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Eikonal Distorted-Wave Calculation for the Excitation of H by He

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The eikonal distorted-wave Born approximation developed recently by Chen, Joachain, and Watson is applied to hydrogen excitation by helium impact in the intermediate-energy range. The differential and total cross sections for the excitation of the hydrogen atom to the $2s$, $2p_{\pm}$, or $2p_0$ state by helium impact are presented. These results are compared to experiment and previous calculations. The differential cross section for the excitation of hydrogen to the $2s$ state compares well with the experimental data of Thomas and Sauers in shape and slope, but has a discrepancy in magnitude.

I. INTRODUCTION

The eikonal distorted-wave Born approximation (DWBA), which was developed by Chen, Joachain, and Watson[1] for inelastic electron-atom scattering at intermediate energies, has recently been applied to inelastic H-H collisions in the intermediate energy range by Shields and Peacher.[2] They found that the total inelastic cross sections obtained from the eikonal DWBA were comparable to the results obtained from the multistate impact-parameter calculations of Flannery.[3] However, the eikonal DWBA yields a differential cross section which could only be compared to a Born calculation since the multistate impact-parameter approach does not yield a differential cross section explicitly.[4] Recently, Thomas and Sauers[5] have experimentally determined the differential cross section for the excitation of hydrogen from the $1s$ to the $2s$ state by impact on helium at 10 keV. In this paper we apply the eikonal DWBA to the excitation of hydrogen in a hydrogen-helium collision. The differential cross section for the $2s$ excitation of hydrogen at 10 keV is compared to the experimental results. The eikonal DWBA gives the correct shape and slope for the differential cross section but there is a discrepancy in the magnitudes.

In 1954 Moisewitch and Stewart[6] applied the first Born approximation to the H-He collision for the processes

$$\mathrm{H}(1s)+\mathrm{He}(1\,^1S)\rightarrow\mathrm{H}(2s,2p_0,2p_{\pm})+\mathrm{He}(1\,^1S)\,. \quad (1.1)$$

In 1969, Orbeli, Andreev, Ankudinov and Dukelskii[7] presented the total cross sections for the processes in Eq. (1.1) in the energy range of 5–40 keV for the incident hydrogen atom. The $2p$ excitation total cross section was also measured by Dose, Gunz, and Meyer.[8] Their results were slightly lower.

More recent measurements of the total excitation cross sections for the processes given by Eq. (1.1) have been carried out by Birely and McNeal[9] for an energy range of 1–25 keV for the incident hydrogen atom. Hughes and Choe[10] have carried out the measurements for an energy range of 20–125 keV for the incident hydrogen atom. Thomas and Sauers[5] have measured the total $2s$ excitation cross section for an energy range of 1–20 keV for the incident hydrogen atom.

Flannery[11] and also Levy[12] have applied the multistate impact parameter method to the processes given by Eq. (1.1). The agreement between the multistate impact parameter treatment and the experimental results is fair. However, the theoretical calculations peak and become smaller as the incident energy decreases whereas the experimental results continue to rise as the incident energy decreases. This discrepancy is not clear at this time. Levy has pointed out that the difference may be due to the neglect of electron exchange and cascade effects. However the most recent measurements of the $2s$ excitation total cross section by Thomas and Sauers[5] indicate that the total cross section peaks at about 3 keV and then decreases as the energy decreases which is more in accord with the existing theoretical calculations.

Thomas and Sauers[5] also measured the differential cross section for the $2s$ excitation of the hydrogen atom at an energy of 10 keV for the incident hydrogen atom. At 10 keV, theory and experiment are essentially in agreement with respect to the total excitation cross sections. The eikonal DWBA provides a differential excitation cross section with which to compare to experiment.

II. BASIC EQUATIONS

The derivation of the theory of the eikonal DWBA has been given by Chen, Joachain, and Watson[1] for a general rearrangement collision. In this section we present only the basic equations to establish our notation.

Let $\vec{k}_i$ and $\vec{k}_f$ be the relative momenta in the center-of-mass coordinate system for the initial and final channels, respectively. The relative coordinate is $\vec{R}$ and is given in cylindrical coordinates as

$$\vec{R} = \vec{b} + Z\hat{k}_i , \quad (2.1)$$

where b and ϕ are the polar coordinates of $\vec{b}$. For direct collisions, in which rearrangement does not occur, the T matrix in the eikonal DWBA is

$$T_{ba}^{(\mathrm{eik})} = (2\pi)^{-3} \int_0^\infty db\, b \int_{-\infty}^{\infty} dZ \int_0^{2\pi} d\phi \times \exp[i(k_i - k_f\cos\theta)Z + i\delta\Phi(\vec{b},Z) - ik_f b \sin\theta\cos\phi] A(\vec{b},z) , \quad (2.2)$$

where θ is the scattering angle between $\vec{k}_i$ and $\vec{k}_f$. Also

$$\delta\Phi(\vec{b},Z) = -\frac{1}{v_i}\int_{-\infty}^{Z} U_i(b,Z')dZ' - \frac{1}{v_f}\int_{Z}^{\infty} U_f(\vec{b},Z')\,dZ' , \quad (2.3)$$

where U_i and U_f are the optical potentials and v_i and v_f are the relative velocities for the initial and final channels, respectively.

The coupling matrix is

$$A(\vec{b},Z) = \langle \psi_b | V | \psi_a \rangle , \quad (2.4)$$

where V is the interaction potential and ψ_a and ψ_b are the electronic wave functions for the atomic systems in the initial and final channels, respectively.

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} M^2 |T_{ba}|^2 , \quad (2.5)$$

where M is the reduced mass.

III. EXCITATION OF HYDROGEN TO THE 2s AND 2p STATES BY HELIUM IMPACT

The eikonal DWBA has been applied to the H-He collisions given by Eq. (1.1) in the energy range of 2.25 keV ($v = 0.3$ a.u.) to 100 keV ($v = 2.0$ a.u.).

The interaction potential was taken as

$$V(\vec{R},\vec{r}_A,\vec{r}_B) = \frac{2}{R} + \sum_{i=1}^{2} \frac{1}{|\vec{R}+\vec{r}_{iA}-\vec{r}_B|} - \sum_{i=1}^{2} \frac{1}{|\vec{R}+\vec{r}_{iA}|} - \frac{2}{|R-\vec{r}_B|} , \quad (3.1)$$

where $\vec{r}_A$ and $\vec{r}_B$ are electronic coordinates for the He and H atoms, respectively.

The wave function of the ground-state helium atom needed in the calculation was taken as the following Hartree-Fock function[13]:

$$\phi_{1\,{}^1S}(\vec{r}_A) = (1.6966/\pi)(e^{-1.41r_{1A}} + 0.799e^{-2.61r_{1A}}) \times (e^{-1.41r_{2A}} + 0.799e^{-2.61r_{2A}}) . \quad (3.2)$$

The hydrogen wave function is given by $\phi_{nlm}(\vec{r}_B)$, where the notation nlm designates the state of the hydrogen atom.

The optical potentials are represented by the static matrix elements. That is,

$$U_i = \langle \phi_{1\,{}^1S}(\vec{r}_A)\phi_{1s}(\vec{r}_B) | V(\vec{R},\vec{r}_A,\vec{r}_B) | \phi_{1\,{}^1S}(\vec{r}_A)\phi_{1s}(\vec{r}_B)\rangle = e^{-2.82R}(-0.0414 - 5.02/R) + e^{-4.02R}(1.20 + 0.403/R) + e^{-5.22R}(0.309 + 0.110/R) + e^{-2R}(-4.25 + 6.50/R) . \quad (3.3)$$

Likewise,

$$U_f^{2s} = \langle \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2s}(\vec{r}_B) | V(\vec{R},\vec{r}_A,\vec{r}_B) | \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2s}(\vec{r}_B)\rangle ,$$

$$U_f^{2s} = e^{-R}(-0.0592R^2 + 0.306R - 0.540 + 0.319/R) + e^{-2.82R}(1.60 + 0.917/R) + e^{-4.02R}(1.33 + 0.642/R) + e^{-5.22R}(0.317 + 0.121/R) . \quad (3.4)$$

Also,

$$U_f^{2p_0} = \langle \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2p_0}(\vec{r}_B) | V(\vec{R},\vec{r}_A,\vec{r}_B) | \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2p_0}(\vec{r}_B)\rangle , \quad U_f^{2p_0} = U_0(R) - (5/4\pi)^{1/2}(3Z^2/R^2 - 1)U_2(R) \quad (3.5)$$

and

$$U_f^{2p_+} = \langle \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2p_+}(\vec{r}_B) | V(\vec{R},\vec{r}_A,\vec{r}_B) | \phi_{1\,{}^1S}(\vec{r}_A)\phi_{2p_+}(\vec{r}_B)\rangle , \quad U_f^{2p_+} = U_0(R) + \tfrac{1}{2}(5/4\pi)^{1/2}(3Z^2/R^2 - 1)U_2(R) , \quad (3.6)$$

where

$$U_0(R) = e^{-2.82R}(1.70 + 1.19/R) + e^{-4.02R}(1.34 + 0.667/R) + e^{-5.22R}(0.318 + 0.121/R) + e^{-R}\times 10^{-2}(-1.98R^2 + 2.29R - 3.99 + 2.27/R) \quad (3.7)$$

and

$$U_2(R) = e^{-2.82R}\times 10^{-2}(1.84 + 7.94/R + 7.75/R^2 + 2.75/R^3) + e^{-4.02R}\times 10^{-3} \times(1.30 + 3.73/R + 2.54/R^2 + 0.633/R^3) + e^{-5.22R}\times 10^{-4}(0.579 + 1.25/R + 0.656/R^2 + 0.126/R^3) + e^{-R}\times 10^{-2}(3.13R^2 - 3.65R + 2.66 + 1.73/R - 2.81/R^2 - 2.81/R^3)\,. \tag{3.8}$$

The coupling matrix elements are given by

$$A_{2s}(\vec{R}) = \langle \phi_{1\,1s}(\vec{r}_A)\phi_{2s}(\vec{r}_B)\,|\,V(\vec{R},\vec{r}_A,\vec{r}_B)\,|\,\phi_{1\,1s}(\vec{r}_A)\phi_{1s}(\vec{r}_B)\rangle = e^{-1.5R}(0.442R - 1.53 + 1.31/R) - e^{-2.82R}(0.414R + 1.23/R) - e^{-4.02R}\times 10^{-2}(4.56 + 7.90/R) - e^{-5.22R}\times 10^{-3}(3.14 + 3.93/R)\,. \tag{3.9}$$

Likewise,

$$A_{2p_0}(\vec{R}) = \langle \phi_{1\,1s}(\vec{r}_A)\phi_{2p_0}(\vec{r}_B)\,|\,V(\vec{R},\vec{r}_A,\vec{r}_B)\,|\,\phi_{1\,1s}(\vec{r}_A)\phi_{1s}(\vec{r}_B)\rangle\,, \quad A_{2p_0}(\vec{R}) = (3/4\pi)^{1/2}(Z/R)A_0(R) \tag{3.10}$$

and

$$A_{2p_+}(\vec{R}) = \langle \phi_{1\,1s}(\vec{r}_A)\phi_{2p_+}(\vec{r}_B)\,|\,V(\vec{R},\vec{r}_A,\vec{r}_B)\,|\,\phi_{1\,1s}(\vec{r}_A)\phi_{1s}(\vec{r}_B)\rangle\,, \quad A_{2p_+}(\vec{R}) = -(3/8\pi)^{1/2}(b/R)e^{i\phi}A_0(R)\,, \tag{3.11}$$

where

$$A_0(R) = e^{-2.82R}(0.451 + 1.61/R + 0.588/R^2) + e^{-4.02R}\times 10^{-2}(3.48 + 7.77/R + 1.93/R^2) + e^{-5.22R}\times 10^{-3}(1.85 + 3.02/R + 0.578/R^2) + e^{-1.5R}(-0.901R + 1.33 - 0.911/R - 0.608/R^2)\,. \tag{3.12}$$

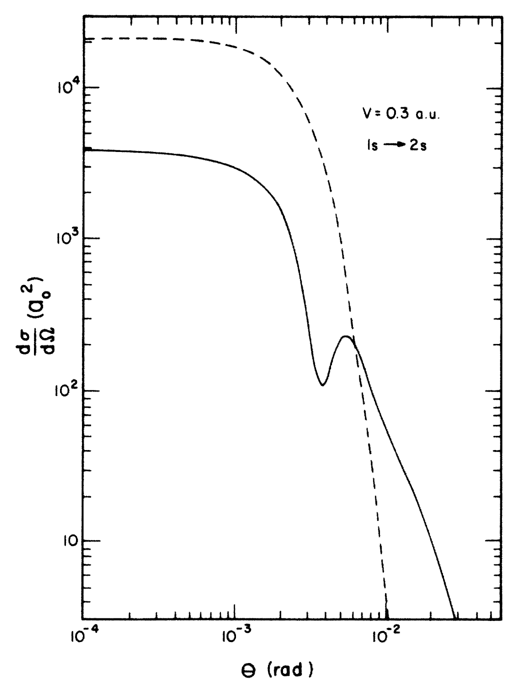

FIG. 1. Differential cross sections for the excitation of hydrogen to the $2s$ state by helium impact for an incident velocity of 0.3 a.u. or for an incident energy of 2.25 keV. The solid line is the eikonal DWBA and the dashed line is the first Born approximation. Both the differential cross section and the scattering angle are given in the center-of-mass coordinate system.

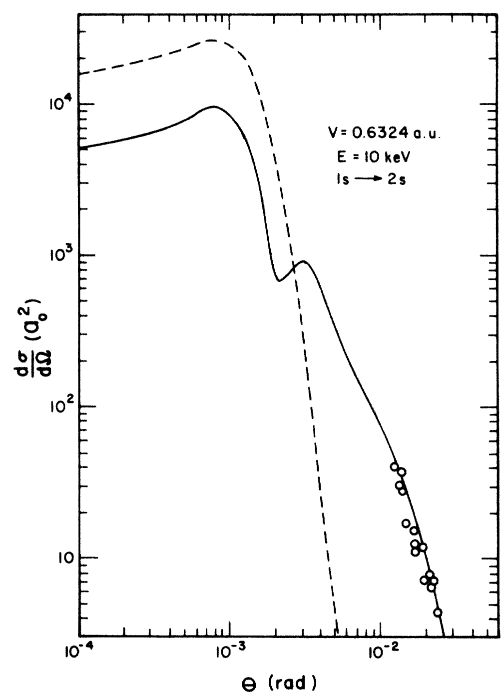

FIG. 2. Differential cross sections for the excitation of hydrogen to the $2s$ state by helium impact for an incident velocity of 0.6324 a.u. or for an incident energy of 10 keV. The solid line is the eikonal DWBA and the dashed line is the first Born approximation. The circles are the experimental data of Thomas and Sauers, Ref. 5, and have been multiplied by a factor of 4. Both the differential cross section and the scattering angle are given in the center-of-mass coordinate system.

The ϕ integration in the expression for the T matrix [Eq. (2.2)] can be carried out analytically and results in either the J_0 or J_1 Bessel function with argument $k_f b \sin\theta$. The remaining two-dimensional integral over b and z is then performed numerically. The details are given in Ref. 2.

IV. RESULTS AND DISCUSSION

A. Differential cross sections

The differential cross sections for the $1s \rightarrow 2s$ excitation are presented in Figs. 1–3 for the incident velocities of $v = 0.3$, 0.632 and 1.0 a.u. for the hydrogen atom. The eikonal DWBA results are compared to the first Born approximation results and in Fig. 2 to the experiment of Thomas and Sauers.[5]

The eikonal DWBA results have the same basic characteristics for the H-He collisions as they did for the H-H collisions.[2] The differential cross section for the eikonal DWBA results lie below the Born results for small angles and remain above them for larger angles. A significant amount of the total cross section is scattered into the larger angle region.

A second peak is also present in the eikonal DWBA results for H-He collisions as it was for H-H collisions. The occurrence of this peak is attributed to the interference of the distortion factor $\delta\Phi(\vec{b}, z)$ [Eq. (2.3)] and the Bessel function resulting from the ϕ integration. This was further discussed with the H-H results (Ref. 2).

In Fig. 2., a comparison is made to the experimental data of Thomas and Sauers.[5] Their experimental data have been normalized to the theoretical cross section by multiplying their results by a factor of 4. The comparison shows good agreement for both the shape and the slope of the curves. The experiment shows that the larger angle scattering is dying off more slowly than the first Born approximation would predict. The factor of four between the magnitudes of the theoretical results and the experimental data could be due to the procedure used in the analysis of the experimental data in arriving at an absolute differential cross section. The integration of the theoretical differential cross section at 10 keV over the solid angle gives a total cross section at 10 keV that compares quite well to experimental data, as shown on Fig. 7. The differential cross section for the $2s$ excitation can be integrated over the solid angle $d\Omega (= 2\pi \sin\theta\, d\theta)$ to yield a total cross section. Since the $\sin\theta$ factor in the integration is rising as θ at these angles, the contribution from large angle scattering is important in the calculations of the total cross sec-

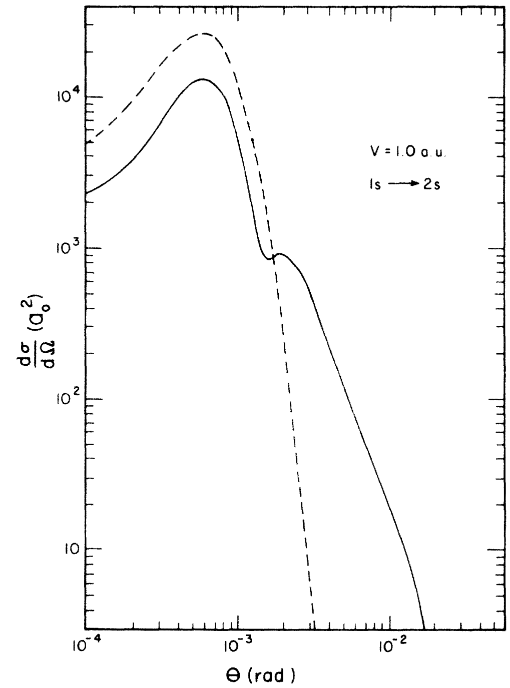

FIG. 3. Same as Fig. 1 but for an incident velocity of 1.0 a.u. or for an incident energy of 25 keV.

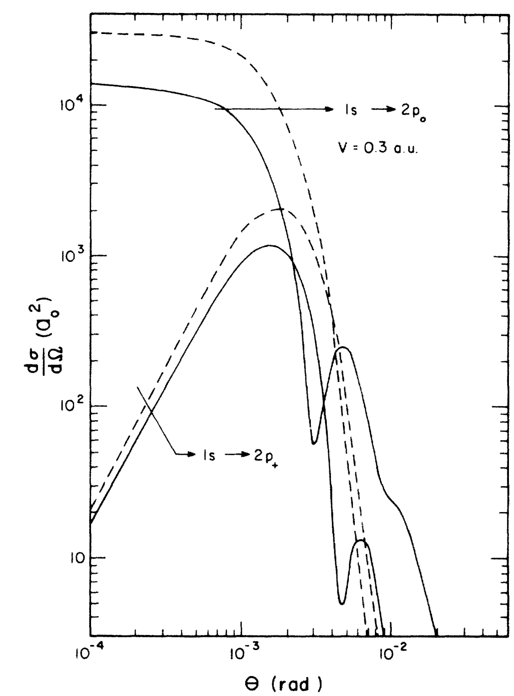

FIG. 4. Differential cross section for the excitation of hydrogen to the $2p_0$ and $2p_+$ states by helium impact for an incident velocity of 0.3 a.u. or for an incident energy of 2.25 keV. The solid line is the eikonal DWBA and the dashed line is the first Born approximation. Both the differential cross section and the scattering angle are given in the center-of-mass coordinate system.

tion. For 10 keV (Fig. 2), the region between 5×10^{-3} rad and 2.5×10^{-2} rad, which contains the experimental data of Thomas and Sauers,[5] contributes 38% of the total cross sections even though the differential cross section in this region is over a factor of 20 below the peak value.

The differential cross sections for the $1s \rightarrow 2p$ excitations are presented in Fig. 4–6 for the incident velocities $v = 0.3$, 0.5, and 1.0 a.u. The eikonal DWBA are compared to the first Born approximation results. The general characteristics are still present. The eikonal DWBA differential cross sections die off much slower in angle than the first Born results and the second peak is still present.

B. Total cross sections

The total cross section for the $1s \rightarrow 2s$ excitation is presented in Fig. 7. The eikonal DWBA is compared to the first Born approximation and to the four-state impact parameter calculation of Flannery[11] or Levy.[12] The experimental data are from the experiments of Orbeli *et al.*,[7] Birely and McNeal,[9] Hughes and Choe,[10] and Thomas and Sauers.[5]

Likewise in Fig. 8, the total cross section is presented for the $1s \rightarrow 2p$ excitation. The source of the experimental data is the same as in the $1s \rightarrow 2s$ excitation with the addition of the experimental data of Dose, Gunz, and Meyer.[8]

The eikonal DWBA results in Figs. 7 and 8 follow closely to the four-state impact-parameter results. This was expected from the analysis of the H-H scattering in Ref. 2. The first Born approximation seems to predict the experimental data better than the other theoretical methods. However, since the validity of the first Born approximation is questionable at lower velocities Levy[12] has pointed out that the agreement may be accidental.

The experimental data are from experiments that use the same general technique. That is, the cross sections are calculated from the intensity of the light emitted from the excited states of the hydrogen atoms. The Lyman-α radiation is emitted spontaneously from the H($2p$) state and the intensity of the radiation gives a relative value for the population of the atoms that were in the $2p$ states. The addition of an electric field quenches the excited H($2s$) atom and the resulting Lyman-α radiation can be used to find the relative population of the $2s$ state. Cascade effects into the $2s$ and $2p$ states could be important in the measurement of these cross sections. However, Birely and McNeal[9] and Hughes and Choe[10] have

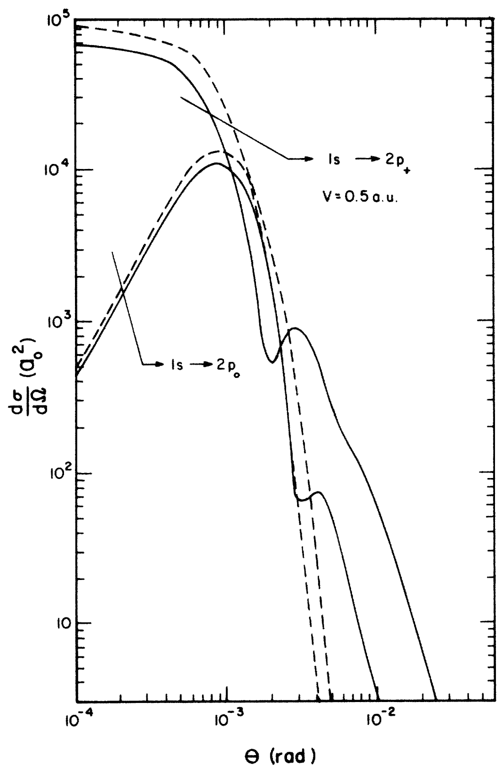

FIG. 5. Same as Fig. 4 except for an incident velocity of 0.5 a.u. or for an incident energy of 6.25 keV.

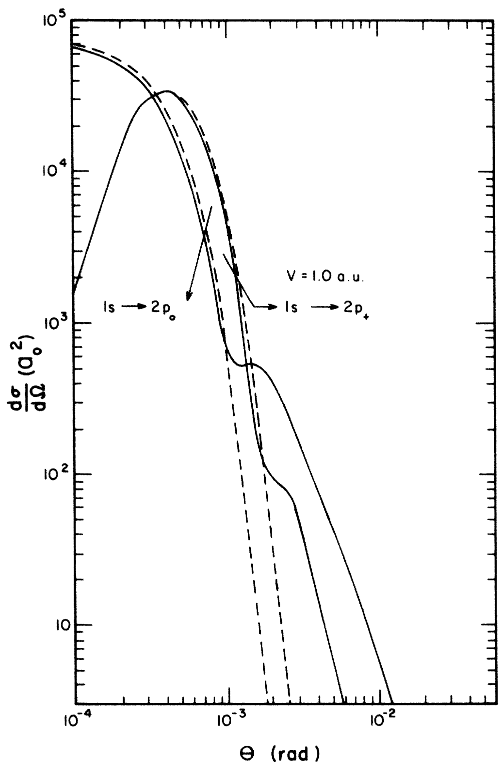

FIG. 6. Same as Fig. 4 except for an incident velocity of 1.0 a.u. or for an incident energy of 25 keV.

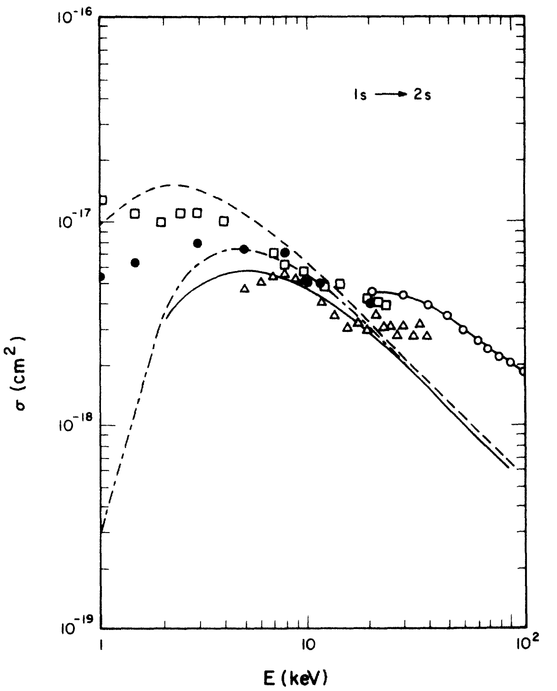

FIG. 7. Total cross section for the excitation of hydrogen to the 2*s* state by helium impact. The solid line is the eikonal DWBA and the dashed line is the first Born approximation. The dash-dot line is the four-state impact parameter calculation of Flannery, Ref. 11, or Levy, Ref. 12. The triangles represent the experimental data of Orbeli *et al.*, Ref. 7; the squares, Birely and McNeal, Ref. 9; the circle line, Hughes and Choe, Ref. 10, and the solid circles, Thomas and Sauers, Ref. 5.

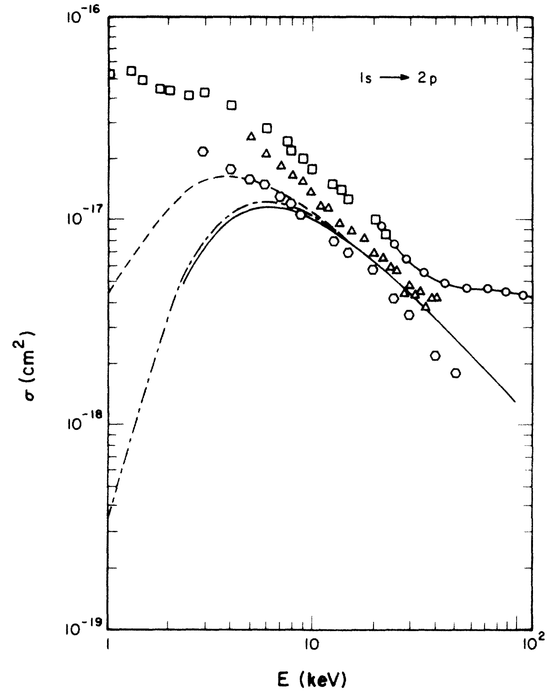

FIG. 8. Total cross section for the excitation of hydrogen to the 2*p* states by helium impact. The solid line is the eikonal DWBA and the dashed line is the first Born approximation. The dash-dot line is the four-state impact-parameter calculation of Flannery, Ref. 11, or Levy, Ref. 12. The triangles represent the experimental data of Orbeli *et al.*, Ref. 7; the squares, Birley and McNeal, Ref. 9; the hexagons, Dose *et al.*, Ref. 8; and the circle line, Hughes and Choe, Ref. 10.

estimated the cascade effect to be small, (3–6)% for H(2*s*) and 10–15% for H(2*p*). The more recent experiments of Birely and McNeal[9] and Hughes and Choe[10] have made several adjustments to improve their results over the earlier experiments of Orbeli *et al.*,[7] and Dose *et al.*,[8] and should be considered to be the more accurate experiments.

The recent experiment of Thomas and Sauers[5] shows the total cross sections for the H(2*s*) excitation to peak at 3 keV and then decrease in value as the incident energy decreases. This is in better agreement with the theoretical calculations. At 1 keV, Birely and McNeal's data are nearly a factor of 3 above the Thomas-Sauers data.

The region of the largest disagreement between the experimental data and the eikonal DWBA results is at low energy where the eikonal DWBA is not expected to be valid. At the lower energies electron exchange may become important.

[1]J. C. Y. Chen, C. J. Joachain, and K. M. Watson, Phys. Rev. A 5, 2460 (1972).
[2]R. H. Shields and J. L. Peacher, Phys. Rev. A 9, 743 (1974).
[3]M. R. Flannery, Phys. Rev. 183, 231 (1969); 183, 241 (1969).
[4]M. R. Flannery and K. J. McCann [Phys. Rev. A 8, 2915 (1973)] recently have shown how a differential cross section can be obtained from a multistate impact-parameter approach.
[5]E. W. Thomas and I. Sauers, *VIII International Conference on the Physics of Electronic and Atomic Collisions*, edited by B. C. Cobic and M. V. Kurepa (Institute of Physics, Boegrad, Yugoslavia, 1973), p. 166.
[6]B. L. Moisewitsch and A. L. Stewart, Proc. Phys. Soc. Lond. A 67, 1069 (1954).
[7]A. L. Orbeli, E. P. Andreev, V. A. Ankudinov, and V. M. Dukelskii, Zh. Eksp. Teor. Fiz. 57, 108 (1969) [Sov. Phys.—JETP 30, 63 (1970)].
[8]V. Dose, R. Gunz, and V. Meyer, Helv. Phys. Acta 41,

264 (1968).
[9]J. H. Birely and R. J. McNeal, Phys. Rev. A 5, 257 (1972).
[10]R. H. Hughes and Song-Sik Choe, Phys. Rev. A 5, 1758 (1972).
[11]M. R. Flannery, J. Phys. B 2, 913 (1969).
[12]H. Levy, Phys. Rev. 187, 136 (1969).
[13]F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. 146, 1 (1966).