Differential cross sections for excitation of atomic hydrogen by proton impact

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The differential cross section for the excitation of the hydrogen atom to the $2s$ and $2p$ states are calculated by applying the Coulomb-projected-Born (CPB) method as proposed by Geltman. The results for the excitations of the hydrogen atom for the incident proton energies of 25, 50, 100, and 150 keV and for the scattering angles θ varying from 0 to 1.5 (in 10^{-3} rad c.m.) obtained by the present CPB approach are compared with the experimental observations and other existing theoretical calculations. At the incident energy 100 keV the present CPB results, except at large scattering angles, are found to be in good agreement with the observed results and are as reliable as the calculated results obtained by applying the many-state close-coupling (CC) approximation. For 50 keV and for scattering angles varying from 0.4 to 1.0 (in 10^{-3} rad c.m.) the present CPB results agree with the observed data and are as reliable as the CC and the Glauber results, however with the decrease of scattering angle ($\theta \leq 0.4$ in 10^{-3} rad c.m.) the results obtained by the CPB method become less reliable compared to the CC or the Glauber results. At 25 keV the present CPB results for the differential cross sections underestimate the observed values throughout the angular region considered except at the large angles, where $\theta \geq 0.5$ in 10^{-3} rad c.m. On the other hand, the Glauber results at this energy give quite good agreement throughout the angular region, whereas the Born results grossly overestimate the observed differential cross sections.

INTRODUCTION

Though a number of independent total-cross-section measurements[1-7] are available for the excitation of atomic hydrogen by proton impact, the measurements of differential cross sections are very few, owing to the difficulty involved in the differential measurements. The data for the differential cross sections, however, provide a better test of the existing theoretical models than do the total-cross-section measurements. The first experiment on the differential cross-section measurements in the low-energy region (less than 2 keV) for the excitation of atomic hydrogen by proton impact was performed by Houver, Fayteton, and Barat.[8] Recently, Park *et al.*[9] have reported the differential cross-section measurements at proton energies of 25, 50, and 100 keV, corresponding to 1.0, 1.4, and 2.0 a.u. of velocity and angles in a range extending from the forward direction to 10^{-3} rad in the center-of-mass system by the method of angular-energy-loss spectrometry. The theoretical models employed in this relatively high-energy range are much different than those which are applicable in the low-energy region of the projectile, studied by Houver, Fayteton, and Barat. A large number of theoretical studies have been undertaken in the H^+-H collision system because the system is simple enough, having one active electron and the initial-and final-state wave functions of the system are well known. However, most of these works are centered around the determination of the total cross sections for the H($n=2$) excitation. The theoretical calculation on the angular differential cross sections is available only in a very few cases because the impact-parameter treatment does not properly lend itself to the calculation of differential cross sections.

Franco and Thomas[10] employed the Born and the Glauber approximation to study theoretically the differential cross sections for the excitation of atomic hydrogen to the $(2s+2p)$ level by the impact of protons at incident energies of 25, 50, and 100 keV. The experimental results of Park *et al.*[9] are found to be in excellent agreement with the Glauber results of Franco and Thomas[10] at all energies and angles except for $0.6\times10^{-3} \leq \theta \leq 0.9 \times 10^{-3}$ rad at 100 keV.

Recently Bransden and Noble[11] have applied a close-coupling pseudostate (CC) calculation to obtain the differential cross sections for the $n=2$ excitation of hydrogen atoms by the impact of proton for impact energies of 50, 100, and 150 keV. At the incident proton energy 100 keV their calculated values[11] for the differential cross sections are in good agreement with the experimental results except at very large scattering angles ($\Theta \geq 0.9\times10^{-3}$ rad), whereas for 50 keV the CC results almost coincide with the observed data throughout the scattering angles considered.

The large-angle scattering is determined by the Coulomb interaction between the nuclei, and this interaction has a vanishing contribution to the scattering amplitude in the first-order Born calculation for the inelastic scattering cases because of the orthogonality of the atomic states. In the impact parameter treatment, the trajectory of the scattered particle will certainly depend on the interaction between the nuclei. Geltman[12] first introduced the idea of the Coulomb-projected-Born (CPB) approximation to calculate the charge-transfer cross section in proton-hydrogen scattering.

Subsequently Geltman and Hidalgo[13-16] applied this method to calculate the excitation cross sections in electron-hydrogen and electron-helium scattering and also in the case of ionization problems. The CPB approximation is essentially a first-order high-energy approximation in which the interaction between the incident particle and the proton in the target atom is represented by a Coulomb-wave final state in the T matrix.

In the present paper we propose to investigate the differential cross section for the H($n=2$) excitation at proton energies of 25, 50, 100, and 150 keV by using the CPB approximation and compare them with the existing theoretical results and the experimental findings. Throughout the calculation, atomic units have been used.

THEORY

The differential cross section for a collision in which the target atom is excited from an initial state i to a final state f is given by

$$d\sigma^d_{if}(\hat{k}_i,\hat{k}_f)=\frac{\mu^2}{4\pi^2}\left(\frac{v_f}{v_i}\right)|T^d_{if}|^2 d\hat{k}_f\,, \quad (1)$$

where $\vec{k}_i$ and $\vec{k}_f$ are the initial and final wave vectors for the relative motion of the center of mass, v_i and v_f are the corresponding relative velocities, μ is the reduced mass of the systems, and T^d_{if} is the T-matrix element,

$$T^d_{if}=\langle\Psi^0_f, V_i\Psi^+_i\rangle\,. \quad (2)$$

Here Ψ^+_i is the exact solution of $(H-E)\Psi^+_i=0$ with proper scattering boundary conditions, and Ψ^0_f and V_i are defined with respect to our choice of splitting the Hamiltonian into $H=H_i+V_i$ and $(H_i-E)\Psi^0_f=0$.

The Hamiltonian for the proton plus hydrogen-atom system is given in the center-of-mass reference frame by

$$H=-\frac{1}{2\mu}\nabla^2_\sigma-\tfrac{1}{2}\nabla^2_{r_2}+\frac{1}{r_1}-\frac{1}{r_2}-\frac{1}{r_{12}}\,, \quad (3)$$

where all the quantities are expressed in atomic units, r_1 and r_2 are the position coordinates of the incident proton and atomic electron, respectively, ∇^2_σ and $\nabla^2_{r_2}$ are the respective kinetic energy operators. $\vec{\sigma}$ is the position vector of the projectile with respect to the center of mass of the atom.

We make the following choices for H_i, V_i, and Ψ^0_f to obtain our present approximation:

$$H_i=-\frac{1}{2\mu}\nabla^2_\sigma+\frac{1}{\sigma}-\tfrac{1}{2}\nabla^2_{r_2}-\frac{1}{r_2}\,,$$

$$V_i=\left(\frac{1}{r_1}-\frac{1}{\sigma}-\frac{1}{r_{12}}\right),$$

$$\Psi^0_f=\exp(-\pi\alpha/2)\Gamma(1-i\alpha)\exp(i\vec{k}_f\cdot\vec{\sigma})\times{}_1F_1(i\alpha;1;-ik_f\sigma-i\vec{k}_f\cdot\vec{\sigma})\Psi_f(\vec{r}_2)\,, \quad (4)$$

where the Coulomb parameter α represents the repulsive proton-proton field and is μ/k_f.

The sum $(1/r_1-1/\sigma)$ of the interaction potential V_i is of the order $\epsilon=1/(M+1)$ smaller than $1/r_{12}$ as can be seen from the Taylor expansion:

$$\frac{1}{r_1}-\frac{1}{\sigma}=\frac{1}{r_1}-\frac{1}{|\vec{r}_1-\epsilon\vec{r}_2|}=\epsilon\left(\frac{\vec{r}_1\cdot\vec{r}_2}{r_1^3}\right)+O(\epsilon^2)\,,$$

M being the mass of proton. The contribution of these terms to the T-matrix element is also of order ϵ, and hence negligible. Making the first Born approximation for Ψ^+_i, the scattering amplitude which is more commonly used than the T matrix is given by

$$f(i\to f)=-\frac{\mu}{2\pi}\left\langle\Psi^0_f,-\frac{1}{r_{12}}\exp(i\vec{k}_i\cdot\vec{\sigma})\Psi_i(\vec{r}_2)\right\rangle\,. \quad (5)$$

If we assume the nucleus to be a fixed origin, the error involved in this assumption will be of order $1/M$ in the cross sections. In most calculations[17] terms of order $1/M$ are neglected compared with unity. The neglect of terms of order $1/M$ implies the replacement of $\vec{\sigma}$ by $\vec{r}_1$. In that case we have for the excitation amplitudes from the initial state as

$$f(i\to f)=\frac{\mu}{2\pi}\exp\left(\frac{-\pi\alpha}{2}\right)\Gamma(1+i\alpha)\times\int d\vec{r}_1 d\vec{r}_2\Psi^*_f(\vec{r}_2)\frac{1}{r_{12}}\Psi_i(\vec{r}_2)\times\exp(i\vec{q}\cdot\vec{r}_1)\,{}_1F_1(-i\alpha;1;ik_f r_1+i\vec{k}_f\cdot\vec{r}_1)\,, \quad (6)$$

where

$$\vec{q}=\vec{k}_i-\vec{k}_f\,.$$

EVALUATION OF AMPLITUDES AND CROSS SECTIONS

Here we first consider the excitation of atomic hydrogen from its ground state to the $2s$ excited state. The bound-state wave functions of the atom are

$$\Psi_i(\vec{r}_2)=(1/\sqrt{\pi})(Z)^{3/2}\exp(-\lambda_1 r_2)\,,$$

$$\Psi_f(\vec{r}_2)=(1/2\sqrt{2\pi})(Z)^{3/2}(1-\lambda_2 r_2)\exp(-\lambda_2 r_2)\,,$$

where

$$\lambda_1=Z \text{ and } \lambda_2=\tfrac{1}{2}Z\,.$$

The integration over $\vec{r}_2$ yields

$$\Psi^*_f(\vec{r}_2)\frac{1}{r_{12}}\Psi_i(\vec{r}_2)d\vec{r}_2=N\left[\left(\frac{16\pi\lambda_2}{\lambda^3}-\frac{4\pi}{\lambda^2}\right)\exp(-\lambda r_1)+\frac{4\pi\lambda_2}{\lambda^2}r_1\exp(-\lambda r_1)\right]\,, \quad (7)$$

where $\lambda=\lambda_1+\lambda_2$ and the normalization constant $N=Z^3/2\sqrt{2}\pi$. The integration over $d\vec{r}_1$ can be performed by using the Nordsieck's[18] integral technique and becomes

$$\int d\vec{r}\exp(-\lambda r + i\vec{q}\cdot\vec{r})\,{}_1F_1(-i\alpha;1;ipr + i\vec{p}\cdot\vec{r}) = -2\pi\frac{d}{d\lambda}[\tfrac{1}{2}(q^2+\lambda^2)]^{-i\alpha-1}[\vec{p}\cdot\vec{q} - i\lambda p + \tfrac{1}{2}(q^2+\lambda^2)]^{i\alpha}\,.$$

Thus

$$f(1s\to 2s) = -\exp\left(\frac{-\pi\alpha}{2}\right)\Gamma(1+i\alpha)N\mu\left[\left(\frac{16\pi\lambda_2}{\lambda^3} - \frac{4\pi}{\lambda^2}\right)\Phi(\lambda) - \left(\frac{4\pi\lambda_2}{\lambda^2}\right)\frac{d}{d\lambda}\Phi(\lambda)\right]\,, \tag{8}$$

where

$$\Phi(\lambda) = \frac{d}{d\lambda}[\tfrac{1}{2}(q^2+\lambda^2)]^{-i\alpha-1}[\vec{k}_f\cdot\vec{q} - i\lambda k_f + \tfrac{1}{2}(q^2+\lambda^2)]^{i\alpha}\,.$$

Now we consider the excitation of the hydrogen atom from its ground state to the $2p$ excited state. We follow a procedure similar to that of Geltman[12] as used in the proton-hydrogen charge-transfer collision in the CPB approximation. Using the Fourier transform of $\Psi_i(\vec{r}_2)$, $\Psi_f^*(\vec{r}_2)$, and $1/r_{12}$ and integrating over $d\vec{r}_2$, we get

$$f(1s\to 2p_{X,Y,Z}) = \lim_{\epsilon\to 0}\exp\left(\frac{-\pi\alpha}{2}\right)\Gamma(1+i\alpha)\frac{\eta\mu}{i2\sqrt{2}\,\pi^3}\,\frac{\partial}{\partial\epsilon_{X,Y,Z}}\int d\vec{r}_1 d\vec{k}\,\frac{\exp[i(\vec{k}+\vec{q})\cdot\vec{r}_1]}{k^2(|\vec{k}-\vec{\epsilon}|^2+\eta^2)^2}\,{}_1F_1(-i\alpha;1;ik_f r_1 + i\vec{k}_f\cdot\vec{r}_1)\,, \tag{9}$$

with $\eta = 1.5$. Introducing the formula for the parametric integration

$$\frac{1}{a^2 b} = 2\int_0^1 dx\,x[ax + b(1-x)]^{-3}\,,$$

we obtain

$$f(1s\to 2p_{X,Y,Z}) = \lim_{\epsilon\to 0}\exp\left(\frac{-\pi\alpha}{2}\right)\Gamma(1+i\alpha)\frac{\eta\mu}{i\sqrt{2}\,\pi^3}\,\frac{\partial}{\partial\epsilon_{X,Y,Z}} \times\int_0^1 dx\,x\int d\vec{k}\,d\vec{r}_1\frac{\exp[i(\vec{k}+\vec{q})\cdot\vec{r}_1]}{[(\vec{k}-\vec{k}_0)^2+\xi^2]^3}\,{}_1F_1(-i\alpha;1;ik_f r_1 + i\vec{k}_f\cdot\vec{r}_1)\,, \tag{10}$$

TABLE I. Angular differential cross sections $d\sigma/d\Omega$ (cm^2/sr) and total cross sections σ (cm^2) for proton excitation of atomic hydrogen on the $n=2$ level. Numbers in parentheses represent powers of ten.

Scattering angles (10^{-3} rad c.m.)	$d\sigma/d\Omega$ (cm^2/sr) $1s\to 2s$	$d\sigma/d\Omega$ (cm^2/sr) $1s\to 2p$	σ (cm^2) $1s\to 2s$	σ (cm^2) $1s\to 2p$
		$E = 25$ keV		
0	2.454(−12)	3.143(−11)		
0.1	2.389(−12)	2.969(−11)		
0.2	2.206(−12)	2.512(−11)		
0.3	1.933(−12)	1.926(−11)		
0.4	1.611(−12)	1.364(−11)		
0.5	1.278(−12)	9.100(−12)		
0.6	9.679(−13)	5.816(−12)		
0.7	7.015(−13)	3.609(−12)	0.387(−17)	2.382(−17)
0.8	4.876(−13)	2.203(−12)		
0.9	3.261(−13)	1.339(−12)		
1.0	2.105(−13)	8.236(−13)		
1.1	1.321(−13)	5.211(−13)		
1.2	8.151(−14)	3.448(−13)		
1.3	5.059(−14)	2.417(−13)		
1.4	3.283(−14)	1.798(−13)		
1.5	2.336(−14)	1.411(−13)		

TABLE I. *(Continued)*

Scattering angles (10^{-3} rad c.m.)	$d\sigma/d\Omega$ (cm^2/sr) $1s\to 2s$	$d\sigma/d\Omega$ (cm^2/sr) $1s\to 2p$	σ(cm^2) $1s\to 2s$	σ(cm^2) $1s\to 2p$
		$E=50$ keV		
0	6.968(−12)	1.941(−10)		
0.1	6.633(−12)	1.598(−10)		
0.2	5.730(−12)	9.844(−11)		
0.3	4.516(−12)	5.282(−11)		
0.4	3.272(−12)	2.679(−11)		
0.5	2.201(−12)	1.329(−11)		
0.6	1.389(−12)	6.561(−12)		
0.7	8.346(−13)	3.278(−12)		
0.8	4.836(−13)	1.690(−12)	0.556(−17)	5.130(−17)
0.9	2.760(−13)	9.179(−13)		
1.0	1.591(−13)	5.339(−13)		
1.1	9.598(−14)	3.350(−13)		
1.2	6.269(−14)	2.257(−13)		
1.3	4.521(−14)	1.612(−13)		
1.4	3.573(−14)	1.202(−13)		
1.5	3.014(−14)	9.236(−14)		
		$E=100$ keV		
0	1.240(−11)	7.277(−10)		
0.1	1.129(−11)	3.833(−10)		
0.2	8.581(−12)	1.307(−10)		
0.3	5.558(−12)	4.509(−11)		
0.4	3.159(−12)	1.599(−11)		
0.5	1.629(−12)	5.855(−12)		
0.6	7.906(−13)	2.258(−12)		
0.7	3.748(−13)	9.483(−13)	0.505(−17)	6.119(−17)
0.8	1.816(−13)	4.461(−13)		
0.9	9.447(−14)	2.373(−13)		
1.0	5.489(−14)	1.408(−13)		
1.1	3.602(−14)	9.077(−14)		
1.2	2.609(−14)	6.207(−14)		
1.3	2.017(−14)	4.423(−14)		
1.4	1.618(−14)	3.246(−14)		
1.5	1.323(−14)	2.437(−14)		
		$E=150$ keV		
0	1.519(−11)	1.355(−9)		
0.1	1.323(−11)	4.339(−10)		
0.2	8.889(−12)	1.026(−10)		
0.3	4.814(−12)	2.749(−11)		
0.4	2.227(−12)	7.832(−12)		
0.5	9.364(−13)	2.391(−12)		
0.6	3.802(−13)	8.179(−13)		
0.7	1.589(−13)	3.276(−13)		
0.8	7.314(−14)	1.556(−13)	0.416(−17)	5.718(−17)
0.9	3.884(−14)	8.554(−14)		
1.0	2.390(−14)	5.217(−14)		
1.1	1.645(−14)	3.414(−14)		
1.2	1.213(−14)	2.344(−14)		
1.3	9.301(−15)	1.667(−14)		
1.4	7.289(−15)	1.218(−14)		
1.5	5.791(−15)	9.109(−15)		

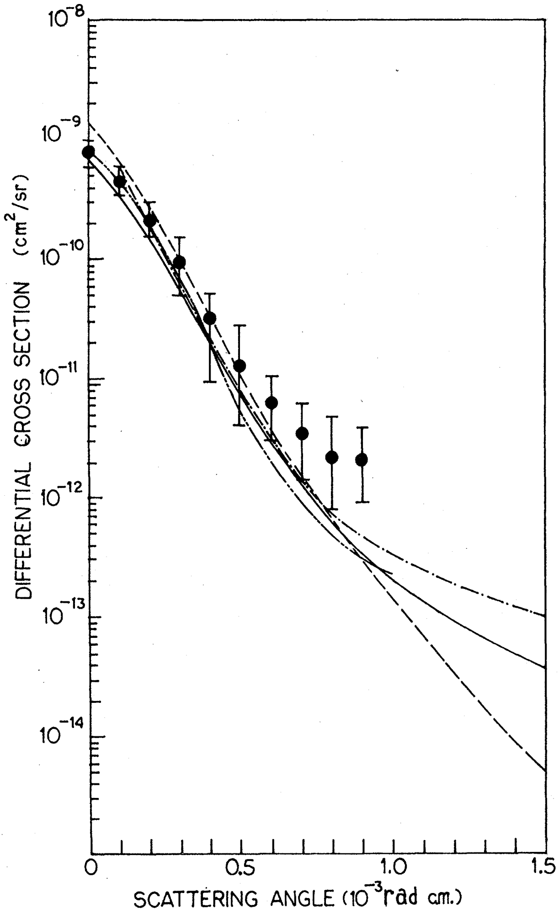

FIG. 1. The angular differential cross sections for 100 keV (laboratory energy) proton excitation of atomic hydrogen to the $n=2$ state. The cross sections and scattering angles are given in center-of-mass coordinates. Experiment: ● Park *et al.*, Ref. 9. Theory — — — first Born approximation, Franco and Thomas, Ref. 10. ---- Glauber theory, Franco and Thomas, Ref. 10. —· — Close-coupling pseudostate model (CC), Bransden and Noble, Ref. 11. — Present CPB approximation.

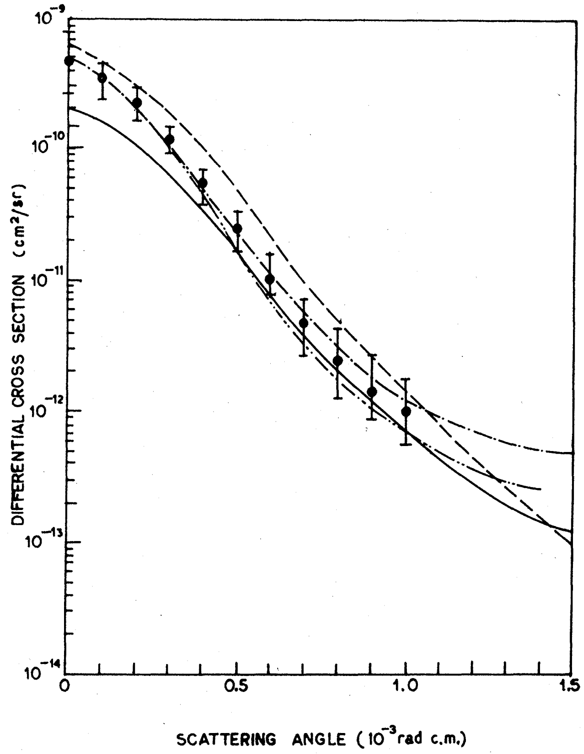

FIG. 2. Same as Fig. 1 but for 50 keV.

where

$$\vec{k}_0 = x\vec{\epsilon},$$

$$\xi^2 = x(\epsilon^2 + \eta^2 - x\epsilon^2).$$

Using the identity

$$\int d\vec{t}\, \frac{\exp(i\vec{t}\cdot\vec{r})}{(t^2+\eta^2)^3} = -\frac{\pi^2}{4\eta}\frac{d}{d\eta}\,\frac{\exp(-\eta r)}{\eta}$$

and then applying the Nordsieck's integral technique the scattering amplitude may be simplified to a simple one-dimensional integral form

$$f(1s\to 2p_{X,Y,Z}) = \lim_{\epsilon\to 0}\exp\left(\frac{-\pi\alpha}{2}\right)\Gamma(1+i\alpha)\frac{\mu\eta}{i2\sqrt{2}}\,\frac{\partial}{\partial\epsilon_{X,Y,Z}} \times \int_0^1 x\,dx\,\frac{1}{\xi}\,\frac{d}{d\xi}\,\frac{1}{\xi}\,\frac{d}{d\xi}\Phi(\xi), \quad (11)$$

where

$$\Phi(\xi) = [\tfrac{1}{2}(Q^2+\xi^2)]^{-i\alpha-1}[\vec{k}_f\cdot\vec{Q} - i\xi k_f + \tfrac{1}{2}(Q^2+\xi^2)]^{i\alpha}$$

and $\vec{Q} = \vec{q} + \vec{k}_0$.

The integral for the scattering amplitude and finally the necessary one-dimensional integral for the total excitation cross sections are performed numerically by applying Gauss-Legendre quadrature method. It may be pointed out here that the calculation for the differential cross sections in the CPB method requires computing an integral such as (11), instead of computing some algebraic functions required in the deduction of the differential cross sections by the Glauber procedure.

RESULTS AND DISCUSSIONS

The differential cross sections for the $1s$-$2s$ and the $1s$-$2p$ transitions calculated by the present CPB approximation for incident proton energies of 25, 50, 100, and 150 keV and the scattering

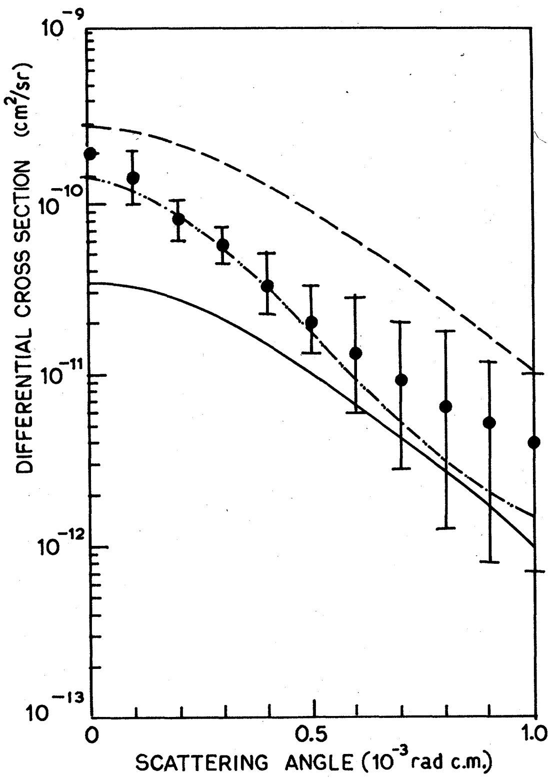

FIG. 3. The angular differential cross sections for 25 keV (laboratory energy) proton excitation of atomic hydrogen to the $n=2$ state. The cross sections and scattering angles are given in center-of-mass coordinates, Experiment: ● Park *et al.*, Ref. 9. Theory: --- First Born approximation, Franco and Thomas, Ref. 10. -·· - Glauber theory, Franco and Thomas, Ref. 10. — Present CPB approximation.

angles varying from 0 to 1.5 (in 10^{-3} rad c.m.) are shown in Table I. We also present in the same table the integrated cross sections obtained by applying the CPB approximation at these energies.

In Figs. 1–3 we present the average experimental data for the differential cross sections for excitation of atomic hydrogen to the $n=2$ state by the incident protons having energies of 100, 50, and 25 keV, respectively. The corresponding theoretical curves obtained by applying the Glauber, the first Born, the close-coupling pseudostate model, and the present CPB approximations are also shown in the same figures. For the incident proton energy of 100 keV it appears that all the theoretical curves for the differential cross sections are more sharply peaked and with the increase of angle fall faster than the experimental curve. At small scattering angles these theoretical results are found to provide good agreement with the experimental findings. With the increase of angle the Born curve, however, shows a considerable deviation from the experiment whereas the present CPB curve, showing a close resemblance with the Glauber and the pseudostate close-coupling models, predicts qualitatively the same behavior as that of the experimental observations. This is expected because the large-angle scattering is mainly determined by the Coulomb interaction between the nuclei and this interaction does not contribute in the first order to inelastic (Born) scattering. The interaction between the incident proton and the target proton has been incorporated in the present CPB calculation by a Coulomb wave final state in the T matrix and as such the present calculated differential cross sections at large angles show a marked improvement over the first Born approximation.

At 50 and 25 keV the present CPB results for the cross sections underestimate the experimental values at small scattering angles and with the increase of scattering angle show a trend similar to the Glauber results, which in the low-angle region give very good agreement with the experi-

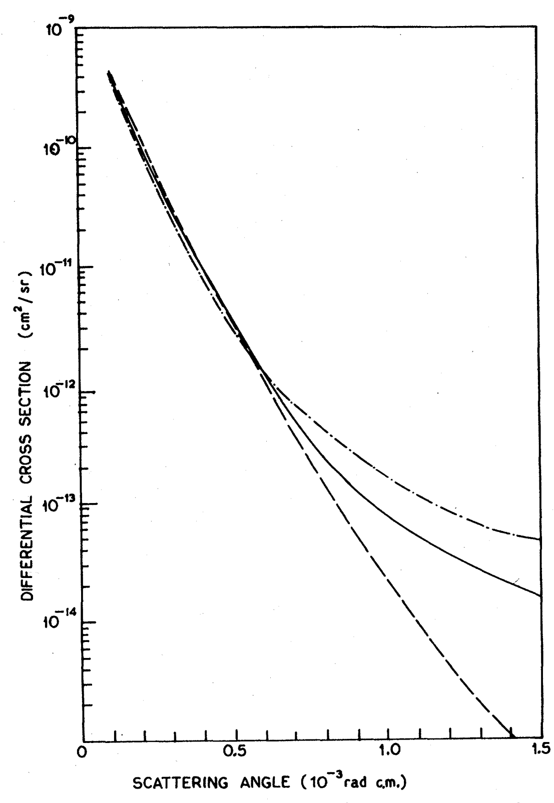

FIG. 4. The angular differential cross sections for 150 keV (laboratory energy) proton excitation of atomic hydrogen to the $n=2$ state. The cross sections and scattering angles are given in center-of-mass coordinates. Theory: --- First Born approximation, Franco and Thomas, Ref. 10. -·- Close-coupling pseudostate model (CC), Bransden and Noble, Ref. 11. — Present CPB approximation.

mental results. The Born curve, on the other hand, lies much above the experimental curve throughout the scattering angles considered. In Fig. 4 we have presented our CPB calculated results for the differential cross sections for the excitation of the $n=2$ state of atomic hydrogen for an incident proton energy of 150 keV with the corresponding theoretical result obtained by applying the Born and close-coupling pseudostate model. Unfortunately, no experimental results are available for comparison at this incident proton energy. From the figure it appears that for small scattering angles (0 to 0.6×10^{-3} rad c.m.) the theoretical results for the differential cross sections obtained by those three approximations are quite close to each other. With the increase of scattering angles the Born results sharply drop down, differing by an order of magnitude from both the present CPB and the pseudostate model results. Though the values for differential cross sections for the excitations obtained by the present CPB approximation become somewhat low with the increase of scattering angle as compared to the results obtained by the close-coupling pseudostate model, these two theoretical curves show a similar trend throughout the range of scattering angles considered.

CONCLUSION

At 100 keV the results obtained by the present CPB calculation, like other existing two-state calculations, do not agree with the observed values at the large-angle region. However, at this region even the many-state close-coupling pseudostate calculations are not in agreement with the observed results. At 50 and 25 keV, where the Glauber results are in good agreement with the experiment, the present CPB results are found to underestimate the observed data especially in the low-angle region, whereas with the increase of scattering angle the present CPB results are found to agree the experimental data within the standard deviation. The validity of the present two-state approximation at high energy could be definitely ascertained if the experimental work for the differential measurements could be extended at incident energy beyond 100 keV and at scattering angles $\Theta \geq 0.7\times10^{-3}$ (rad c.m.).

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