct electron affinities into adiabatic hyperspherical calculations has greatly improved their accuracy near threshold, at least in the case of multiphoton detachment processes for H^- [18]. For two- and three-photon detachment of H^- such results [18] agree very well with alternative calculational results of Proulx and Shakeshaft [19] as well as with results using state-of-the-art R-matrix methods [20]. For these reasons we feel the semiempirical, adiabatic hyperspherical method is a good one to employ for process (3).

In Sec. II we discuss briefly our theoretical method. In Sec. III we present our results for process (3), compare them with results of Ref. [15], and discuss in some detail the validity of the semiempirical adiabatic hyperspherical approximation for this process.

II. THEORY

This section can be very brief, as nearly all of the relevant theory has been presented elsewhere. Specifically, the type of wave functions employed in the current calculations have been described in detail in Ref. [21]. The adiabatic hyperspherical method has been presented in detail by several authors [22–25]. Formulas for the calculation of electric dipole transition matrix elements using adiabatic hyperspherical wave functions have been published [26]. Furthermore, a complete summary of the relevant theory for single-photon detachment of H^- has been given in Ref. [17]; in particular, Eqs. (3) – (19) of that reference apply directly to the current calculations and a summary is also given of the long-range dipole field effects [27,28] arising from the degeneracy of the H-atom energy levels. Moreover, the importance of semiempirically ensuring that the initial state has the correct electron affinity has been emphasized in Ref. [18].

In this section, then, we simply indicate the changes entailed in calculating the cross section for process (3) from the procedure described in Ref. [17]. These changes stem from the initial state's having $^3P^e$ symmetry in process (3) rather than the $^1S^e$ symmetry of the ground state considered in Ref. [17]. Thus, the differential cross sections for the $H(2s)$ and $H(2p)$ states resulting from the detachment process (3) are given by

$$\frac{d\sigma_{2\ell}}{d\Omega} = 4\pi^2 \omega\alpha k \sum_m |T^{(1)}_{2\ell m k}|^2 . \tag{4}$$

Here the transition amplitude $T^{(1)}_{2\ell mk}$ is defined in Eq. (17) of Ref. [17]. Through use of the Wigner-Eckart theorem, the angular integral in Eq. (19) of Ref. [17] may be expressed in terms of a reduced angular integral [29]. This allows one to express the amplitude $X^{(1)LM}_{n\ell,k\ell'}$ in Eq. (18) of Ref. [17] in terms of an amplitude $X^L_{n\ell,k\ell'}$, which is independent of magnetic quantum numbers, as follows:

$$X^{(1)LM}_{n\ell,k\ell'} \equiv (-1)^{L-M} \begin{pmatrix} L & 1 & L_0 \\ -M & 0 & M_0 \end{pmatrix} X^L_{n\ell,k\ell'} . \tag{5}$$

Here L_0, M_0 are the orbital angular-momentum quantum numbers for the initial $^3P^e$ state of H^-. Substituting Eq. (5) into Eq. (17) of Ref. [17], averaging over the initial state, and integrating over angles, we may express the $H(2s)$ and $H(2p)$ partial cross sections as

$$\sigma_{2\ell} = \frac{4\pi^2\omega\alpha}{3} \sum_{l',L} |X^L_{2\ell,k\ell'}|^2 \quad \text{for} \quad \ell = 0, 1, \tag{6}$$

where use has been made of standard formulas of angular-momentum algebra [30].

III. RESULTS AND DISCUSSION

Electric dipole selection rules restrict the final states for process (3) to $^3P^o$ for $H(2s)$ and to $^3P^o$ and $^3D^o$ for $H(2p)$. There are several adiabatic hyperspherical channels having these LS-coupling symmetries. Effective radial potentials for two important final-state channels are shown in Fig. 1 together with the effective radial potential for the $^3P^e$ initial state. One sees in Fig. 1 that the $^3P^o+$ channel is attractive, whereas the $^3D^o$ channel shown is repulsive. Other relevant potentials are the $^3P^o-$ and $^3P^o$(pd) radial potentials, which are shown elsewhere [31]. These are both repulsive $^3P^o$ potentials. The other $^3D^o$ potentials are not shown. They are so

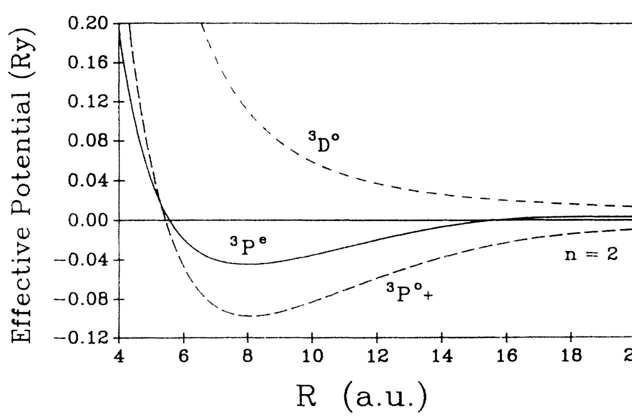

FIG. 1. Effective radial hyperspherical potentials $V_\mu(R)$ (in rydbergs) plotted vs the hyperradius R. All potentials converge asymptotically to the $H(n = 2)$ threshold, which is chosen as the zero of energy. Shown is the $^3P^e$ potential, which describes the H^- $2p^2(^3P^e)$ state, and two of the important potentials, $^3D^o$ and $^3P^o$ +, for describing the $H(n = 2)$ + e^- final states reached by photodetachment of the H^- $2p^2$ ($^3P^e$) state.

repulsive that they have no effect on the cross section results presented here. Note that the $^3P^e$ effective radial potential has been semiempirically lowered near its minimum so that the bound initial state has an electron affinity of 3.50×10^{-4} a.u., in agreement with that calculated by Drake [3].

Normally, the fact that there is only one attractive final state channel (i.e., $^3P^o$ +, shown in Fig. 1) would mean that essentially all of the transition amplitude could be accounted for by the transition $^3P^e \rightarrow {}^3P^o +$. Such is not the case here, however. The reason is the very broad radial extent of the $^3P^e$ state. As shown in Fig. 2(a), the $^3P^e$ state still has an amplitude of about 14% of its peak amplitude at a hyperspherical radius of 60 a.u. Furthermore, transitions to the attractive $^3P^o$ + channel are subject to extensive cancellations because of the first node in the continuum $^3P^o$ + radial wave function, shown in Fig. 2(b). (At higher energies, additional nodes play a role.) It turns out that the transition amplitude to the repulsive channels is actually about an order of magnitude stronger than to the attractive channel at the cross section maximum. The continuum radial wave function for one of these repulsive channels, $^3P^o$ −, is shown in Fig. 2(b).

Our adiabatic hyperspherical result for the photodetachment cross section for process (3) is shown in Fig. 3. Our predictions are compared with the three-state close-coupling results of Jacobs, Bhatia, and Temkin [15]. One sees quite good agreement between our results and the close-coupling results, except near threshold. At threshold (actually at a photoelectron kinetic energy of 3.4×10^{-3} meV), we predict a cross section value of 1.092×10^{-18} cm^2 which rises by a factor of 441 to a maximum of 4.816×10^{-16} cm^2 at a photoelectron kinetic energy of 25.7 meV above the H($n = 2$) threshold. This factor of 441 increase has two components. First, the photon frequency factor ω in Eq. (6) increases by about a factor of 4 from threshold to the cross section maximum (i.e., from $\omega = 3.50 \times 10^{-4}$ a.u. to 1.30×10^{-3} a.u.). Second, whereas the transition amplitude to the attractive $^3P^o$ + final-state channel is fairly constant over this energy range, the transition amplitude to the repulsive $^3P^o$ and $^3D^o$ channels become an order of magnitude more important, thereby increasing the cross section by two orders of magnitude.

Our results indicate that effects of attractive long-range dipole fields are of minor importance for this process. The $^3P^o$ + channel (whose effective radial potential is shown in Fig. 1) has such an attractive dipole field, which occurs in part because of the degeneracy of the H(2s) and H(2p) final-state energy levels [27,28]. Consequently the cross section at threshold is finite and may exhibit oscillations on a scale of $\ln k$, where k is the photoelectron's kinetic energy [28]. Reference [15] attributed the large cross section at its maximum to this

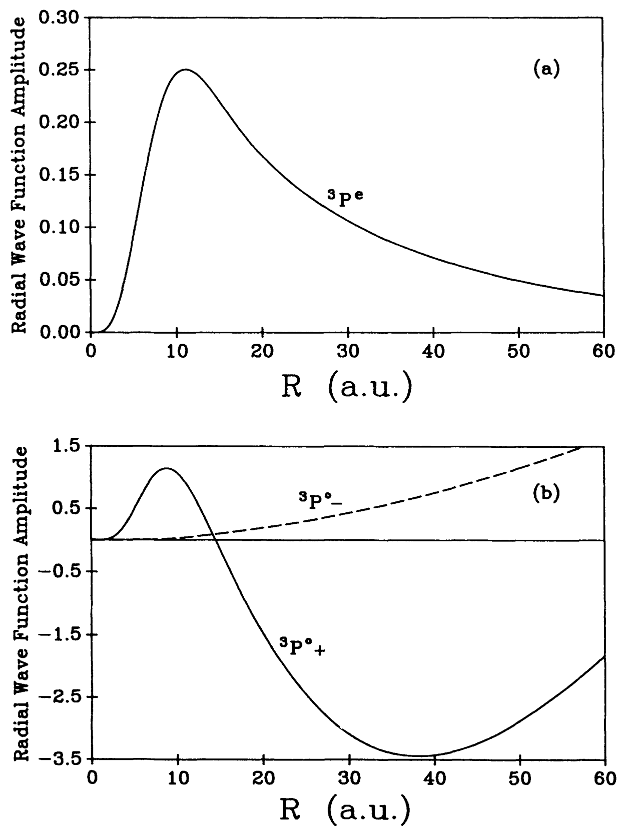

FIG. 2. Hyperspherical radial wave functions plotted vs hyperspherical radius R. (a) The bound $^3P^e$ radial wave function. (b) The continuum radial wave functions in the $^3P^o$ + and $^3P^o$ − final-state channels (normalized per unit energy in a.u.) for an electron kinetic energy $\frac{1}{2}k^2 = 1.36$ meV (i.e., $k = 10^{-2}$ a.u.).

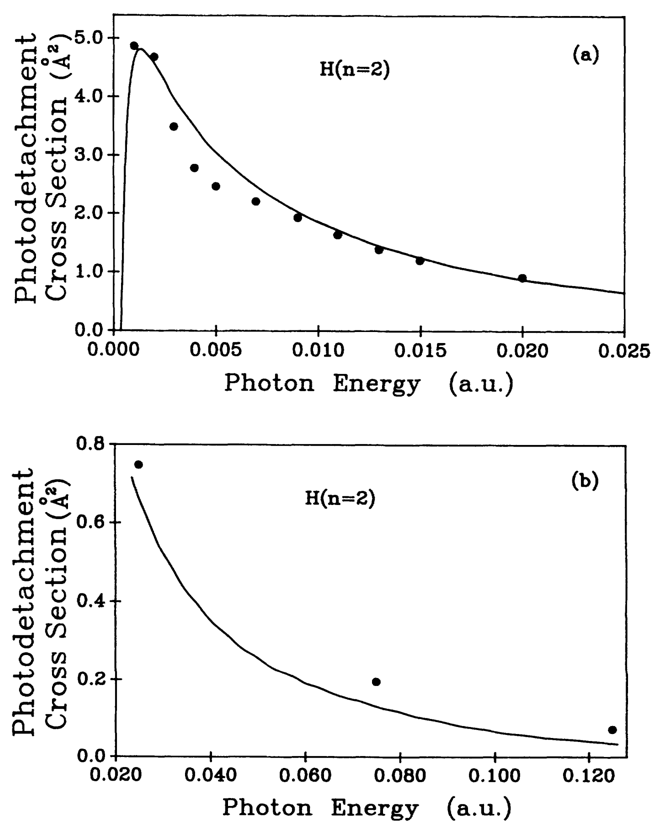

FIG. 3. Total photodetachment cross section for the process H$^-$ $2p^2$ ($^3P^e$) + $\gamma \rightarrow$ H($n = 2$) + e^-.

finite threshold value. Our calculations show that the cross section at threshold is very small. Rather, we find the long-range dipole field effect to be of minor importance for process (3) because of the large transition amplitudes at energies above threshold to channels having repulsive effective potentials. Processes for which effects of attractive long-range dipole interactions may be more observable are discussed elsewhere [17,29].

Last, we have considered the influence of nonadiabatic interactions upon our results. The good agreement (above the cross section maximum) between our results for process (3) and the close-coupling results [15] indicate the nonadiabatic effects are not very important for the *total* detachment cross section. They are, however, expected to be important for the *partial* cross sections for populating the $2s$ and $2p$ states. Such partial cross sections are highly sensitive to electron correlations, particularly since the $2s$ partial cross section is so much smaller than the $2p$ partial cross section and hence involves differences of alternative transition amplitudes. Because of the broad extent of the initial ${}^3P^e$ state, its wave function overlaps final-state wave functions for the interacting ${}^3P^o+$, ${}^3P^o-$, and ${}^3P^o$ (pd) channels. Even weak nonadiabatic interactions can strongly influence the magnitude of a small partial cross section. The adiabatic hyperspherical approximation predicts an H($2p$) partial cross section that agrees within about 10% with that predicted by Ref. [15]; it predicts an H($2s$) partial cross section, however, that is nearly an order of magnitude smaller than predicted by Ref. [15] in the vicinity of the cross section maximum. We expect that this large difference for the rather small H($2s$) cross section stems from our neglect of nonadiabatic coupling and that the close-coupling results [15] are more reliable (above the cross section maximum). For this reason, we only present total detachment cross sections. Recently, we have learned of hyperspherical close-coupling results [32] which confirm our expectations. Specifically, these results [32] confirmed the sharp rise we predict for the total cross section at threshold as well as our predicted magnitudes over the energy region shown in Fig. 3, thereby indicating that nonadiabatic effects are not significant for the total cross section. They confirm also the close-coupling results [15] for the partial cross sections (above the cross section maxima), thereby indicating the importance of nonadiabatic effects for the partial cross sections.

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