

stant, and that use of a Mott screening constant seems appropriate.

There is little indication that the octahedral sites remain occupied for any appreciable length of time in the deficient ( $x < 1.94$ ) concentrations. The hydride lanthanum resonance shows no quadrupolar effects, even as the protons start to diffuse. One can conclude, using a typical quadrupolar interaction as  $\omega_{Q0} \approx 3 \times 10^6$  sec<sup>-1</sup>, that the lifetime of a diffusing proton in an octahedral site in  $x < 1.94$  concentrations must be considerably less than  $10^{-7}$  sec at temperatures greater than 300°C where diffusion is evident. Diffusion-dependent quadrupolar effects exist only in concentrations with  $x > 2$  and are consistent with a treatment of the occupied octahedral site as a point defect.

The vanishing Knight shift of the proton resonance and the ease of diffusion of protons are not incompatible with the model of a positive hydrogen ion or proton.<sup>36</sup> We assume that the electron from the hydrogen is ionized to the conduction band localized on the La

<sup>36</sup> J. Friedel, *Phil. Mag.* **43**, 153 (1952); I. Isenberg, *Phys. Rev.* **79**, 736 (1950).

ions. This picture is consistent with the susceptibility and conductivity data if the conduction band, part of the  $6s-5d$  bands of La, becomes filled when  $3H/La$  are added. Martin and Rees<sup>19</sup> have suggested a similar band-structure for Zr-H. It is here suggested that in La-H the  $5d$  band of La is *split* into two bands in which the lower energy band can accommodate four electrons. A maximum of about four electrons in the lower part of the  $d$  band is consistent with the maximum solubility of hydrogen in the other group IIIB to VB transition metals.

#### ACKNOWLEDGMENTS

We express our appreciation to D. F. Holcomb for the use of a Varian NMR rf unit used in some of the measurements. Professor V. A. Fassel of Iowa State University kindly identified the hydrogen content in a La metal sample early in this work. E. L. Wolf and S. H. Christensen examined the impurity electron spin resonance of some of the hydride samples, and D. H. Smith helped construct the pulse apparatus used. We thank Dr. David Zamir for informative discussions.

## Empirical Analysis of the H<sup>-</sup> Photodetachment Cross Section\*

BAXTER H. ARMSTRONG

*Lockheed Missiles and Space Company, Palo Alto, California*

(Received 6 February 1963; revised manuscript received 1 April 1963)

The zero-range photoelectric cross section of Bethe and Peierls, corrected according to effective range theory, is fitted to the H<sup>-</sup> photodetachment cross section. The value of  $2.64 a_0$  obtained for the effective range agrees with values obtained from the wave-function calculations of Schwartz, Burke and Schey, and others. A more accurate formula for the detachment cross section is obtained by allowing for distortion in the final  $\rho$  state by means of an approximate formula for the phase shift. This formula agrees qualitatively with the close-coupling theory phase-shift results of Burke and Schey, and provides a photodetachment cross section that fits the experimental data slightly better than the results recently obtained by Geltman with an elaborate variational treatment. There are two adjustable parameters: the binding energy, and one parameter in the phase-shift formula. By a slightly different choice of the parameters than is required to fit the experimental data, close agreement can also be obtained with the Geltman results.

### I. INTRODUCTION

SINCE the original suggestions of Wildt<sup>1</sup> concerning the importance of H<sup>-</sup> photoabsorption in stellar atmospheres, much effort has gone into the calculation of H<sup>-</sup> wave functions and the H<sup>-</sup> photodetachment cross section. Since the early estimates<sup>2</sup> of the photodetachment cross sections were not very satisfactory, Chandrasekhar undertook a series of increasingly more elaborate

calculations.<sup>3</sup> He used successively better variational bound-state functions, with a plane-wave continuum function and with more accurate versions that allowed for distortion.

In 1956, Geltman<sup>4</sup> obtained a usefully accurate representation of the H<sup>-</sup> photodetachment cross section by means of a very simple model. He obtained both bound- and free-state wave functions for a cutoff Coulomb potential, and computed the cross section from these. Since then, renewed effort has been spent in obtaining

\* Supported by the Lockheed Missiles and Space Company Independent Research Program.

<sup>1</sup> R. Wildt, *Astrophys. J.* **89**, 295 (1959); **90**, 611 (1939).

<sup>2</sup> H. S. W. Massey and R. A. Smith, *Proc. Roy. Soc. London* **A155**, 472 (1936); D. R. Bates and H. S. W. Massey, *Astrophys. J.* **91**, 202 (1940).

<sup>3</sup> S. Chandrasekhar, *Astrophys. J.* **102**, 223 (1945); **102**, 395 (1945); **128**, 114 (1958); S. Chandrasekhar and D. D. Elbert, *ibid.* **128**, 633 (1958).

<sup>4</sup> S. Geltman, *Phys. Rev.* **104**, 346 (1956).

more accurate wave functions and in obtaining dipole-velocity and acceleration cross sections, in order to improve the agreement between theory and experiment.<sup>5</sup> Until recently, this effort had not yielded a completely satisfactory cross section: in fact, the results as reviewed by Branscomb<sup>5</sup> were very little better than Geltman's 1956 results.<sup>4</sup>

Geltman<sup>6</sup> has now carried the elaborate calculations still further; by use of a 70-parameter bound-state function and a many-term correlated free-state function, he has obtained essential agreement between theory and experiment within the errors of each. In obtaining agreement in this fashion, he concluded that one cannot expect high accuracy from a simple model such as he had used in 1956, or as Tietz proposed in 1961.<sup>7</sup> Although one might expect this *a priori*, at the expense of being somewhat empirical a simple model can be constructed that fits the data as well as Geltman's recent results. The wave functions are analytic, and the integrals leading to the photodetachment cross section are elementary. Because of its analytical simplicity, this model should be very useful in radiation transport calculations and in investigating other closely related photodetachment processes. The complicated polarization and correlation effects that require the many-parameter wave functions used by Geltman for explicit representation can be implicitly represented by use of the *p*-state phase shift and the binding energy as adjustable parameters.

The basis of this model was first used extensively for the deuteron.<sup>8</sup> Apparently, the emphasis on many-parameter variational wave functions has led to the neglect of this simple model in the H<sup>-</sup> problem.<sup>8a</sup> Its use can provide a coherent framework for the wide variety of elaborate calculations and perhaps yield more physical insight into the structure of H<sup>-</sup>.

Since it has been suggested<sup>9</sup> that an excited state affects the detachment process, our method can be used to ascertain if an empirical selection of the *p*-wave phase shift will yield a fit to the photodetachment cross section, with perhaps a different type of phase shift than a ground-state calculation would imply. In addition, the analytical simplicity of our approach yields another result that is obscured in the more detailed approaches: namely, a simple approximate relationship between the binding energy and the position of the maximum in the

photodetachment cross section. This result is useful from the experimental standpoint, since the threshold is difficult to observe. The position of the maximum is a much more accessible measure of the binding energy.

## II. ANALYSIS

### A. The Bound-State Wave Function

For a short-range potential  $V$ , such as exists in a negative ion, the solution to the Schrödinger equation with  $V=0$  should yield a fairly accurate representation (except for normalization) of the wave function of one of the two electrons<sup>10</sup> outside the range of this potential. Furthermore, for the photodetachment process, the region close to the origin, where this wave function becomes inaccurate, should not contribute appreciably to the matrix element. It is essentially weighted by a factor of  $r$  in addition to the volume element, and also the final continuum state has a long "range." Hence, we will use the<sup>11</sup>  $V=0$  solution for all  $r$ , rather than just for  $r>r_0$  (where  $r_0$  is some small matching radius) as did Geltman.<sup>1</sup>

This situation is well known in nuclear physics where it has been exploited particularly in application to the deuteron.<sup>8</sup> In the atomic case, ample evidence that the region near the coordinate origin may not contribute to radiative cross sections is provided by the success of the Coulomb approximation of Bates and Damgaard<sup>12</sup> (and its extension to the photoelectric case by Burgess and Seaton<sup>13</sup>).

The solution that we propose to use for H<sup>-</sup> is well known to be, for a bound *s* state,

$$\psi_b(r) = N e^{-\epsilon^{1/2}r}/r = \epsilon^{1/2} N h_0^{(1)}(i\epsilon^{1/2}r),$$

where  $N$  is a normalization constant,  $\epsilon = 2mE_b/\hbar^2$ , where  $E_b$  is the binding energy, and  $h_0^{(1)}$  is a spherical Hankel function. If we normalize  $\psi_b(r)$  to unity over all  $r$ , we obtain for the normalization constant  $N$  the value  $\epsilon^{1/4}/(2\pi)^{1/2}$ . Because of the singular behavior of  $h_0^{(1)}$  at the origin, this normalization will be incorrect. Therefore, we take for  $N$  the value  $\epsilon^{1/4}f/(2\pi)^{1/2}$ , where the error factor  $f$  can be evaluated by comparison with a wave function accurate for small  $r$ , or by empirical adjustment of the photodetachment cross section. This normalization is discussed in detail by Bethe and

<sup>5</sup> This work is reviewed and extensive references cited by L. M. Branscomb, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962).

<sup>6</sup> S. Geltman, *Astrophys. J.* **136**, 935 (1962).

<sup>7</sup> T. Tietz, *Phys. Rev.* **124**, 493 (1961).

<sup>8</sup> H. A. Bethe and R. Peierls, *Proc. Roy. Soc. London* **A148**, 146 (1935); H. A. Bethe and C. Longmire, *Phys. Rev.* **77**, 647 (1950).

<sup>8a</sup> *Note added in proof.* After this paper was submitted, the paper of Ohmura and Ohmura [*Phys. Rev.* **118**, 154 (1960)], of which I was unaware, was brought to my attention. In this paper, the authors have already pointed out the relatively good agreement with the Smith and Burch data of the zero-range approximation with  $r_0 \cong 2.64$ . Our Eq. (5) is thus identical with their Eq. (8). The *p*-state phase shift correction is the essentially new contribution of the present article.

<sup>9</sup> A. Dalgarno and R. W. Ewart, *Proc. Phys. Soc. (London)* **80**, 616 (1962).

<sup>10</sup> H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press Inc., New York, 1957). The discussion of Sec. 34 enables one to draw this conclusion. See especially Eqs. (34.3), (34.6), and (34.7).

<sup>11</sup> We will presently show, in Tables II and III, that the extra effort of including potential structure near the origin does not necessarily improve the fit to the experimental data. This, however, is an *a posteriori* conclusion and could not have been verified prior to the experimental work of Burch and Smith in 1959 (Ref. 15). Also, of course, a more accurate treatment near the origin is required in order to obtain theoretically the proper normalization of the wave function.

<sup>12</sup> D. R. Bates and A. Damgaard, *Phil. Trans. Roy. Soc. London* **A242**, 101 (1949).

<sup>13</sup> A. Burgess and M. J. Seaton, *Mon. Not. Roy. Astron. Soc.* **120**, 121 (1960).

Longmire,<sup>8</sup> who also show explicitly that our  $f^2$  is given by

$$f^2 = (1 - \epsilon^{1/2} r_0)^{-1}, \quad (1)$$

where  $r_0$  is the well-known "effective range."

The complete bound-state wave function that we will use is therefore given by

$$\psi_b(r) = \frac{\epsilon^{1/2} f}{(2\pi)^{1/2}} \frac{e^{-\epsilon^{1/2} r}}{r}. \quad (2)$$

### B. Plane-Wave Final-State Cross Section

If we compute the cross section using Eq. (2) for the bound-state wave function and a plane wave  $e^{i\mathbf{k}_e \cdot \mathbf{r}}$  for the final continuum state of an electron with momentum  $\mathbf{p}_e = \hbar \mathbf{k}_e$  according to the well-known rules,<sup>14</sup> the differential cross section per electron turns out to be

$$\frac{d\sigma_{pw}}{d\Omega} = \frac{16e^2 f^2}{mc\omega} \frac{E_b^{1/2} (\hbar\omega - E_b)^{3/2} \sin^2\theta \cos^2\varphi}{[2\hbar\omega + (\hbar\omega)^2/mc^2 - 2\hbar\omega p_{ec} \cos\theta/mc^2]^2}. \quad (3)$$

We have used the conservation relation

$$\hbar\omega = E_b + p_e^2/2m \quad (4)$$

between the photon energy  $\hbar\omega$  and the sum of the electron binding and kinetic energies. If  $\mathbf{\kappa}_\gamma$  is the photon propagation vector ( $|\mathbf{\kappa}_\gamma| = \omega/c$ ) and  $\mathbf{e}$  is a unit photon polarization vector, then  $\theta$  is the angle between  $\mathbf{\kappa}_\gamma$  and  $\mathbf{p}_e$ , and  $\varphi$  lies between the  $\mathbf{p}_e$ ,  $\mathbf{\kappa}_\gamma$  plane and the  $\mathbf{e}$ ,  $\mathbf{\kappa}_\gamma$  plane.

At present, we are interested in photon and electron energies for which  $\hbar\omega/mc^2$  and  $p_e/mc$  are both small. With this restriction, Eq. (3) can be integrated easily to yield the following approximate expression for the total photodetachment cross section per electron:

$$\begin{aligned} \sigma_{pw}(\omega) &= \frac{16\pi f^2}{3} \left( \frac{e^2 \hbar}{mc} \right) \frac{E_b^{1/2} (\hbar\omega - E_b)^{3/2}}{(\hbar\omega)^3} \\ &= 0.93163 f^2 \times 10^{-16} (\text{eV cm}^2) \frac{E_b^{1/2} (\hbar\omega - E_b)^{3/2}}{(\hbar\omega)^3}. \end{aligned} \quad (5)$$

This result is the zero-range photoelectric cross section of Bethe and Peierls. A factor of two difference appears in  $\text{H}^-$  relative to the deuteron for which their calculations were made. In the  $\text{H}^-$  case, the coordinate system for the two electrons is fixed on the proton which is very heavy in comparison so that the reduced mass of each electron is effectively its laboratory mass. In the case of the deuteron, the two constituents are almost equally massive so that the reduced mass that enters the formula is  $M_p/2$ , where  $M_p$  is the mass of the proton. The dipole moment for the proton in the deuteron is  $r/2$  rather than  $r$  as in  $\text{H}^-$  and the parameter  $\epsilon$  in the wave function depends on the reduced mass. Some of

<sup>14</sup> W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1954), 3rd ed.

TABLE I. Comparison of the asymptotic bound-state wave function  $\psi_b(r)$  (with binding energy  $E_b = 0.747$  eV) for  $\text{H}^-$  with Geltman's 1956 wave function  $\varphi_G(r)$ .  $f$  is the normalization correction factor that is shown by this comparison to be 1.14.

$r$	$\psi_b(r)/f$	$\varphi_G(r)$	$\frac{\varphi_G(r)}{\psi_b(r)/f}$
0.5	0.3435	0.266	0.775
1.0	0.1528	0.171	1.12
2.0	0.06043	0.0689	1.14
3.0	0.03187	0.0364	1.14

these effects cancel so that only a net factor of two difference appears.

Differentiation of Eq. (5) yields the relation (independent of the normalization error factor  $f$ )

$$\lambda_m = hc/2E_b, \quad \text{or} \quad h\omega_m = 2E_b, \quad (6)$$

between the binding energy  $E_b$  and the wavelength or photon energy at the maximum of the cross section.

The experimental data<sup>15</sup> have a maximum that appears to lie between

$$1.4 \leq h\omega_m \leq 1.6 \text{ eV}.$$

Taking the mean of these values yields  $E_b = 0.75 \pm 0.5$  eV; however, a least-squares analysis, for example, could be performed on the data to reduce the error considerably below that of this visual estimate.

### C. The Normalization Factor $f$

We now come to a discussion of the normalization problem. In Table I we present a comparison of  $\psi_b(r)/f$  and Geltman's 1956 wave function. His binding energy value of 0.747 eV was used in making this comparison. The value of  $f$  obtained thereby is  $f = 1.14$ . Using the slightly larger value 1.15 in the cross-section formula Eq. (5) multiplied by two to account for the two electrons (presumed equivalent in Geltman's formulation), and the binding energy value  $E_b = 0.75$  eV, we obtain the results shown in Table II. Our formula, Eq. (5), for  $\sigma_{pw}$  is compared to Geltman's 1956 cross section, labeled  $\sigma_G'$  in this table. The two are seen to agree quite closely. Furthermore, this curve is in approximate agreement (10% or better) with the normalized experimental data on the basis of any reasonable normalization of the latter (on this point, cf., Ref. 5). A plot of formula (5) for the cross section versus photon energy in eV is shown in Fig. 1 along with the experimental data (open circles) normalized according to the theoretical results listed by Branscomb.<sup>5</sup> Now the effective-range formula, Eq. (1), is valid for the one-body problem, rather than the two-body formulation employed by Geltman<sup>4</sup> in obtaining the wave function we have listed in column 3 in Table I. Also, as stated in Sec. II A (cf. footnote 10) it is the one-body model

<sup>15</sup> Stephen J. Smith and David S. Burch, Phys. Rev. **116**, 1125 (1959).

that we propose to use here. That is to say, for purposes of the present analysis one electron can be considered to be represented by a delta function at the origin, and the other to be represented by Eq. (2). With this in mind, we must multiply the value of  $f^2$  obtained from the above comparison by two to account for the fact that in our formulation only one electron participates in the detachment process (at the energies we consider). Therefore, the value of  $f^2$  to be inserted into Eq. (1) is given by  $f^2 \cong 2 \times (1.15)^2 = 2.65$ . This value of  $f^2$  yields  $r_0 = (1 - 1/f^2)/\epsilon^{1/2} = 2.64a_0$ .

Burke and Smith<sup>16</sup> give a plot of  $\kappa \cot \delta$  for the singlet electron-hydrogen atom state according to four different methods of calculation. The slopes of all four results are in reasonable agreement yielding  $r_0 = 2.6a_0$  to  $3.0a_0$  (calculated directly from the plots give by Burke and Smith). Therefore, our empirical value is in agreement with the theoretical effective-range values.

#### D. Distorted Final-State Cross Section

As can be seen from Fig. 1, Eq. (5) for the photodetachment cross section is too small on the low-frequency side of the maximum and too large on the high-frequency side. An attempt to improve this result is made by using the final-state ( $l=1$ ) wave function<sup>17</sup>

$$u_f(r) = \cos \delta_1 j_1(\kappa_e r) - \sin \delta_1 n_1(\kappa_e r), \quad (7)$$

TABLE II. Comparison of our plane-wave result  $\sigma_{pw}$  from Eq. (5) with Geltman's 1956 result, labeled  $\sigma_{G'}$ , for the photodetachment cross section as a function of the wavelength  $\lambda$  in microns.

$\lambda$ ( $\mu$ )	$\sigma_{G'}$ ( $10^{-17}$ cm <sup>2</sup> )	$\sigma_{pw}$ ( $10^{-17}$ cm <sup>2</sup> )
1.6533	...	...
1.5158	0.69	0.686
1.3994	1.54	1.53
1.2996	2.26	2.25
1.2131	2.83	2.82
1.0706	3.57	3.56
0.9581	3.95	3.93
0.8669	4.09	4.05
0.7916	4.10	4.07
0.6744	3.91	3.87
0.5874	3.62	3.58
0.5204	3.31	3.27
0.4236	2.76	2.72
0.3572	2.31	2.28
0.2566	1.58	1.55
0.2002	1.15	1.13
0.1391	0.69	0.698
0.0864	0.33	0.360

<sup>16</sup> P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).

<sup>17</sup> The present analysis has been based on a pure short-range formalism for simplicity, and because the results suggest that short-range effects dominate the over-all corrections to the zero-range photodetachment cross section. Very near the threshold, long-range polarization forces may be expected to become important. For high accuracy in the threshold region our analysis will probably require modifications along the lines suggested by T. F. O'Malley, L. Spruch, and C. Rosenberg, J. Math. Phys. **2**, 491 (1961).

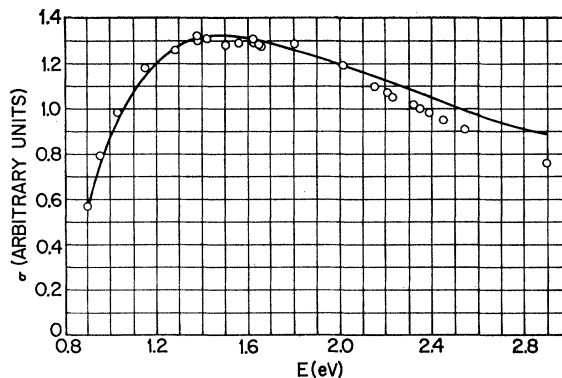


Fig. 1. H<sup>-</sup> plane-wave photodetachment cross section  $\sigma_{pw}$  in arbitrary units versus photon energy  $E$  in eV. The theoretical curve (solid line) is normalized to the experimental data in the vicinity of the maximum. A plane-wave final state and a binding energy  $E_b = 0.745$  eV have been assumed.

instead of a plane wave ( $j_1$  and  $n_1$  are spherical Bessel and Neumann functions, respectively, and  $\delta_1$  is the  $p$ -state phase shift). We note, for purposes of normalization, that Eq. (7) has the asymptotic form  $[\sin(\kappa_e r - \pi/2 + \delta_1)]/\kappa_e r$ . The appropriate formula for the total dipole-length cross section has been given by Geltman. In our notation, it becomes, per electron,

$$\sigma_{dl} = \frac{32\pi^2}{3} \left( \frac{\omega \kappa_e}{a_0 c} \right) \left| \int \psi_0(r) u_f(r) r^3 dr \right|^2, \quad (8)$$

where  $\psi_b(r)$  is given by Eq. (2) and  $u_f(r)$  is given by Eq. (7). The integration is elementary and leads to the Bethe-Longmire<sup>8</sup> result (except that we have not made the small-angle approximation as did those authors):

$$\sigma_{dl}(\omega) = \frac{16\pi f^2 E_b^{1/2} (\hbar\omega - E_b)^{3/2}}{3 (\hbar\omega)^3} \left( \frac{e^2 \hbar}{mc} \right) \times \left[ \cos \delta_1 + \frac{(\epsilon + 3\kappa_e^2) \epsilon^{1/2}}{2\kappa_e^3} \sin \delta_1 \right]^2. \quad (9)$$

We note that the same result is obtained whether one uses Eq. (7) for the free wave function or its asymptotic form, as did Bethe and Longmire. This lends further verification to the relative independence of the matrix element in Eq. (8) on the value of its integrand near the origin.

The factor in brackets represents the correction to the Bethe-Peierls result, Eq. (5). If we set

$$\begin{aligned} \chi_0 &\equiv E_b/Ry, \\ \chi &\equiv \hbar\omega/Ry, \\ \alpha &\equiv e^2/\hbar c, \\ a_0 &\equiv \hbar^2/me^2, \\ g(\chi) &\equiv \tan \delta_1 / \kappa_e^3 a_0^3, \end{aligned}$$

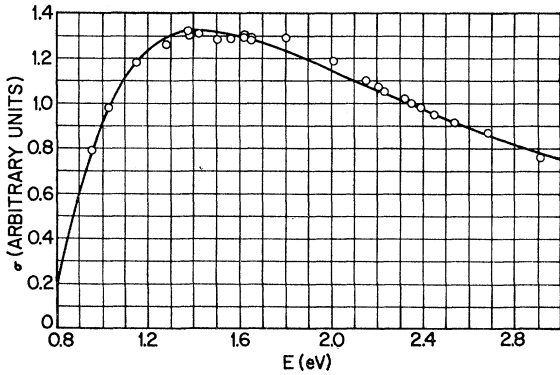


FIG. 2.  $H^-$  dipole-length photodetachment cross section  $\sigma_{d1}$  in arbitrary units versus photon energy  $E$  in eV. The theoretical curve (solid line) is normalized to the experimental curve in the vicinity of the maximum. A one-parameter ( $g_0$ ) empirical formula for the phase shift is assumed. The values  $g_0=4.7$  a.u. and binding energy  $E_b=0.745$  eV have been selected for a best fit to the data.

in Eq. (9), the result is

$$\sigma_{d1}(\chi) = \frac{32\pi}{3} f^2 \alpha a_0^2 \frac{\chi_0^{1/2} (\chi - \chi_0)^{3/2}}{\chi^3} \times \cos^2 \delta_1 [1 + (3\chi - 2\chi_0) \chi_0^{1/2} g(\chi) / 2]^2. \quad (10)$$

Now in the small-angle, low-energy approximation<sup>18</sup>

$$\sin \delta_1 \cong \tan \delta_1 = g_0 \kappa_e^3 a_0^3,$$

where  $g_0$  is a constant,  $g(\chi)$  is just the constant  $g_0$ . The correction to the plane-wave result is then

$$[1 + (3\chi - 2\chi_0) \chi_0^{1/2} g_0 / 2]^2.$$

This correction will not materially improve the over-all fit to the cross section. Figure 1 shows that what is needed is a correction that increases the plane-wave result on the low-frequency side of its maximum (at  $\chi = 2\chi_0$ ) and decreases it on the high-frequency side. For example, a correction factor  $[1 + \beta(2\chi_0 - \chi)]^2$ , with  $\beta$  a constant, will perform this service. We, therefore, set

$$g(\chi) \equiv \tan \delta_1 / \kappa_e^3 a_0^3 \cong (2\chi_0 - \chi) g_0 / (3\chi - 2\chi_0), \quad (11)$$

where  $g_0$  is a constant, in order to obtain an empirical fit to the data valid at energies somewhat higher than the threshold approximation  $g(\chi) = \text{const}$ . With this relationship, Eq. (10) now becomes, for small  $\delta_1$ ,

$$\sigma_{d1}(\chi) = \frac{32\pi f^2}{3} \alpha a_0^2 \frac{\chi_0^{1/2} (\chi - \chi_0)^{3/2}}{\chi^3} \times [1 + g_0 \chi_0^{1/2} (2\chi_0 - \chi) / 2]^2. \quad (12)$$

The solid line in Fig. 2 is a plot of Eq. (12) versus photon energy in eV for  $g_0=4.7$ , and  $E_b=0.745$  eV. It has been normalized to fit the experimental data (open circle)

<sup>18</sup> This is the pure short-range form consistent with Eq. (7). We have neglected polarization effects as stated in the preceding footnote.

as given by Smith and Burch<sup>15</sup> and appears to give a slightly better fit than Geltman's<sup>6</sup> recent elaborate treatment. The discrepancy of the two experimental points at 1.8 and 2.0 eV (6900 and 6200 Å) with the theoretical curve also appears in Geltman's results (Figs. 5 and 6 of Ref. 6). Table III presents a comparison of our  $\sigma_{d1}$  as given in Eq. (12) with the recent "best" theoretical results (dipole velocity) labeled  $\sigma_G$  as quoted by Geltman.<sup>6</sup> Column (a) of Table III lists the ratio  $\sigma_{d1}/\sigma_G$  for our "best" choice of parameters  $E_b=0.745$  eV and  $g_0=4.7$ , and column (b) lists this ratio for  $g_0=3.6$  and the variational value of  $E_b=0.75416$  eV. This value of  $E_b$  and the smaller value of  $g_0$  appear to give the best fit to Geltman's results. Our  $\sigma_{d1}$  has been normalized to agree with  $\sigma_G$  in the region around the peak of the curve. Over the frequency region where experimental data exist (set off by asterisks in Table III), the relative agreement of the two calculations is within 6% for our choice of parameters in column (a), and within 1% for the choice of variational energy and smaller phase shift of column (b). From the form of our result, Eq. (12), it can be readily determined that manipulation of the phase-shift parameter  $g_0$  results in increasing  $\sigma$  on one side of the peak and decreasing it on the other. Thus, the arbitrariness of the fit is limited. The two calculations differ significantly outside the region for which experimental data exist. On the high-frequency side (beyond  $h\nu=2.9$  eV) our result undoubtedly becomes poor, as we cannot expect the simple expression, Eq. (11), for the phase shift to remain valid over an extensive energy range. Indeed, this expectation is borne out by a comparison, presented in the next section, of Eq. (11) with the phase shift as determined theoretically.

Consequently, one cannot expect our analysis to be carried on to higher energy without some modification or improvement in the representation of the phase shift.

On the low-frequency side, the last entry in column (b) of Table III at  $\lambda=1.6 \mu$  does not fit smoothly onto the others. (Although it is sensitive to the exact value

TABLE III. A comparison of the distorted dipole-length  $H^-$  photodetachment cross section  $\sigma_{d1}$  [Eq. (12)] with the "best" dipole-velocity values  $\sigma_G$  as given by Geltman.<sup>6</sup>  $\sigma_{d1}$  has been normalized to  $\sigma_G$  at the peak. The experimental data<sup>b</sup> lie in the wavelength range between the asterisks (\*). For column (a), the parameters are  $E_b=0.745$  eV,  $g_0=4.7$ ; for column (b),  $E_b=0.75416$  eV and  $g_0=3.60$ .

$\lambda(\mu)$	$\sigma_{d1}/\sigma_G$ (a)	$\sigma_{d1}/\sigma_G$ (b)	$\lambda(\mu)$	$\sigma_{d1}/\sigma_G$ (a)	$\sigma_{d1}/\sigma_G$ (b)
0.1	0.40	0.57	0.9	1.00	0.989
0.2	0.84	0.94	1.0	1.01	0.991
0.3	0.94	0.997	1.1	1.02	0.987
0.4*	0.96	1.00	1.2	1.04	0.989
0.5	0.99	1.01	1.3*	1.06	0.990
0.6	0.99	1.01	1.4	1.11	1.00
0.7	1.00	1.00	1.5	1.24	1.04
0.8	1.00	0.994	1.6	1.40	0.81

<sup>a</sup> Ref. 6.  
<sup>b</sup> Ref. 15.

of  $E_b$ , since it is so near threshold, the small difference between the more appropriate Schwartz value<sup>6</sup> of  $E_b$  and the Pekeris value that we have used is not significant.) This discrepancy may arise from our neglect of polarization effects.

The normalization situation for Eq. (12) is essentially the same as in the plane-wave case. The phase-shift correction does not alter the value of  $f^2$  appreciably relative to the plane-wave case. This is particularly true in view of the uncertainty in the absolute normalization of the experimental data.

### E. Independent Tests and Comparisons

Our approximate plane-wave cross section, Eq. (5), can be tested in the sum rules<sup>5</sup>

$$(mc/e^2\pi) \int \sigma(\nu) d\nu < 2, \quad (13)$$

$$(mc/\pi\hbar a_0) \int [\sigma(\nu)/\nu] d\nu < 14.2, \quad (14)$$

quite easily, since the integrations can be performed analytically. The result for the integral in Eq. (13) is  $1.99 f^2$ , or  $2.63$ , and for the integral in Eq. (14) is  $12.1 f^2$ , or  $\sim 16$ . As might be expected, the uncorrected cross section overestimates these sums. Our corrected cross section, Eq. (12), cannot be tested with our approximation, Eq. (11), for  $\sin \delta_1$  (unless a cutoff is employed), as the integral diverges. In order to make this test, the correct high-energy behavior of  $\delta_1$  would be required.

The phase-shift result we have obtained does turn out to be quite different from the results obtained if the hydrogen atom is assumed to be in its ground state. The solid line in Fig. 3 shows a plot of  $\delta_1$  as given by Eq. (11) versus  $\kappa_e^2$ , the energy of the ejected electron (in a.u.). The dashed line is the close-coupling result of Burke and Schey<sup>19</sup> with which it is in qualitative agreement, and this close-coupling model includes virtual excitation to the  $2s$  and  $2p$  states. Qualitative agreement is all that can be expected, as the close-coupling results, while probably the best available, are still very approximate. The phase shifts obtained in the static (ground-state) approximation are shown in Fig. 14 of Ref. 16 and they are quite different from the curves presented here in Fig. 3.

As we have noted in Sec. II C, our result for the

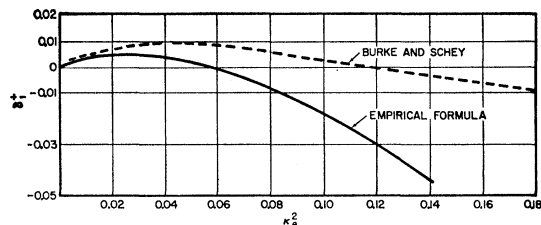


FIG. 3. A comparison of the empirical phase-shift formula (in a.u.)  $\delta_1^+ = g_0(\epsilon - \kappa_e^2)\kappa_e^3 / (\epsilon + 3\kappa_e^2)$  for the singlet  $p$  state with the close-coupling results of Burke and Schey (Ref. 19).

effective range  $r_0$  is in agreement with the scattering-theory predictions if we assume that just one of the two H<sup>-</sup> electrons participate in the detachment process (up to  $\hbar\omega = 2.9$  eV, the upper limit of our analysis). Presumably the other electron is nearly hydrogenic, with a much more rapid asymptotic decline of its wave function than the one we consider. Its contribution to the total cross section then would not become significant until the photon energy approaches the magnitude of the hydrogen binding energy.

### III. CONCLUSION

Although it appears possible to fit the experimental data somewhat more closely by our method than by the first-principles method of Geltman, it is doubtful that the slight difference in binding energy obtained thereby can as yet be considered significant. When more experimental data are available, such a fit can become more conclusive. We note, however, that this difference is not merely a result of the approximate mathematics of the fit. The much closer agreement with Geltman's result, which is obtained when the binding energy is taken to be (very nearly) the value appropriate to this calculation, bears out this conclusion.

The comparisons and simple analytic formulas we have given should make the method presented a useful exploratory tool for stellar atmospheres and for other detachment processes of the  $l=0$  to  $l=1$  type. However, without a first-principles computation of  $\delta_1$ , this method remains empirical and is merely a useful adjunct of the more detailed methods. Its usefulness is augmented by its simplicity and intuitive clarity compared to the elaborate variational calculations.

### ACKNOWLEDGMENTS

The author acknowledges with appreciation the valuable suggestions and criticism of Dr. Sydney Geltman, and the computational assistance of Mrs. Carole Chase.

<sup>19</sup> P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).