Anal. Acad. Nac. Cs. Ex. Fís. Nat., Buenos Aires, tomo 37, 1985

ELECTRON CAPTURE AT MEDIUM AND HIGH COLLISION ENERGIES. DIFFERENTIAL CROSS SECTIONS THEORETICAL SITUATION

por *Roberto Daniel Rivarola* * * *

ABSTRACT

In this work we present recent progress on theoretical differential cross sections for one-electron capture in ion-atom collisions at small angles and intermediate and high energies. Results obtained from different theoretical models (for monoelectronic as well as multielectronic targets) are compared with experimental data.

Recent theoretical differential cross sections $d\sigma/d\Omega$ for one electron capture in ion-atom collisions are reviewed in this work. The energy range here considered is divided in two regions: a first one at intermediate velocities ($v \sim v_e$, where v is the relative collision velocity and v_e the initial or final electron orbital velocity) and a second one at high velocities ($v >> v_e$). In the first region, close-coupling methods between the most significant states of the collision (see Bates, 1958) and Classical-Trajectory-Monte Carlo calculations (CTMC; Olson, 1983) appear to be adequate to describe the symmetrical (homonuclear) systems. In the high energy region, perturbative models (which must include the presence of the continuum of the target and/or the continuum of the projectile as intermediate states) are found to describe appropriately the physical processes. These perturbative models appear to give also a good agreement with experimental data at intermediate velocities for asymmetric systems.

a. Intermediate energies

In figures 1 and 2, $d\sigma/d\Omega$ is shown for $H^+ + H\ (1s) \rightarrow H + H^+$ at 25keV and 125keV Experimental points are those ones obtained by Martin *et al.* (1981a). Three different perturbative models are presented: i) the (CDW) Continuum Distorted Wave (Belkić *et al.*, 1979), which

* Instituto de Física Rosario (CONICET - UNR), Av. Pellegrini 250, 2000 Rosario, Argentina.

* * Invited talk at the VIII International Seminar on the Physics of Ion-Atom Collisions (Castle of Neijenrode in Breukelen near Utrecht, The Netherlands, August 1983).

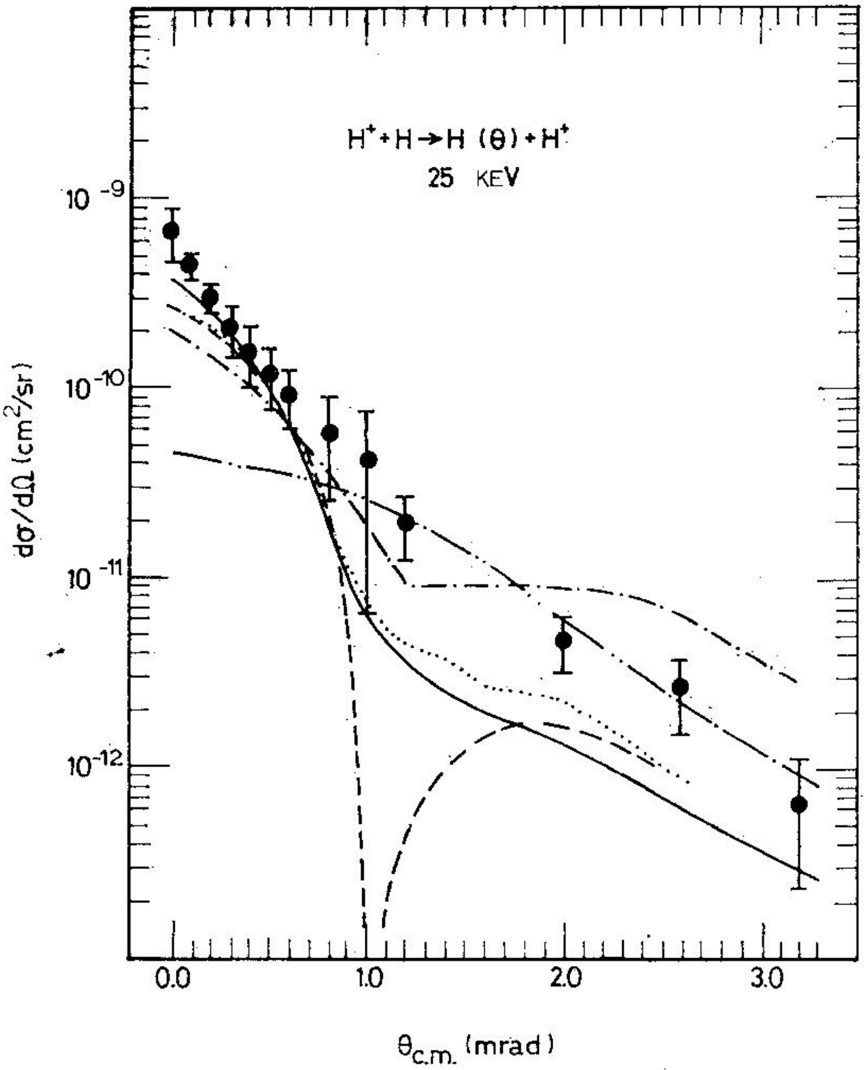

FIG. 1. — Electron capture-differential cross sections for the H^+ + H (ls) reaction in center-of-mass coordinates at 25keV laboratory energy. Experimental points: (Φ) from Martin *et al.* (1981a). Theoretical results: (——) MS, (. . . .) TSAE, (- . - . - . -) CDW, (- - - - -) JS, (— . . —) EA models.

is the first order of a perturbative series where the initial and final functions are chosen as a product of the electron-bounded wave function on a nucleus with the electron-continuum intermediate state on the other nucleus; ii) the (EA) eikonal approximation (Ho *et al.*, 1982), where this product is chosen only on the entrance or exit channel and the continuum state is approached by a coulombic exponential phase and iii) the (JS) Jackson-Schiff approximation (Martin *et al.*, 1981a), where initial and final wave functions are taken as bounded and the nucleus-nucleus interaction is included in the perturbation potential. In CDW and EA, this internuclear potential is considered to affect the scattering amplitude as a phase factor for each impact parameter (in an impact parameter approximation) and $d\sigma/d\Omega$ is obtained using the eikonal

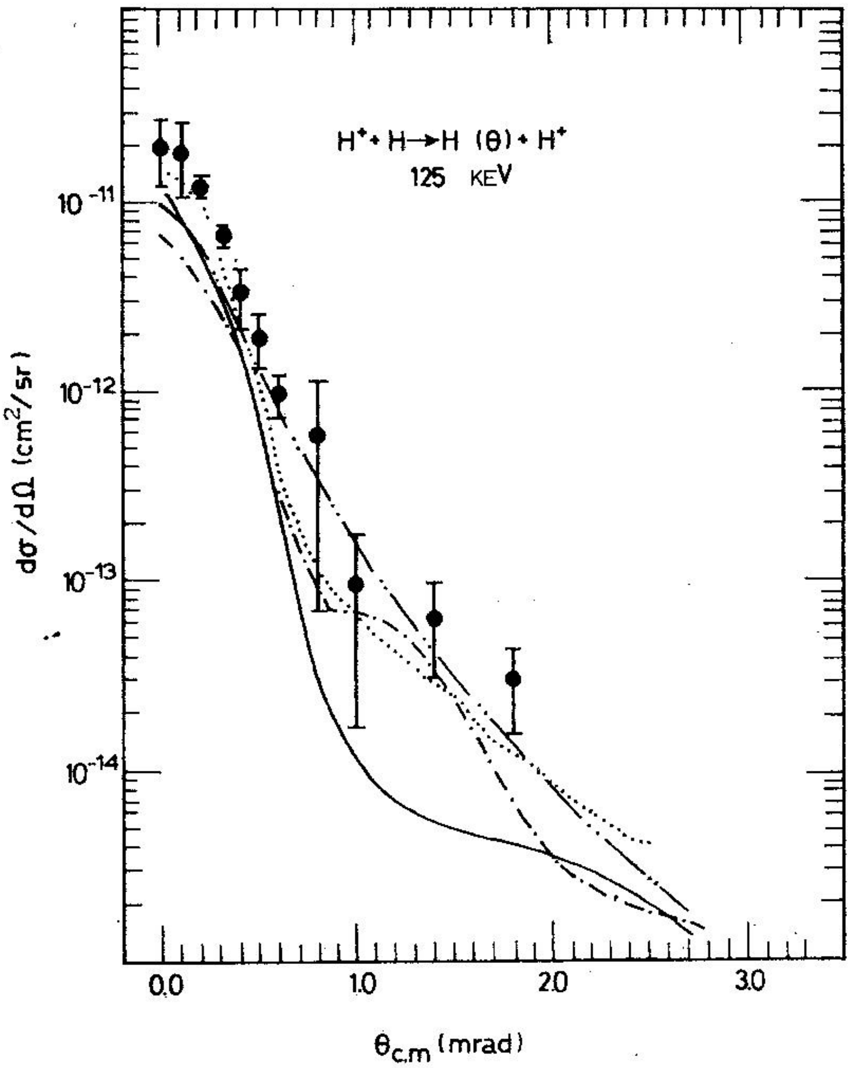

FIG. 2. — Same that in figure 1, but for 125 keV laboratory energy.

expression for it (McCarroll and Salin, 1968). The JS results (including only capture to a H (ls) state) present a deep not shown by the experiments. The EA (including capture to all H states) and CDW (including capture only to the H (ls) state) models even when not adequate for the lowest energy case, give a reasonable agreement with data when the energy increases. The best accordance between theory and experiment is obtained using the (TSAE) Two-State-Atomic-Expansion (Lin and Richard, 1981) for the resonant H^+ + H (ls) collision. Surprinsingly, a (MSAE) Multiple-State-Atomic-Expansion (Shakeshaft, 1978), where twelve Sturmian wave functions are considered on each nucleus gives a poorer comparison with the results of Martin *et al.* (1981a) than the TSAE ones. Maidagan *et al* (1982) have also studied this system at 25keV into the TSAE model but with pseudo-states included at finite internuclear distances by introduction of dynamical

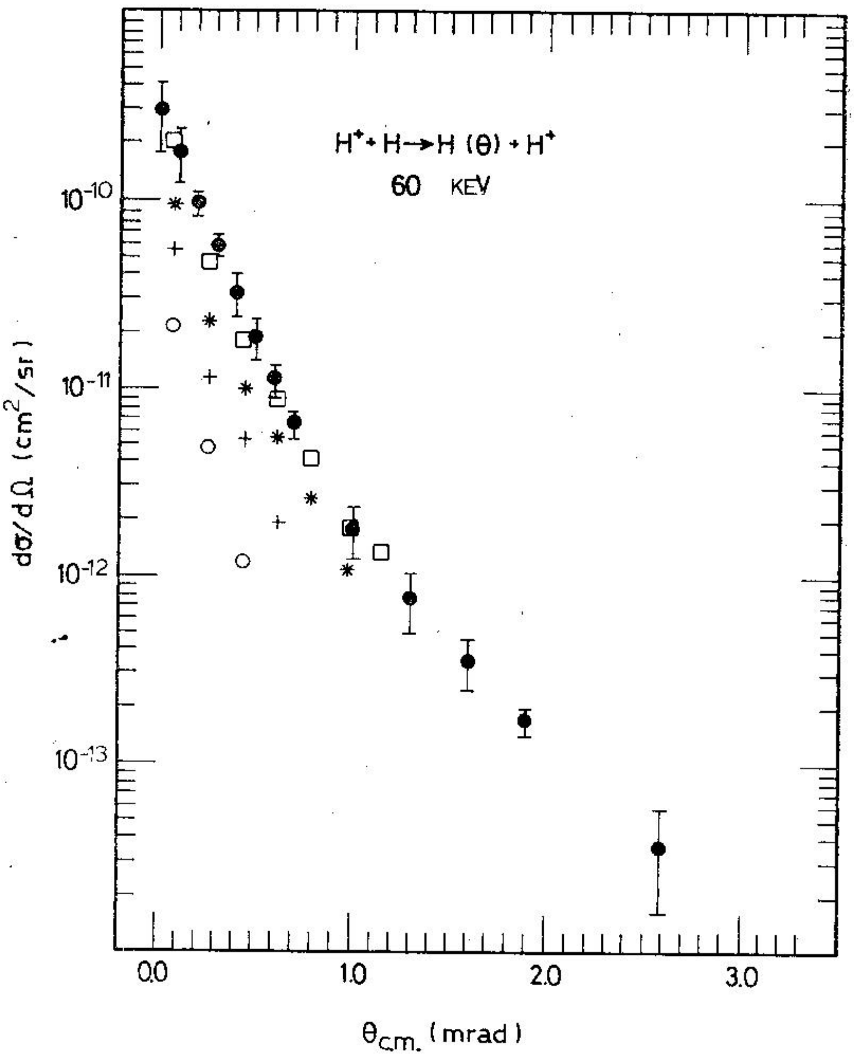

FIG. 3. — Same that in figure 1, but for 60 keV laboratory energy and theoretical results obtained using CTCM calculations for capture to: (□) all H states, (*) H (ls) state, (+) H (n = 2) states, (○) H (n = 3) states.

variable nuclear charges. The results differ at most by 18 percent from the case of using constant nuclear charges. Thus, they are not shown in the figure. In figure 3, very recent CTMC calculations (Olson, 1983) are compared with H^+ + H – experimental data (also from Martin *et al.*, 1981a) but for 60 keV. The agreement is very good when using up to 60,000 trajectories. Theoretical results are obtained for capture to all states and also for each η principal quantum number At 25 KeV, the CTMC values lie below the data at small angles and this effect has been attributed (see Olson, 1983) to the fact that the classical description of the radial distribution of the electron of the target does not allow the electron to penetrate into the classical forbidden region ($r > 2a_0$, where a_0 is the Bohr's radius). Naturally, this effect becomes less important when the energy increases, that is when the collision becomes closer.

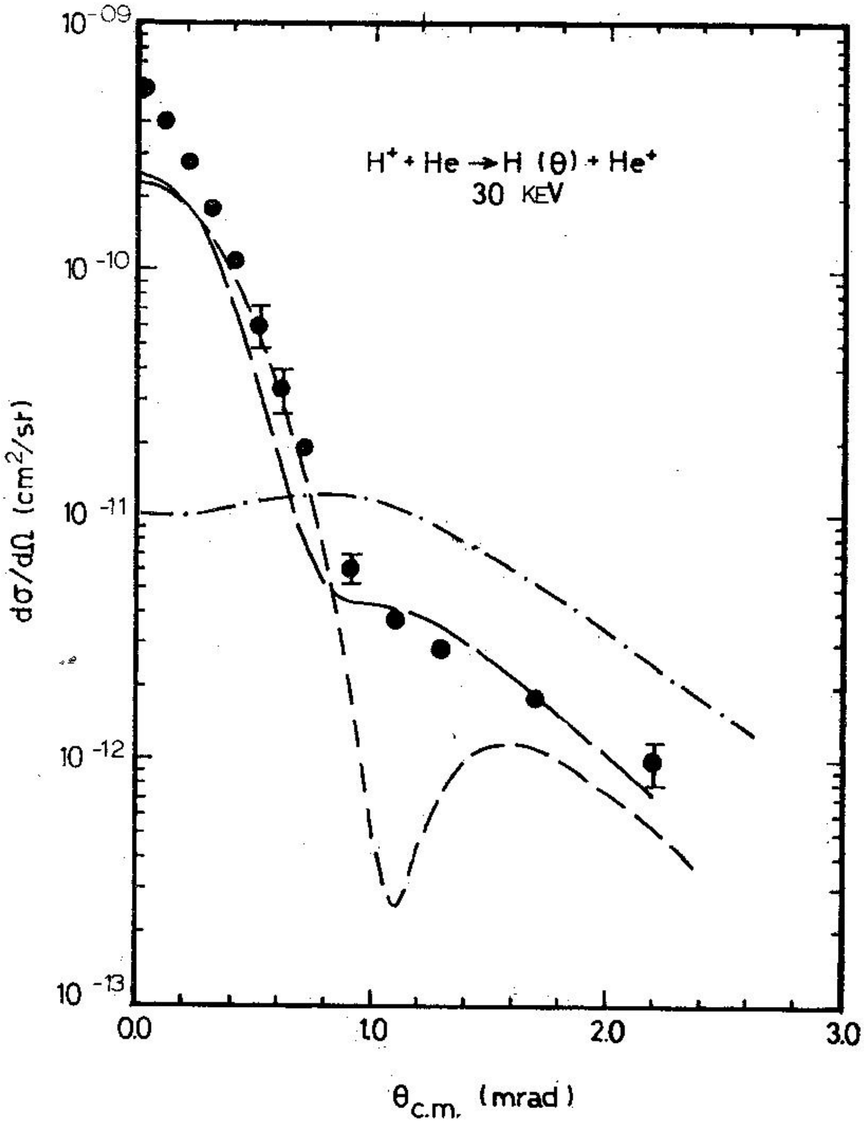

FIG. 4. — One electron capture-differential cross sections for the H^+ + He reaction in center-of-mass coordinates at 30 keV laboratory energy. Experimental (Φ) and theoretical points from Martin *et al.* 1981b). Calculations are obtained using the static potentials i), ii) and iii) of the text.

Other CTCM calculations have been also reported by Eichenauer *et al.* (1982) but not so good accordance with experiments is obtained (for a detailed discussion, see Olson, 1983).

Another interesting point to be analysed is the influence of the presence of "passive electrons" (those not captured) on $d\sigma/d\Omega$ in bare ions on multielectron targets collisions. At these energies it is appropriate to consider these electrons as "frozen" (i.e. their orbital states do not change throughout the collision) and the "active" electron as an independent particle of the core composed by the passive electrons. Thus, different static potentials (which take into account the internuclear potential and/or the projectile-passive electrons and/or the projectile-

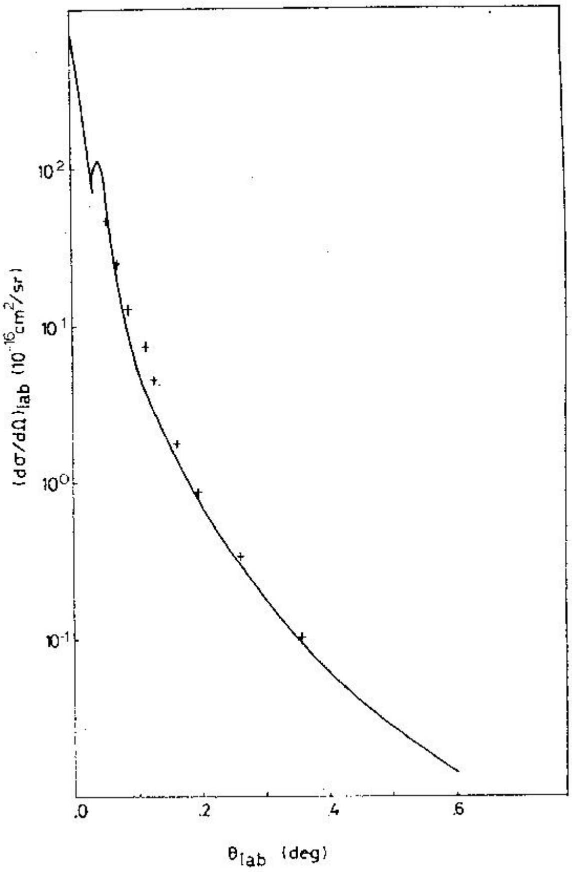

FIG. 5. — K-shell one electron capture-differential cross sections for $H^+ + C$ at 0.6 MeV. All quantities in the laboratory system. Experimental points (Φ) from Horsdal-Pedersen *et al.* (1982). Theoretical results are calculated with the CDW model (——).

active electron interactions, modifiying the trajectory of the projectile) are introduced into the scattering amplitude. Calculations using the TSAE approximation have been compared by Martin *et al.* (1981b) with their own experimental points for $H^+ + He \rightarrow H + He^+$ at 30 keV (figure 4). Three static potentials were used by including: i) only internuclear potential (as proposed by Belkić and Salin, 1976) ; ii) the internuclear potential plus the interactions between the projectile and passive and active electrons (as proposed by Rogers and McGuire, 1977) ; iii) the internuclear potential plus the interaction between the projectile and the passive electron (as formally obtained by Rivarola *et al.*, 1980). The best agreement with the data is obtained in the case iii), showing the interesting physical conclusion that only the projectile-active electron interaction is responsible for the capture of the electron and that the projectile-passive electron and internuclear interactions affect the trajectory of the incident particle.

Differential cross sections for more asymetric systems at intermediate

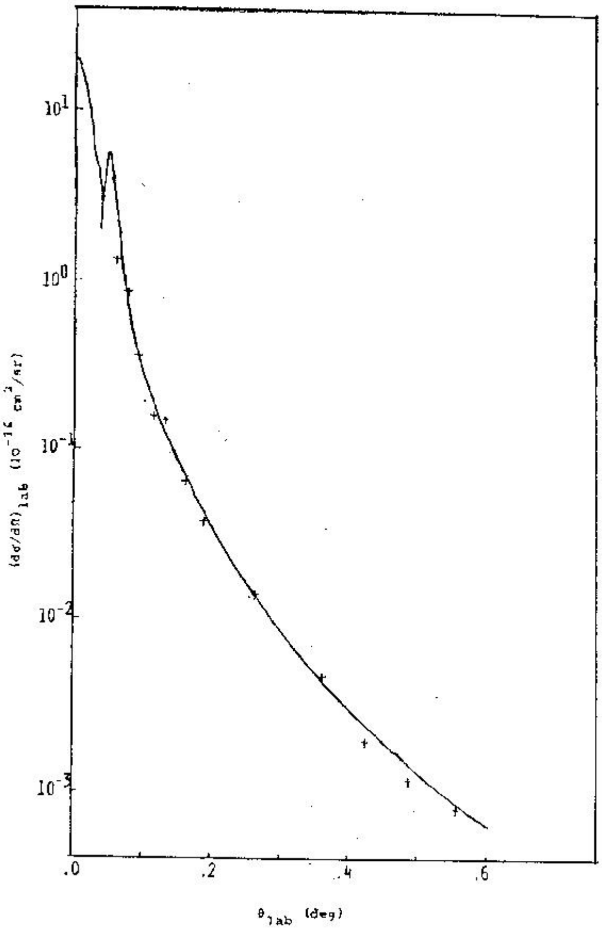

FIG. 6. — Same that in figure 5, but for the $H^+ + Ne$ system at 1.5 MeV.

energies are shown in figures 5 and 6. Calculations using the CDW model (Rivarola and Salin, 1983) show a close agreement with experimental data from Horsdal-Pedersen *et al* (1982) for the $H^+ + C \rightarrow H + C^+$ (K^{-1}) and $H^+ + Ne \rightarrow H + Ne^+$ (K^{-1}) systems at 0.6 MeV and 1.5 MeV laboratory energies respectively. TSAE calculations from Horsdal-Pedersen *et al.* (1982) on the last system at 0.7 MeV do not compare well their own experimental values.

b. **High energies**

The more important feature in electron capture-differential cross sections at high energy is the presence of a peak (the Thomas' peak; Thomas, 1927) around the critical angle θ_c (which depends only of the projectile mass in the laboratory system). This peak is due to a two step-collision process: a first one between the projectile and the electron (such that the projectile nucleus is deflected and angle θ_c from the

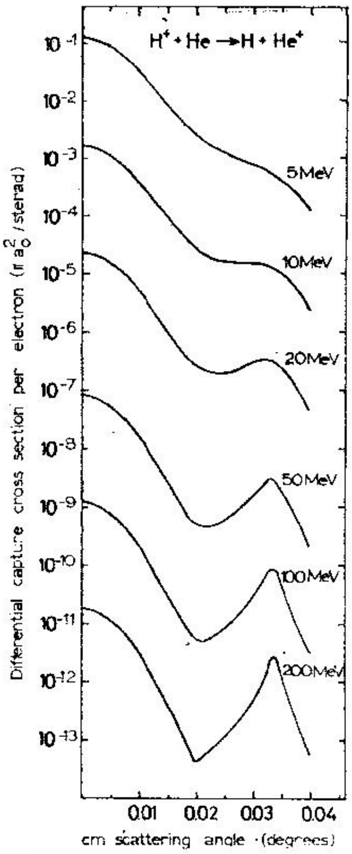

Fig. 7. — Theoretical electron capture-differential cross sections for the resonant H^{+} + H(ls) collision at 10MeV. All quantities in the laboratory system. The approximations used are: (———) CDW (without nucleus-nucleus interaction), (—.—) IA, (—..—) B2.

incident direction) and a second one between the electron and the target nucleus, after which the electron is captured by the projectile (Shakeshaft and Spruch, 1978, 1979). This peak becomes more pronounced when the energy increases, as can be seen in figure 7 from the calculations of Simony *et al.* (1982). They calculated the H^{+} + He (ls^{2}) → H (ls) + He^{+} (ls) collision into the Second Born approximation (B2, using a free particle-Green's function) from 5 MeV up to 200 MeV laboratory energies. The resonant H^{+} + H (ls) case at 10 MeV has been studied by Simony and McGuire (1981) into the B2 approximation and by Miraglia *et al.* (1981) into the CDW model. Results are shown in figure 8 and are compared with the recent Impulse approximation (IA; Briggs *et al.*, 1982a) ones, where only one channel is distorted by a continuum state. A deep appears in the CDW calculations overlaping the Thomas' peak. This structure has been interpreted by Rivarola (1981; see also Rivarola

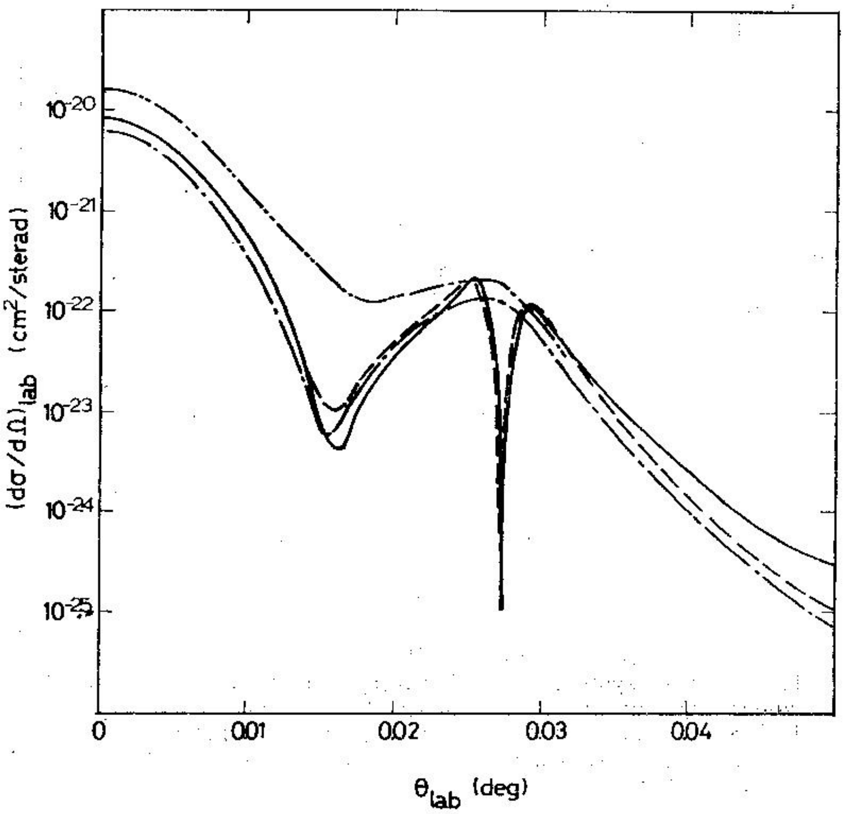

FIG. 8. — Theoretical one electron capture-differential cross sections for the $H^+ + He$ system in center-of-mass coordinates. Calculations are obtained using the B2 approximation. Laboratory energies are indicated in the figure.

and Miraglia, 1982) as an interference between two processes: i) the electron initially in a bound state of the target is firstly excited to an intermediate state of the continuum of the target and then captured to a bound state of the projectile, and ii) the electron is firstly captured to an intermediate state of the continuum of the projectile and then into a bound state of the projectile. This interference is produced at large impact parameters (Rivarola, 1983). This deep must disappear for non-hydrogenic targets as recently pointed out by Rivarola and Salin (1983). Very recent experimental data (Stockli *et al.*, 1983) on the $H^+ + H_2 \rightarrow H + H_2^+$ shows a smooth depression on $d\sigma/d\Omega$ in the predicted angular region for the existence of the deep when using a H target. For K-K shell capture (for asymmetric as well as for symmetric systems) the T-matrix element appears to depend as v^{-5} in the peak's angular region (which will give the velocity dependence of the total cross sections σ for asymptotic high energies). It depends as v^{-7} in the sorroundings of $\theta \simeq \theta_c/\sqrt{3}$, where an interference between the first- and higher-orders of the Born series takes place (Briggs *et al.*, 1982a). It must be pointed out that the second-order term that interferes comes from the contribution

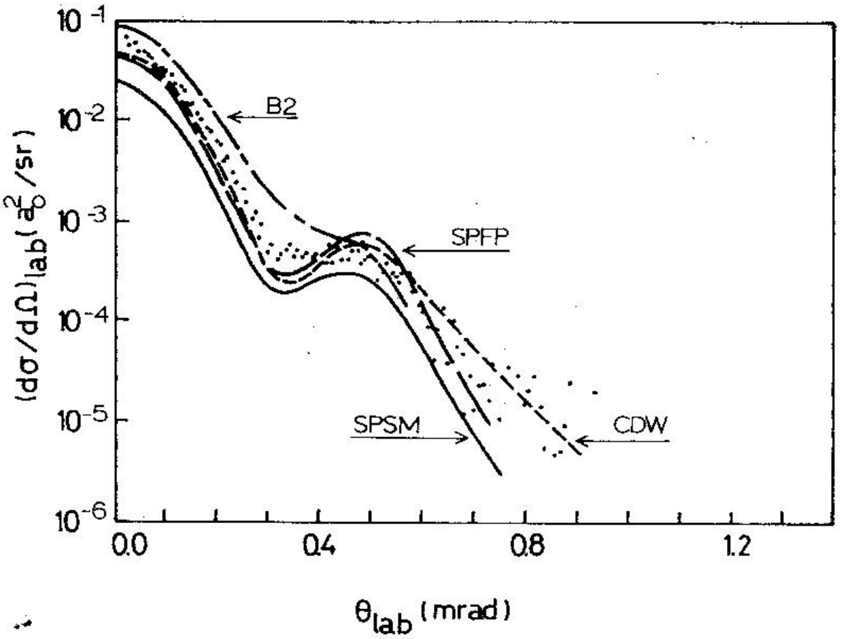

FIG. 9. — One electron capture-differential cross sections for the $H^+ + He$ system in laboratory coordinates at 7.4 MeV laboratory energy. Experimental data (dots) from Horsdal-Pedersen *et al.* (1983). Theoretical results obtained using the following approximations: (- - - -) CDW, (— —) SPFP, (——) SPSM and (— - —) B2.

of the off-the-energy shell inermediate states. In the other angular regions T depends as v^{-6} (for the CDW model, T goes as v^{-6} also at $\theta \simeq \theta_c$ when the impact energy increases; Rivarola and Miraglia, 1982). The influence of higher-order than the second one of the Born series on $d\sigma/d\Omega$ is clearly shown in figure 8. There, the B2 results are compared with the IA and CDW ones. In these two latter models, higher-orders are considered approximately by the inclusion of intermediate continuum states. The influence becomes dominant at $\theta \simeq \theta_c/\sqrt{3}$. The effect of nucleus-nucleus ineraction on $d\sigma/d\Omega$ is also shown in figure 8, where CDW calculations including or excluding this interaction are presented.

Experimental differential cross sections (Horsdal-Pedersen *et al.*, 1983) are shown in figure 9 for the $H^+ + He \rightarrow H + He^+$ system at 7.4 MeV laboratory energy. These measurements, which constitute perhaps the more important recent contribution to the study of these high energy processes, confirm the theoretical predictions about the existence of the Thomas' peak. Theoretical results shown in this figure are calculated with the strong Potential Born (SPFP; McGuire, 1983, into the full-peaking version; SPSM; McGuire and Sil, 1983, into a more exact calculation), CDW (Rivarola and Salin, 1983) and B2 (McGuire, 1983) approximations. All the theoretical results have been convoluted on the angular resolution by Horsdal-Pedersen *et al.* (1983). The Strong Potential calculations include all terms of the Born series in the strong potential but only the first one in the weak potential. The best agreement between theory and experiment is found with the CDW calculations, where the influence of the internuclear potential is more evident at larger angles. It is the only model where this interaction has been included. Also, it includes approximately the infinite terms of the Born series corresponding to the strong and weak potentials. Consequently, the model is well adapted for this quasi-symmetric system. The B2 results appear to overestimate $d\sigma/d\Omega$ and the SPSM to understimate it at small angles (the Strong Potential theory has been developed for asymmetric systems; Briggs *et al.*, 1982b).

New experimental data for other systems and energies will be welcomed, particularly for monoelectronic systems, where as has been explained above, other structure could appear.

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