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Electron capture into arbitrary n, l levels of fast projectiles

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The approach to electron capture previously developed by the authors is extended to describe the capture of hydrogenic 1s electrons into arbitrary hydrogenic n, l excited states of fast projectiles. A simple formula for n, l distributions is derived. Capture occurs mainly into states around $n_{\rm res} \approx Z_p/Z_t$ (Z_t and Z_p are the target and projectile charges) and $l \approx n_{\rm res} - 1$. The n, l distributions for $O^{8+} + H(1s) \rightarrow O^{7+}(nl) + H^+$ and for $O^{8+} + He(1s^2) \rightarrow O^{7+}(nl) + He^+(1s)$ are graphically displayed as representative examples. For the reactions $H^+ + H(1s) \rightarrow H(nl) + H^+$ and $H^+ + He(1s^2) \rightarrow H(nl) + He^+(1s)$ (nl = 2s, 2p, 3s, 3p, 3d, and 4s), good agreement is obtained with experimental cross sections.

I. INTRODUCTION

Electron capture into multicharged ions has attracted considerable attention in recent years. In particular, experimental and theoretical effort has been focused on total capture cross sections, which are relevant for astrophysical plasmas and magnetically confined fusion plasmas. Thus in a previous investigation[1] (hereafter called paper I) we have studied capture of 1s electrons into arbitrary principal shells n of energetic projectiles using an approach based on the eikonal approximation. Our motivation for extending the treatment so as to specify the contributions of various subshells is twofold. Firstly, the role played by impurities in neutral-beam heating of tokamak fusion plasmas is now being examined[2] by optical spectroscopy. This requires a knowledge of subshell populations. Secondly, specification of n, l levels should allow for a more critical test of the approach developed in paper I and at the same time it furnishes information that is not unambiguously available from classical-trajectory Monte Carlo calculations.[3]

In paper I we derived a simple formula for the total capture cross section and showed that it is in agreement with a large body of experimental data. The reason why this approach works so well can be understood as follows.[1] The eikonal approximation requires that the collision time be small compared to the transition time (i.e., the inverse of the transition energy in atomic units). For capture reactions this condition is satisfied over a wide energy range because for high projectile velocities the collision time is short and for lower velocities capture is predominantly resonant and hence the transition time is long. This argument holds as well for capture into the dominant sublevels so that the methods of paper I should also be suitable for the present investigation.

It may furthermore be understood why the approach of paper I yields a considerable reduction of the cross section as compared to the cross section calculated in the Oppenheimer–Brinkman–Kramers (OBK) approximation, thus bringing it in accord with experiment.[1] While (the prior form of) the OBK approximation confines itself to treating the electron-projectile nucleus interaction in first order, the prior form of the eikonal approximation adopted in paper I in addition includes the interaction between the captured electron and the target nucleus left behind. This interaction (treated to infinite order, yet in the specific form of an eikonal phase factor) tries to hold the electron back near the target nucleus and thus reduces the capture cross section. Obviously, this reduction is different in origin from the familiar reduction caused by the interference between the first-order and second-order terms in the Born expansion.[4]

Over the years, many theoretical papers[4-13] have dealt with electron capture. The cross section for capture from hydrogen atoms into arbitrary n, l levels of energetic ions has been given by Omidvar[5] in the OBK approximation. Golden *et al.*[6] have performed numerical calculations based on this formulation and in some cases they compare the results with those of full Born calculations. Toshima[7] calculated the cross section for capture from H(nl) to H($n'l'$) within the OBK approximation and for s-s and s-p transitions in the full Born approximation. Belkić and Gayet[8,9] used the "continuum-distorted-wave" method[10] to calculate electron capture from atomic hydrogen[8] and helium[9] into specific subshells (with $n \leq 4$) of fast protons. In the lower velocity range the classical-trajectory Monte Carlo method has been used by Salop[11] to obtain classical distributions of angular momenta and binding energies. Subsequently, these distributions have been converted into n, l distributions, a procedure which may not be fully justified for small n and l values.

In Sec. II we start from an expression for the transition amplitude derived in paper I to calculate the capture into a specific n, l final state. In Sec. III we give some representative n, l distributions for O^{8+} ions on H and He targets. For the reactions $H^+ + H(1s) \to H(nl) + H^+$ and $H^+ + He(1s^2) \to H(nl) + He^+(1s)$, with $2 \leq n \leq 4$, we compare our results with existing experimental data. Finally, in Sec. IV some concluding remarks are made.

II. CALCULATION OF CAPTURE CROSS SECTION

We consider the capture of an electron initially bound in the $1s$ shell of a hydrogenic target atom with charge Z_t into a specific n, l shell of a bare projectile ion with charge Z_p. Although this case is more complicated than the situation considered in paper I, we found that the same methods can also be used when there is no summation over subshells, and that again one obtains the cross section in a closed form. Below we outline the calculations only where they differ from those of paper I.

Let the projectile propagate along a rectilinear trajectory $\vec{R}(t) = \vec{b} + \vec{z}_R(t) = \vec{b} + \vec{v}t$ with respect to the target nucleus. The cross section is then written as

$$\sigma_{1s-nl} = \sum_m \int |A_{1s-nlm}(\vec{b}, v)|^2 d^2b \,, \qquad (1)$$

with Eq. (18) of paper I defining the exact eikonal transition amplitude

$$A_{1s-nlm}(\vec{b}, v) = i\,\frac{2^{5/2} Z_p Z_t^{3/2}}{v\Gamma(-i\eta Z_t')} \int g^*_{nlm}(\vec{p}+\vec{v})\Bigg|_{p_z = p_{0z}} \frac{(\lambda + Z_t)\,\lambda^{-i\eta Z_t' - 1} e^{-i\vec{b}\cdot\vec{p}_b}}{(p_b^2 + p_{0z}^2 - 2i\lambda p_{0z} + 2\lambda Z_t + Z_t^2)^2}\, d^2p_b\, d\lambda \,. \qquad (2)$$

We use atomic units throughout the paper unless otherwise stated. In Eq. (2) the following definitions are used: $\eta = 1/v$ and $p_{0z} = -\frac{1}{2}v + \epsilon\eta$, with $\epsilon = -\frac{1}{2}(Z_p^2/n^2 - Z_t^2)$ being the energy difference between initial and final bound states. Furthermore, while Z_t is the target charge in the initial state (associated with the binding energy), we also introduce the effective target charge Z_t' in the final state (associated via the eikonal phase[1] with the interaction between target nucleus and captured electron), thus allowing $Z_t' \neq Z_t$ for multielectron atoms. Finally, the momentum function $g_{nlm}(\vec{q})$ is the Fourier transform of $\varphi_{nlm}(\vec{r})/r$, where φ_{nlm} is the wave function of the hydrogenic state nlm.

The basic point in our previous treatment[1] is the observation that the density matrix $\sum_{n,l} g^*_{nlm}(\vec{q})\, g_{nlm}(\vec{q}\,')$ occurring in the expression for the cross section enters only at momenta $\vec{q}\,' = \vec{q}$ after carrying out $\sum_{n,l}\int d^2b$. Moreover, this diagonal part becomes very simple. A similar conclusion holds for the present case: It follows from Eqs. (1) and (2) that only $\vec{q}\,' = \vec{q}$ contributes to σ_{1s-nl}. It is therefore sufficient to consider the diagonal part of the density matrix defined by

$$G_{nl}(q) = \sum_m |g_{nlm}(\vec{q})|^2 \,. \qquad (3)$$

By inserting the Fourier transform[1] $\tilde{\varphi}_{nlm}(\vec{q})$ of $\varphi_{nlm}(\vec{r})$ into the Schrödinger equation one arrives at the relation

$$G_{nl}(q) = \frac{\frac{1}{4}(q^2 + q_n^2)^2}{Z_p^2} \sum_m |\tilde{\varphi}_{nlm}(\vec{q})|^2 \,, \qquad (4)$$

with $q_n = Z_p/n$. Here one may readily introduce the standard expression[14] for $\tilde{\varphi}_{nlm}(\vec{q})$ to rewrite Eq. (4) as

$$G_{nl}(q) = \frac{2l+1}{\pi^2}\, 2^{4l+1} \frac{(n-l-1)!\,(l!)^2}{Z_p(n+l)!} \frac{q^{2l} q_n^{2l+4}}{(q^2+q_n^2)^{2l+2}} \times \left[C_{n-l-1}^{l+1}\left(\frac{q^2 - q_n^2}{q^2 + q_n^2}\right)\right]^2 . \qquad (5)$$

By expressing the Gegenbauer polynomials[15] $C_n^\lambda(x)$ in terms of hypergeometric functions and expanding the latter into terminating power series, one arrives at a finite sum of elementary expressions

$$G_{nl}(q) = \frac{2l+1}{\pi^2 Z_p}\, 2^{4l+1} \frac{(n+l)!}{(n-l-1)!} \left(\frac{l!}{(2l+1)!}\right)^2 \times \sum_{\nu=0}^{l} (-1)^\nu \frac{l!}{(l-\nu)!\,\nu!} \sum_{\mu,\mu'=0}^{n-l-1} B_\mu(n,l) B_{\mu'}(n,l) \times \frac{q_n^{2(l+2+\nu+\mu+\mu')}}{(q^2+q_n^2)^{l+2+\nu+\mu+\mu'}} \,. \qquad (6)$$

The quantities

$$B_\mu(n,l) = \frac{(-n+l+1)_\mu (n+l+1)_\mu}{(l+\frac{3}{2})_\mu\, \mu!} \,, \quad \text{with } (a)_\mu = \frac{\Gamma(a+\mu)}{\Gamma(a)} \,, \qquad (7)$$

obviously result from the hypergeometric functions[15] and lend themselves to easy recursive computation. Having established the form of $G_{nl}(q)$, one derives the capture cross section from Eqs. (1), (2), and (6), following the procedure outlined in paper I. The final result is

$$\sigma_{1s-nl} = \alpha_{nl}\sigma^{\mathrm{OBK}}_{1s-n}\,, \tag{8a}$$

where the OBK cross section for electron capture into a complete principal shell n has the usual form

$$\sigma^{\mathrm{OBK}}_{1s-n} = \frac{2^8\pi Z_p^5 Z_t^5}{5n^3v^2[Z_t^2+(\frac{1}{2}v-\epsilon\eta)^2]^5} \tag{8b}$$

and the subshell scaling factor is

$$\alpha_{nl} = \frac{\pi\eta Z_t'}{\sinh(\pi\eta Z_t')}\exp\left[-2\eta Z_t'\tan^{-1}\left(\frac{\frac{1}{2}v-\epsilon\eta}{Z_t}\right)\right]2^{4l}(2l+1)\frac{(n+l)!}{n(n-l-1)!}\left(\frac{l!}{(2l+1)!}\right)^2$$
$$\times\sum_{\nu=0}^{l}(-1)^l\frac{l!}{(l-\nu)!\,\nu!}\sum_{\mu,\mu'=0}^{n-l-1}B_\mu(n,l)B_{\mu'}(n,l)\left(\frac{Z_p^2}{n^2[Z_t^2+(\frac{1}{2}v-\epsilon\eta)^2]}\right)^{l+\nu+\mu+\mu'}\Lambda_{l+\nu+\mu+\mu'}\,, \tag{8c}$$

where the last factor is defined as

$$\Lambda_\lambda = 5\left\{\frac{1}{\lambda+5}-\frac{1}{2(\lambda+4)}\frac{Z_t'}{Z_t}+\frac{1}{16(\lambda+3)}\frac{Z_t'^2}{Z_t^2}+\left[\left(\frac{1}{\lambda+5}-\frac{1}{\lambda+4}+\frac{1}{4(\lambda+3)}\right)Z_t'^2+\frac{1}{\lambda+4}\frac{Z_t'}{Z_t}\epsilon-\frac{1}{4(\lambda+3)}\frac{Z_t'^2}{Z_t^2}\epsilon\right]\eta^2\right.$$
$$\left.+\frac{1}{4(\lambda+3)}\frac{Z_t'^2}{Z_t^2}\epsilon^2\eta^4\right\}. \tag{8d}$$

This result is exact within the eikonal approximation. The OBK cross section $\sigma^{\mathrm{OBK}}_{1s-nl}$ is immediately obtained as a special case of Eq. (8) by choosing $Z_t'=0$. In particular, for $n=1,2$, and 3 we recover the results explicitly given by Omidvar[5] for these cases. In general, it appears that Eq. (8) with $Z_t'=0$ is simpler to evaluate than Omidvar's expression, which involves a transformation from parabolic to spherical coordinates. As a check on Eq. (8), we verified analytically for $n\leq 3$ that l summation yields the same result as Eq. (22) of paper I for the complete principal shell. Furthermore, in a computer program based on Eq. (8) we performed the l summation numerically; in each of a large variety of cases we found agreement with the independently calculated[1] value for the complete n shell.

III. RESULTS AND DISCUSSION

A. n,l distributions

The final formula given in Eq. (8) is rather easy to program on a computer, so that one may readily obtain numerical values for the cross section for any given set of parameters v, Z_t, Z_t', Z_p, n, and l. Therefore, and because of the number of para-

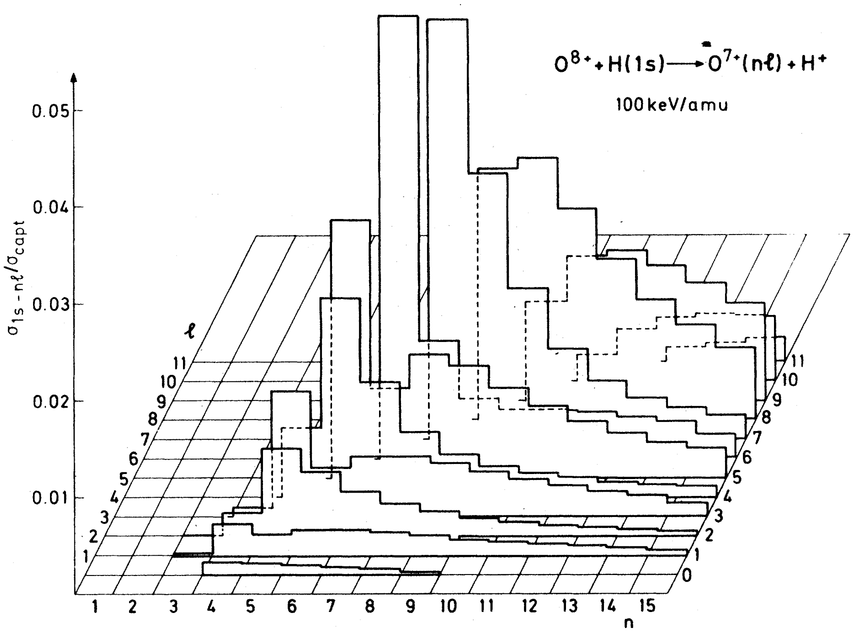

FIG. 1. Calculated relative contributions of various sublevels n,l to the total cross section for electron capture in the reaction $O^{8+}+H(1s)\rightarrow O^{7+}(nl)+H^+$ at a projectile energy of 100 keV/amu.

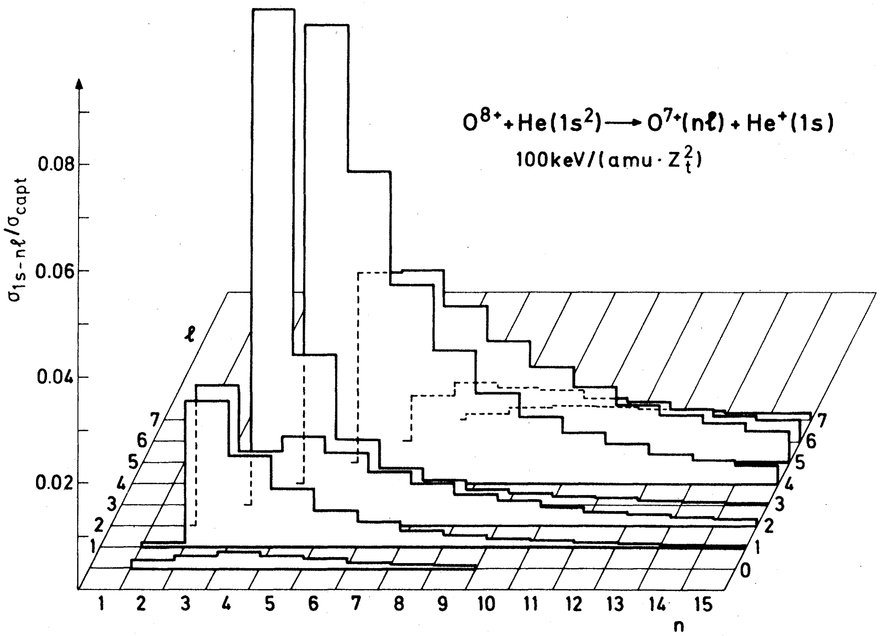

FIG. 2. Calculated relative contributions of various sublevels n,l to the total cross section for electron capture in the reaction $O^{8+}+He(1s^2) \rightarrow O^{7+}(nl)+He^+(1s)$ at a projectile energy of 100 keV/$(amu Z_t^2)$. The effective target charge $Z_t=Z_t'=1.6875$ has been used (Ref. 1).

meters involved, we confine ourselves to displaying just two representative n,l distributions. Figure 1 and 2 show the relative contributions of various n,l shells to the total cross section for capture of electrons initially bound in 1s states of H and He atoms, respectively, into n,l shells of O^{8+} projectiles moving with an energy of 100 keV/

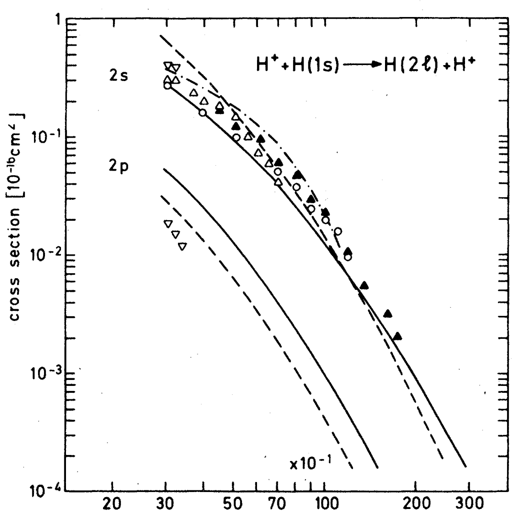

FIG. 3. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + H(1s) \rightarrow H(2l)+H^+$. Theory:—present work; --- Belkić and Gayet (Ref. 8); •-•-• Gallaher and Wilets [Refs. 12 and 4(b)]. Experiment: ○ Hughes *et al.* (Ref. 17); △ Bayfield (Ref. 18); ▲ Ryding *et al.* (Ref. 19) normalized to Bayfield (Ref. 18) at 44 keV; ▽ Andreev *et al.* (Ref. 20). Results for σ_{2p} are multiplied by 10^{-1}.

$(amu Z_t^2)$. In both cases it is seen that "resonant" levels with $\epsilon \approx 0$ or $n \approx Z_p/Z_t$ and with maximum $l=n-1$ are predominantly populated at this energy. A similar trend has also been observed by Golden *et al.*[6] in their OBK calculations. In fact, in our numerical calculations we always determine the OBK cross section along with the eikonal cross section and find that the ratios $\sigma_{1s-ln}/\sigma_{capt}$ are not much different (deviations are below 30% in most cases) in the two approximations. Of course, the absolute OBK cross sections have to be scaled down by the usual factor[1] $\alpha = 0.1-0.4$ in order to match our eikonal cross sections.

It should be mentioned that we get noticeable disagreement with the eikonal results of Dewangan[16] for capture into H(2s) and into H(2p) in the low-energy range. He uses the post form of the eikonal approximation in conjunction with an incorrect sign for the eikonal phase (see Ref. 15 of paper I). Hence for nonsymmetric charge transfer his results are incorrect. On the other hand, considering the checks (mentioned at the end of Sec. II) to which we have subjected our formulas and our computer program, we believe that our results are correct.

B. Comparison with experimental results

It appears that systematic measurements of absolute cross sections for capture into specific subshells are available only for the collision systems $H^+ + H(1s)$ and $H^+ + He(1s^2)$. In Figs. 3–8 we compare the results of Eq. (8) with experimental data[17-28] for these systems compiled in the theoret-

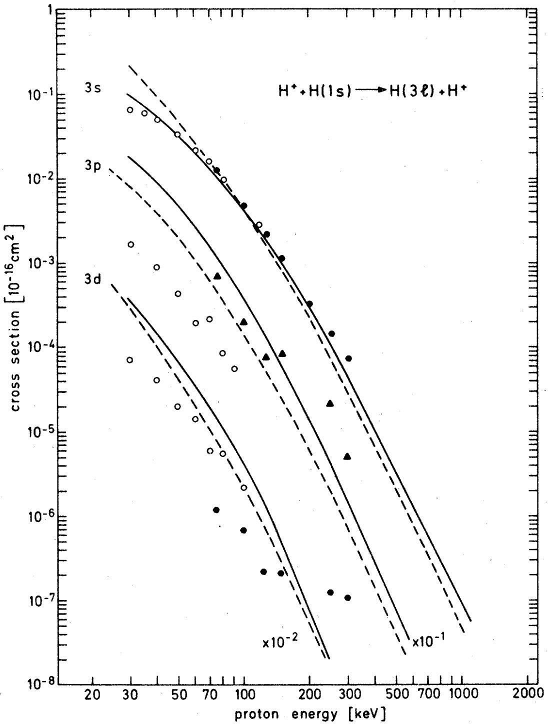

FIG. 4. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + H(1s) \rightarrow H(3l) + H^+$. Theory:—present work; --- Belkić and Gayet (Ref. 8). Experiment: ○ Hughes *et al.* (Ref. 21); ● and ▲ Ford and Thomas (Ref. 22). Results for σ_{3p} and σ_{3d} are multiplied by 10^{-1} and 10^{-2}, respectively.

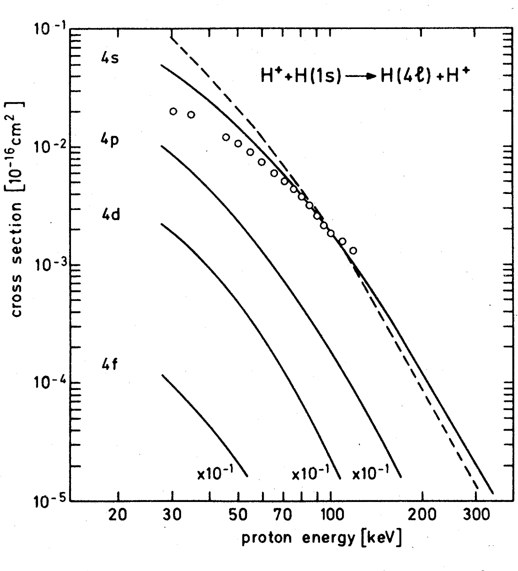

FIG. 5. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + H(1s) \rightarrow H(4l) + H^+$. Theory:—present work; --- Belkić and Gayet (Ref. 8). Experiment: ○ Hughes *et al.* (Ref. 23). Results for σ_{4p}, σ_{4d}, and σ_{4f} are multiplied by 10^{-1}.

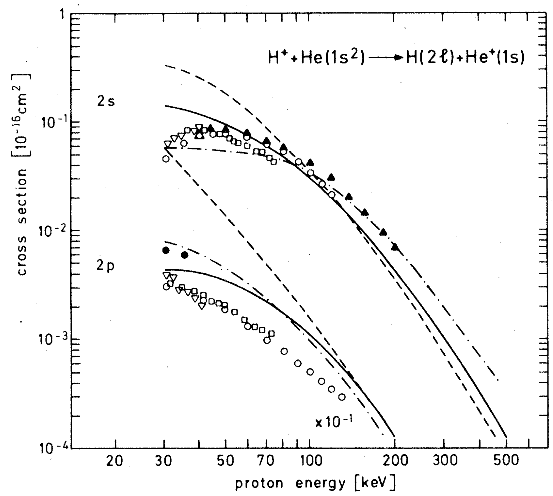

FIG. 6. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + He(1s^2) \rightarrow H(2l) + He^+(1s)$. Theory:—present work with $Z_t = Z_t' = 1.6875$; --- Belkić and Gayet (Ref. 9); -·-·- Sin Fai Lam [Refs. 13 and 4(b)]. Experiment: ○ Hughes *et al.* (Ref. 17); ▲ Ryding *et al.* (Ref. 19) normalized to Hughes *et al.* (Ref. 17) at 40 keV; ▽ Andreev *et al.* (Ref. 24); □ Dose (Ref. 25) normalized to Andreev *et al.* (Ref. 24) at 27 keV; ● de Heer *et al.* (Ref. 26). Results for σ_{2p} are multiplied by 10^{-1}.

ical work of Belkić and Gayet.[8,9] The reader is referred to this work for a detailed discussion of the data.

Figures 3–5 show experimental and theoretical cross sections for the reactions $H^+ + H(1s) \rightarrow H(nl) + H^+$ with $n = 2, 3$, and 4, respectively. Besides our theoretical results, the figures contain those of the continuum-distorted-wave method,[8] and for capture into $H(2s)$, results for coupled-state calculations by Gallaher and Wilets.[12,4(b)] The experimental data seem to be fairly consistent for capture into the $2s$ and $3s$ states, but for final $3p$ and $3d$ states the data are conflicting and hence not very conclusive. Considering these uncertainties, the overall agreement between our calculated cross sections and the measured cross sections is quite good, in particular for the transitions into the $2s$, $3s$, and $4s$ final states. This holds down to projectile energies of 40 keV, corresponding to velocities roughly equal to the $1s$ electron orbital velocity in hydrogen. It is also observed that in the low-energy range our theoretical curves reproduce the trend of the data somewhat better than the curves of Ref. 8.

Figures 6–8 show experimental and theoretical cross sections for the reactions $H^+ + He(2s^2) \rightarrow H(nl) + He^+(1s)$ with $n = 2, 3$, and 4, respectively. Besides our results [see Eq. (8)] and the theoretical curves of Belkić and Gayet,[9] we have also in-

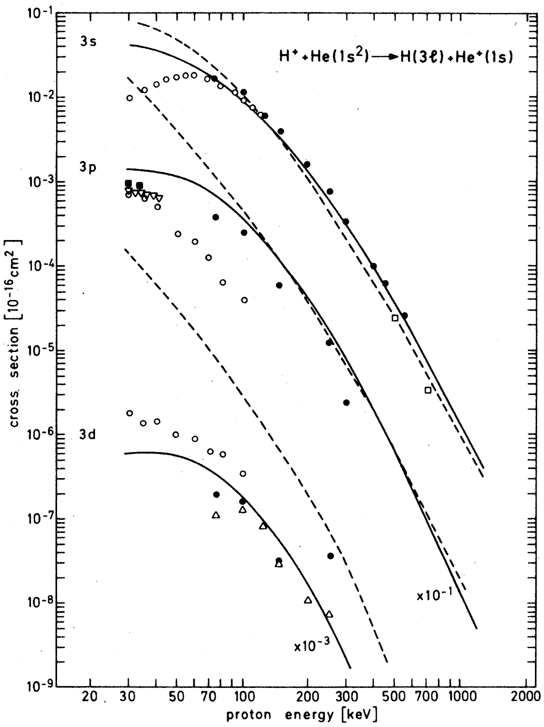

FIG. 7. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + He(1s^2) \rightarrow H(3l) + He^+(1s)$. Theory:—present work with $Z_t = Z_t' = 1.6875$; --- Belkić and Gayet (Ref. 9). Experiment: ○ Hughes *et al*. (Ref. 17); ● Ford and Thomas (Ref. 22); △ Edwards and Thomas (Ref. 27); ▽ Andreev *et al*. (Ref. 24); ■ de Heer *et al*. (Ref. 26); □ Conrads *et al*. (Ref. 28). Results for σ_{3p} and σ_{3d} are multiplied by 10^{-1} and 10^{-3}, respectively.

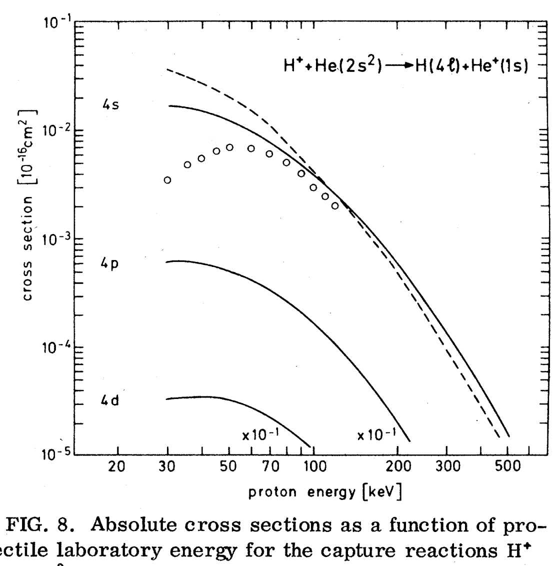

FIG. 8. Absolute cross sections as a function of projectile laboratory energy for the capture reactions $H^+ + He(1s^2) \rightarrow H(4l) + He^+(1s)$. Theory:—present work with $Z_t = Z_t' = 1.6875$; --- Belkić and Gayet (Ref. 9). Experiment: ○ Hughes *et al*. (Ref. 23). Results for σ_{4p}, σ_{4d}, and σ_{4f} are multiplied by 10^{-1}.

cluded calculated curves by Sin Fai Lam[13,4(b)] for $2s$ and $2p$ final states as examples for elaborate coupled-states calculations. Again, for the $2s$ and $3s$ final states our calculated curves are in good agreement with experimental values down to 40 and 70 keV, respectively. Also the data for final $2p$, $3d$, and $4s$ states are reasonably well reproduced, while for the $3p$ final state conflicting sets of data preclude a definite comparison. Note that for the $2p$ and $3d$ final states the cross sections calculated by Belkić and Gayet[9] considerably exceed both our cross sections and the experimental ones. Again, in the low-energy range our calculated curves show a curvature that is quite similar to the trend followed by the experimental data. In fact, the behavior of the data seems to be well described down to proton velocities even less than the $1s$ electron orbital velocity in helium.

We conclude this section by noting that the simple Eq. (8) gives an impressive overall agreement with experimental data for electron capture into the $2s, 2p, 3s, 3p, 3d$, and $4s$ shells of H^+ projectiles impinging on H and He targets. The agreement appears to be better than for the more involved calculations[8,9] in the continuum-distorted-wave method[10] and is comparable with the agreement achieved by existing coupled-states calculations.[12,13,4(b)]

IV. CONCLUDING REMARKS

In the present work we have extended the approach developed in paper I to electron capture into arbitrary n, l states of fast projectiles. As a result, we obtain more detailed theoretical predictions, which in turn might be checked in experiments studying radiative transitions and radiative cascades following electron capture. In this respect, our approach, being based on quantum theory, is expected to reach beyond the regime of applicability of classical-trajectory Monte Carlo calculations.[3] The latter method should be reliable whenever classical momentum distributions coincide with the corresponding quantal distributions (as is the case for initial hydrogenic $1s$ states) and when classical space distributions (which are different from the quantal distributions) do not enter because they are integrated over. That these conditions have been satisfied in the applications[3] may explain the striking success of the method. Conversely, the classical method should be less reliable if space distributions, subshells, and impact parameters enter explicitly. Thus, for example, electron capture from initial $2s$ states[29] would not be well described by a classical theory and n, l distributions of the captured electron derived from classical quantities[11] have to be viewed with some care, in particular for low quantum states.

It is important to stress that our final result, Eq. (8), is very simple to evaluate for arbitrary n,l, while any other known method going beyond the OBK approximation becomes prohibitively tedious to apply.[6] Experimental results are still scarce and more systematic data are definitely needed to assess the validity of our approach. So far, for the capture from H(1s) and He(1s^2) into H(nl) with $n,l = 2s$, $2p$, $3s$, $3p$, $3d$, and $4s$ we obtain a good overall agreement with existing data. This fact, taken together with the success of our theory to predict total cross sections,[1] may be encouraging enough to use Eq. (8) for estimating unknown cross sections for capture into n,l states. This may prove to be helpful for the diagnostic techniques currently being developed[2] for examining the role played by impurities in neutral-beam heating of fusion plasmas.

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